Universidad Zaragoza
1542

Trabajo Fin de Grado

Modelado de la combustión de sulfuro de hidrógeno adicionado a metano a presión atmosférica

Autor:

Martín Leciñena Andrés

Director:

Juan Manuel Colom

Ponente:

Dra. Mª Ujué Alzueta Anía

Universidad de Zaragoza

2018

Modelado de la combustión de sulfuro de hidrógeno adicionado a metano a presión atmosférica

Debido a la creciente importancia de los recursos energéticos obtenidos en procesos como el *fracking*, y a la presencia de H_2S en el gas de *fracking*, así como en el gas natural, gases de refinería, etc, así como el hecho de que la combustión de combustibles que contienen H_2S pueda dar lugar a contaminantes como el SO_2, precursor de lluvia ácida y que puede generar corrosión, es importante estudiar la combustión de los gases que contienen H_2S en diferentes concentraciones, con el fin de evitar procesos de limpieza cuyos costes asociados son muy elevados y, en ocasiones, pueden llegar a ser inadmisibles.

En el presente trabajo de final de grado se pretende modelar la oxidación de sulfuro de hidrógeno en presencia de metano a presión atmosférica, con diferentes concentraciones de oxígeno (condiciones reductoras, estequiométricas y oxidantes) y en un rango de temperaturas entre 500 y 1100 ℃, cuya finalidad es la de desarrollar un mecanismo cinético que prediga la conversión de gas ácido. Se utilizarán datos experimentales disponibles en el grupo de investigación de la conversión de mezclas representativas de gases ácidos. El modelado cinético se va a realizar usando el programa Chemkin-PRO para el cálculo e interpretación del mecanismo de reacción desarrollado.

La primera fase de trabajo fue un estudio bibliográfico del tema con el objetivo de leer y entender en lo que se está trabajando. Posteriormente, partiendo de un mecanismo base, se introdujeron y actualizaron reacciones del mecanismo de CH_4 y H_2S con el fin de mejorar el modelado cinético del proceso de oxidación. Para ello, se introdujeron nuevas reacciones de interacción de azufre y carbono con el objeto de mejorar la reproducción de los resultados experimentales disponibles. Para conocer las reacciones más importantes dentro del mecanismo y los caminos de reacción que tienen lugar durante la oxidación de la mezcla de CH_4/H_2S estudiadas, se usaron las herramientas de análisis de reacción y de sensibilidad del software Chemkin-PRO.

Finalmente, se obtuvieron las conclusiones del trabajo realizado.

TRABAJOS DE FIN DE GRADO / FIN DE MÁSTER

Escuela de Ingeniería y Arquitectura Universidad Zaragoza

DECLARACIÓN DE AUTORÍA Y ORIGINALIDAD

(Este documento debe acompañar al Trabajo Fin de Grado (TFG)/Trabajo Fin de Máster (TFM) cuando sea depositado para su evaluación).

D./Dª. Martín Leciñena Andrés,

con nº de DNI 73417557-B en aplicación de lo dispuesto en el art. 14 (Derechos de autor) del Acuerdo de 11 de septiembre de 2014, del Consejo de Gobierno, por el que se aprueba el Reglamento de los TFG y TFM de la Universidad de Zaragoza,

Declaro que el presente Trabajo de Fin de (Grado/Máster) Grado, (Título del Trabajo) Modelado de la combustión de sulfuro de hidrógeno adicionado a metano a presión atmosférica,

es de mi autoría y es original, no habiéndose utilizado fuente sin ser citada debidamente.

Zaragoza, 9 de Septiembre de 2019

Fdo: Martín Leciñena Andrés

Índice

1 Introducción y objetivos

El gas natural tiene una gran importancia en la actualidad, tiene un uso muy extendido en todo el mundo y sus aplicaciones son diversas, entre ellas podemos destacar su uso como combustible o como materia prima para la creación de productos químicos.

Los yacimientos de gas natural se pueden encontrar tanto en tierra firme como bajo el mar, aunque a gran profundidad bajo el subsuelo. Actualmente existen técnicas novedosas como la fractura hidráulica (*fracking*) que permite obtener el (*shale gas)* proveniente de pizarra y esquisto, las cuales son formaciones minerales procedentes de sedimentos ricos en arcilla.

El gas natural esta principalmente formado por metano. Sin embargo, puede incluir grandes cantidades de gases ácidos, los cuales principalmente son dióxido de carbono (CO_2) y sulfuro de hidrogeno (H_2S). El primero de ellos tiene un efecto negativo, ya que disminuye el poder calorífico y puede formar hielo seco. Por otro lado, el segundo es un compuesto muy contaminante, ya que, además de que puede corroer las tuberías para el transporte del gas natural, puede plantear problemas derivados de su combustión.

Con el fin de eliminar el H_2S del gas natural se han propuesto numerosas alternativas, las cuales tienen un gran gasto de energía y dinero o tienen problemas de contaminación secundaria. Entre estas alternativas se encuentra la separación por membranas, que tiene poco gasto energético, pero es muy inestable; o los procesos Rectisol y Selexol, utilizando metanol y dimetil eter de polietilenglicol, respectivamente. Sin embargo, estos procesos deben realizarse a presión por lo que tienen un coste elevado. El uso de aminas también posee problemas por la baja selectividad de interacción con H_2S/CO_2, la corrosividad y la regeneración y pérdida de disolvente [1].

Debido a estos problemas se está planteando el abandono de estos procesos de limpieza y el uso de los gases combustibles tal y como se obtienen, con concentraciones apreciables de

gases ácidos, avanzando tanto en la tecnología que lo haga posible como en los modelos cinético químicos que reproduzcan su comportamiento.

En este contexto, el presente trabajo de fin de grado pretende llevar a cabo el estudio del modelado de la combustión de la mezcla metano-sulfuro de hidrógeno con el fin de obtener un mecanismo cinético que describa correctamente el resultado de esa combustión para diferentes temperaturas y estequiometrias (atmósfera reductora, estequiométrica y oxidante).

El modelo obtenido podrá ser usado para evaluar la posibilidad de combustión directa de mezclas ácidas para su uso en determinadas situaciones.

2 Antecedentes

2.1 Limpieza de impurezas de H_2S

Debido a los múltiples problemas que se generan debido a la presencia de sulfuro de hidrógeno como impureza en los gases combustibles, la tendencia general ha sido separarlos de manera previa a la combustión. Como consecuencia, la oxidación de esta especie no ha sido profundamente estudiada.

Para eliminar las impurezas de H_2S, se acude a métodos de separación tales como la absorción usando disolventes como el metanol (proceso Rectisol), el cual trabaja a temperaturas entre -40 y -62 ºC o el dimetil eter de polietilenglicol (proceso Selexol) para temperaturas de -18 a 175 ºC, entre otros [2].

El tratamiento del gas ácido se realiza comúnmente mediante el proceso Claus, el cual es ampliamente conocido y muy usado desde hace aproximadamente 100 años. El proceso Claus se lleva a cabo en dos etapas, en la primera de ellas ocurre la oxidación térmica del

sulfuro de hidrógeno formando dióxido de azufre y agua (Ec.1) y es llevada a cabo en hornos. En esta etapa se oxida una tercera parte del H_2S a SO_2 y todos los hidrocarburos presentes a una temperatura aproximada de 965 °C. Posteriormente, la reacción entre el H_2S y SO_2 para formar azufre y agua (Ec.2) se lleva a cabo en convertidores catalíticos. El calor generado en las etapas se aprovecha para generar vapor de agua.

$$H_2S + 3/2\, O_2 \rightarrow SO_2 + H_2O$$ **Etapa de Oxidación térmica**. Ec. 1

$$2H_2S + SO_2 \rightarrow 3/2\, S_2 + 2H_2O$$ **Etapa de Conversión.** Ec.2

Este proceso tiene una eficiencia limitada debido al equilibrio que se establece en las etapas que lo comprenden, por tanto, a pesar de no tener una conversión total, alcanza eficiencias de entre el 94 y 97 % [3].

En este contexto y, como se ha mencionado anteriormente, cobran importancia los estudios que abordan la combustión del gas ácido directamente, con objeto de evitar los costosos procesos de limpieza, en particular en aquellos casos donde su aplicación puede ser compleja debido a que se trate de pequeños yacimientos de gas.

2.2 Estudios realizados sobre el proceso de oxidación de H_2S

Zhou et al. [4] llevaron a cabo estudios de oxidación de H_2S en concentraciones comprendidas entre 100 y 520 ppm en un reactor de flujo de cuarzo a presión atmosférica. Para distintas concentraciones de oxígeno (200 a 1000 ppm) y temperaturas comprendidas entre 950 y 1150 K. Una vez realizados estos experimentos, trataron de predecirlos mediante el uso de un mecanismo de reacción, en el que introdujeron nuevos caminos de reacción y se actualizaron algunos ya existentes, en relación con el S_2, el HSS y el HSSH.

Posteriormente, el estudio de Colom-Díaz et al. [5] incluye experimentos para diferentes relaciones estequiométricas y a presión atmosférica en un reactor de flujo pistón, evidenciando la importancia de las reacciones de SH con oxígeno y obteniendo un mecanismo cuyas predicciones se asemejan a los datos experimentales y del cual se ha partido como inicio en este TFG.

Finalmente, los autores llegan a la conclusión de que es de vital importancia en el proceso de oxidación de H_2S el proceso de isomerización del HSOO a HSO_2, el cual no se había tenido en cuenta en estudios anteriores, aunque se había propuesto teóricamente

2.3 Estudios sobre la combustión de CH_4 con impurezas de H_2S

Una gran parte de las reservas de gas natural no son utilizables sin tratamientos previos, ya que de la extracción se obtiene gas ácido, es decir, gas que además de tener una gran cantidad de metano, también posee otras impurezas como sulfuro de hidrógeno y dióxido de carbono. Estas sustancias al no ser deseables han de ser separadas previamente. Sin embargo, debido a que se quieren reducir costes, se plantea estudiar el comportamiento de estas dos especies juntas en el proceso de combustión.

El estudio de Bongartz et al. [6] sobre la cinética y modelado de la oxi-combustión de CH_4 con H_2S analiza la interacción entre las especies de carbón y azufre señalando cómo su mecanismo de mezcla CH_4/H_2S podía capturar el efecto inhibidor del SO_2 en la oxidación de CO en condiciones estequiométricas, un efecto ya visto experimentalmente por Giménez-López et al. [7]. Por otro lado, se comprobó en su estudio el efecto ya observado por Fleig et al. [8] en el que el metano introducido en el reactor de flujo pistón afectaba a la oxidación de SO_2 a SO_3, aumentando la formación de SO_3 a temperaturas intermedias a medida que se introduce más CH_4.

Finalmente, los autores señalaron la falta de datos experimentales de la velocidad de la deflagración laminar y de estructura de llama de H_2S, sobre todo a altas presiones y la falta de datos de la oxi-combustión de H_2S/CH_4.

Gersen et al. [9] desarrollaron un mecanismo para la oxidación de la mezcla H_2S/CH_4 a presiones altas, para ello se llevan a cabo experimentos en una máquina de compresión rápida (RCM) a presiones entre 30 y 80 atmósferas y en un intervalo de temperaturas de 930 a 1050 K y en un reactor de flujo pistón a 50 bares y en un intervalo de temperaturas de 600 a 900 K.

En los experimentos observaron que la adición de un 1% de H_2S al CH_4 reducía el tiempo de autoignición en un factor de 2 si se compara con el H_2S puro.

Con respecto al modelo desarrollado por Gersen et al. [9] se concluye que la reacción $H_2S + O_2 = SH + HO_2$ es la causante de la oxidación de H_2S y que las reacciones de H_2S y SH con el radical CH_3OO son las causantes de estimular dicha oxidación.

3 Metodología experimental

Los datos experimentales de este trabajo han sido obtenidos de forma previa en el laboratorio de Reacciones de Combustión del Grupo de Procesos Termoquímicos (GPT) del Instituto de Investigación en Ingeniería de Aragón (I3A). Los experimentos se llevaron a cabo en una instalación que permite el estudio de reacciones en fase gas a presión atmosférica (fase homogénea).

3.1 Descripción del sistema experimental

Los experimentos de investigación llevados a cabo se desarrollaron en una instalación experimental como la esquematizada en la Figura 3.1. Esta instalación puede dividirse a su vez en tres partes principales que son el sistema de alimentación, el sistema de reacción y el sistema de detección y análisis de gases.

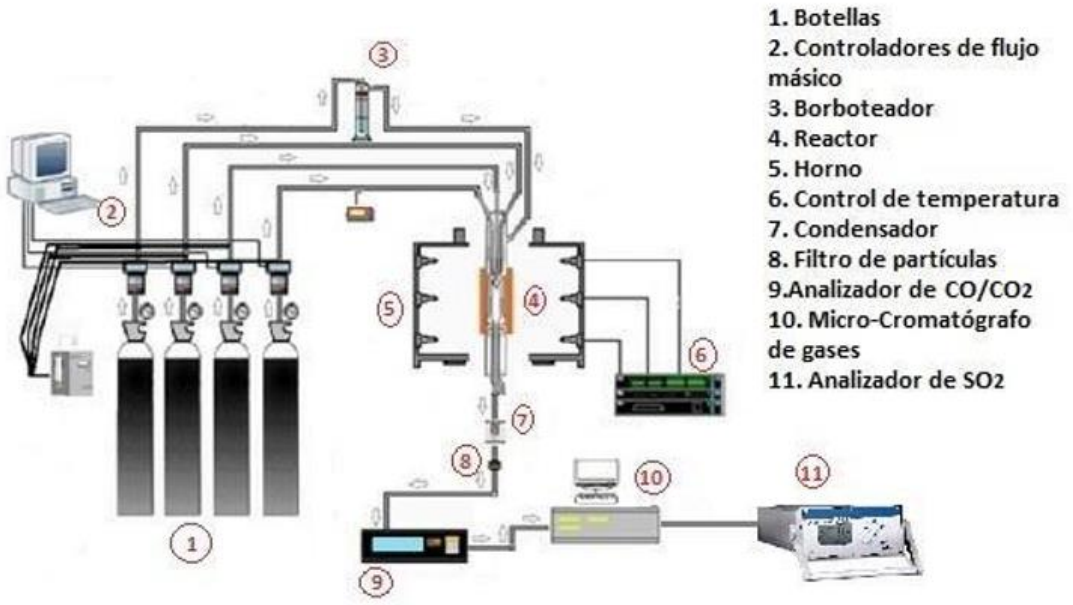


Figura 3.1 Esquema de la instalación experimental

Sistema de alimentación de gases: En este sistema se incluyen las botellas de gases a presión, los controladores de flujo másico, el medidor de caudal volumétrico (burbujímetro) y el borboteador. Los gases salen de las botellas presurizadas y se miden sus caudales, los cuales

son controlados mediante controladores de flujo másico, usando un burbujímetro digital. Después de los controladores de flujo, los gases son direccionados hacia un panel de válvulas, tras el cual los gases se dirigen hacia el reactor, equipos de medición o hacia el exterior.

Sistema de reacción: Esta sección comprende los equipos necesarios para que la reacción se lleve a cabo. Incluye un reactor de flujo de cuarzo de cuatro entradas que opera en condiciones de flujo pistón y un horno eléctrico de tubo vertical abierto con tres zonas calefactoras independientes con su correspondiente sistema de control de temperatura.

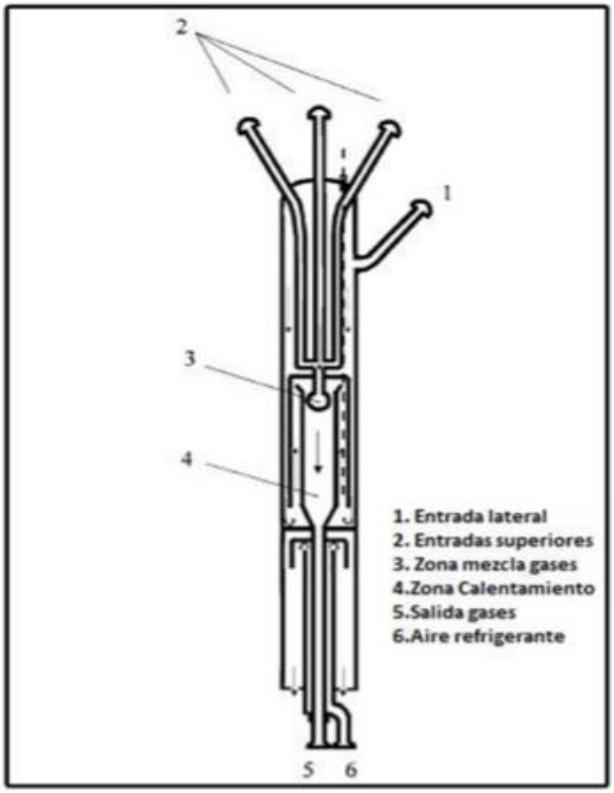


Figura 3.2 Reactor de flujo de cuarzo

Sistema de detección y análisis de gases: Los gases de combustión que salen del reactor deben ser acondicionados antes de ser analizados para no ocasionar daños a los equipos ni interferir con los resultados. Por ello, tras producirse la reacción de oxidación y ser paralizada por el aire de refrigeración, los gases de salida pasan por un condensador y un filtro de partículas. Los análisis cualitativos y cuantitativos de los gases se realizan usando un micro-cromatógrafo de gases, un analizador en continuo con sensor infrarrojo (IR) de CO/CO_2 y un analizador en continuo de SO_2 con sensor ultravioleta (UV) [10].

3.2 Planteamiento de los experimentos

En el presente trabajo de final de grado se plantea el uso de combustibles con presencia de sulfuro de hidrógeno, con el objetivo de que se realice la combustión en las mejores condiciones posibles. Debido a que actualmente solo se puede conocer el resultado de la combustión de manera experimental, se ha desarrollado un mecanismo cinético que pueda predecir estos resultados utilizando el software Chemkin-Pro [11], de esta manera, se ahorrarían costes y tiempo de realizar experimentos. En concreto, se van a simular los resultados a presión atmosférica y a un rango de temperaturas entre 500 y 1100 ºC y con diferentes composiciones de alimentación.

Debido a que se va a estudiar un proceso de combustión, es de vital importancia conocer la estequiometria de la reacción, ya que dependiendo del porcentaje de oxigeno aportado, los resultados serán diferentes. Así pues, se define el parámetro lambda (λ) como el cociente entre el oxígeno introducido y el oxígeno estequiométrico. Los moles de oxígeno estequiométrico necesarios vienen determinados por las siguientes reacciones químicas:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \qquad \text{R. 2.1}$$

$$H_2S + 3/2\, O_2 \rightarrow SO_2 + H_2O \qquad \text{R. 2.2}$$

Sustituyendo el valor del oxígeno estequiométrico por el metano y sulfuro de hidrógeno introducido, en la ecuación de λ, obtenemos la ecuación 2.1.

$$\lambda = \frac{[O_2]\ introducido}{2[CH_4]+3/2[H_2S]} \qquad \text{Ec. 2.1}$$

En el presente trabajo se va a considerar la concentración de H_2S como despreciable frente a la concentración de CH_4 en los cálculos de λ, esta condición da como resultado la ecuación 2.2.

$$\lambda = \frac{[O_2]\ introducido}{2[CH_4]} \qquad \text{Ec. 2.2}$$

Una vez definido lambda se puede concluir que se van a dar tres tipos de condiciones diferentes, dependiendo del valor de lambda:

- Atmósfera reductora λ< 1
- Condiciones estequiométricas λ=1
- Atmósfera oxidante λ>1

En el anexo A se pueden encontrar los datos experimentales utilizados para la comparación, y en la tabla 3.1 unos datos generales sobre ellos.

Tabla 3.1 Datos generales sobre los experimentos

Experimentos	**Tª (°C)**	**H_2S (ppm)**	**SO_2 (ppm)**	**CH_4 (ppm)**	**H_2O (ppm)**	λ	Fuente
H_2S/CH_4 cond. red.	500-1100	279	1,6	1508	14470	0,25	[10]
H_2S/CH_4 cond. est.	500-1100	273	1,9	1516	14470	1	[10]
H_2S/CH_4 cond. oxi.	500-1100	253	18	1537	10294	2	[10]
CH_4 cond. red.	500-1100	177	75	1504	20	0,25	[10]
CH_4 cond. est.	500-1100	132	138	1517	20	1	[10]
CH_4 cond. oxi.	500-1100	85	177	1503	20	2	[10]

El tiempo de residencia (τ) en la zona de reacción se calcula aplicando la ecuación 2.3.

$$\tau(s) = \frac{V_{sr}}{Q_T(P_{sr}, T_{sr})} \qquad \text{Ec. 2.3}$$

Donde:

V_{sr} → Volumen del reactor = 11,89 cm^3

P_{sr} → Presión en el reactor = 1013,25 mbar

T → Temperatura del reactor en (K)

Q_T → Caudal de alimentación al reactor (mL/min)

El tiempo de residencia para cada temperatura alcanzada por el horno durante los experimentos que se han llevado a cabo, teniendo en cuenta un caudal normal (temperatura de 273 K y presión de 1 bar) de 1000 mLN/min, se recoge en la Tabla 3.2

Tabla 3.2 Tiempos de residencia

Temperatura (°C)	τ (s)	Temperatura (°C)	τ (s)
500	0,25	800	0,18
550	0,24	900	0,17
600	0,22	950	0,16
650	0,21	1000	0,15
700	0,20	1100	0,14
750	0,19		

Como se puede observar, la temperatura juega un papel muy importante en el valor del tiempo de residencia, resultando una diferencia de 0,1 segundos entre los 500 y 1100 ºC.

4 Modelado cinético

Partiendo del mecanismo base de Colom-Díaz et al. [5], se ha desarrollado un mecanismo mejorado capaz de prever mejor el comportamiento de la combustión de CH_4 con H_2S. Con dicho mecanismo, se mostrará la comparación de las simulaciones, obtenidas tanto en el mecanismo de partida como en el modificado en el presente trabajo, con los datos experimentales para diferentes condiciones (reductoras, estequiométricas y oxidantes), con el fin de conocer la mejora que supone el nuevo mecanismo con respecto al de partida.

4.1 Software y modelos utilizados

Para llevar a cabo las simulaciones se ha utilizado el software ANSYS – ChemkinPro, con un modelo de reactor de Flujo Pistón. Se ha utilizado la versión comercial CHEMKIN-Pro, de la compañía Reaction Design [11]. Este software permite calcular la evolución en el tiempo de una mezcla homogénea de gases reactantes en un sistema cerrado. Además, ofrece la posibilidad de realizar análisis de velocidad de reacción, mediante la herramienta Reaction Path Analyzer Tool. Una información más detallada del software se encuentra en el Anexo A.

El modelo cinético de partida utilizado en este estudio fue desarrollado por Colom-Díaz et al. [5] y se ha actualizado en el presente trabajo con varios mecanismos de reacción, entre los que se puede destacar el mecanismo de Jorge Giménez et al. [12] de CH_4, y los de Gersen et al. [9] y Mulvihill et al. [13] para la combustión de CH_4 y H_2S, además de otras fuentes que se han utilizado para agregar y actualizar reacciones y que están detalladas en el Anexo B.

4.2 Mecanismo de partida utilizado

Como se ha mencionado anteriormente, se ha partido del mecanismo desarrollado por Colom-Díaz et al. [5] para el proceso de oxidación del H_2S. Este mecanismo de partida es una versión modificada del mecanismo de Abián et al. [14], al cual se añadieron reacciones químicas de los compuestos de azufre enfocándose en las reacciones de SO_2. Además, los autores [5] tomaron reacciones del mecanismo de H_2S a presión de Song et al. [15] y las incorporaron al mecanismo.

En el mecanismo inicial se determinaron también los parámetros cinéticos de reacciones importantes, como la isomerización del HSOO a HSO_2 y la interacción de H_2S con HO_2.

Las simulaciones del mecanismo desarrollado por Colom-Diaz et al. [5] predicen bastante bien los resultados experimentales de los experimentos de oxidación de solamente H_2S a diferentes condiciones realizados por los autores.

Utilizando los experimentos de combustión de la mezcla H_2S/CH_4, se realizó una simulación de todos ellos para comprobar el funcionamiento previo del modelo, y para tener un punto de partida sobre el que valorar los posteriores resultados. Las simulaciones obtenidas son las correspondientes a las figuras 4.2.1 a 4.2.3.

Los resultados experimentales se muestran como símbolos y los cálculos mediante líneas continuas.

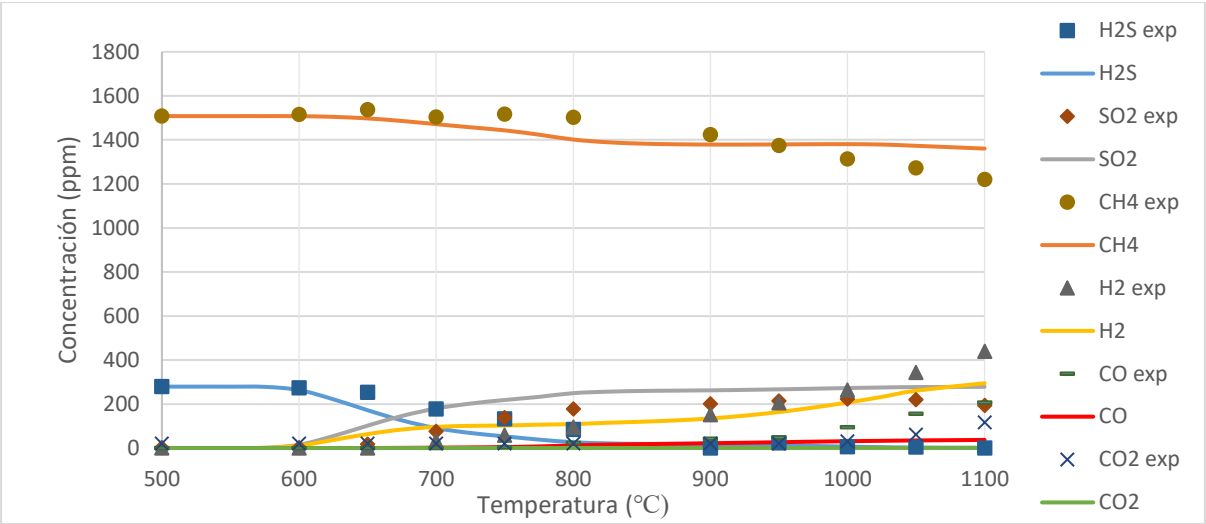


Figura 4.2.1 Resultados con el mecanismo inicial en el experimento H_2S/CH_4 en condiciones reductoras

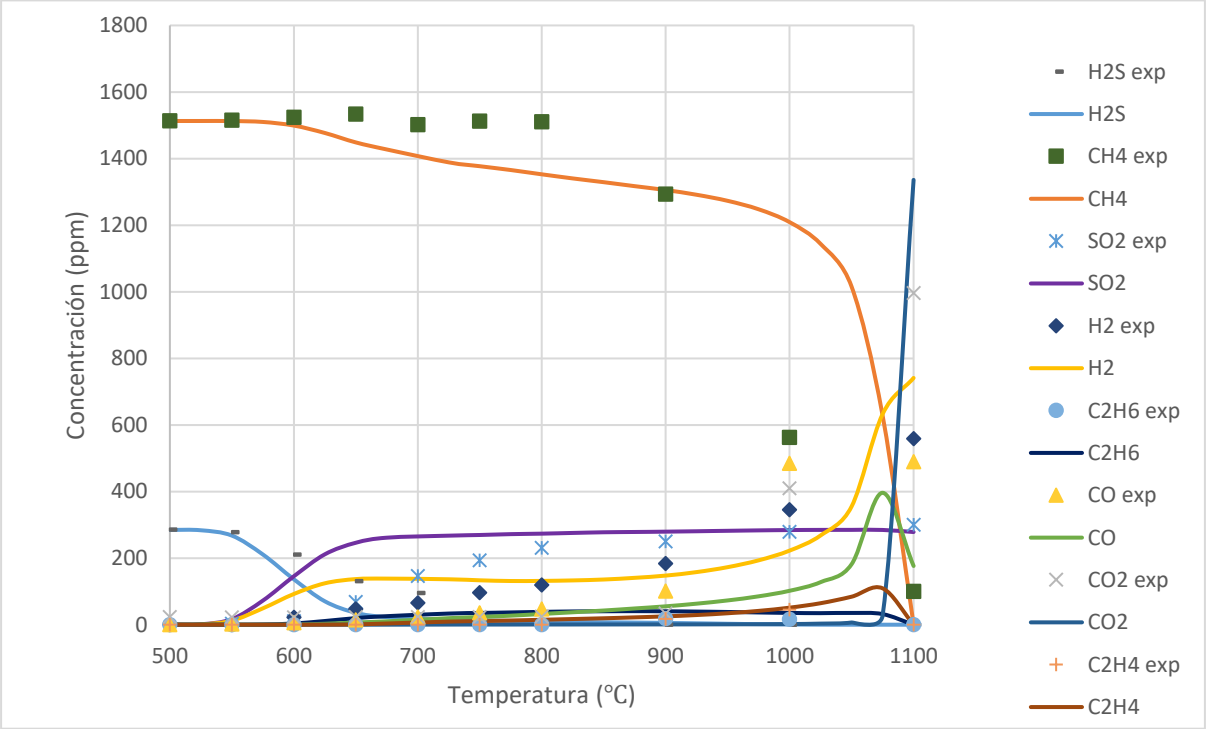


Figura 4.2.2 Resultados con el mecanismo inicial en el experimento H_2S/CH_4 en condiciones estequiométricas

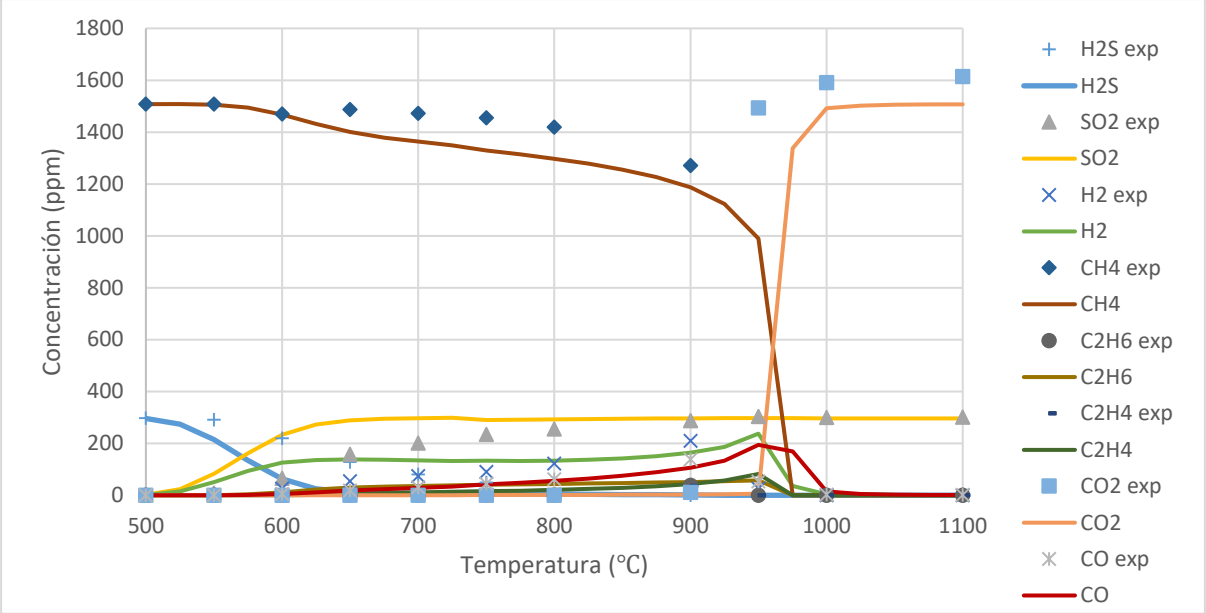


Figura 4.2.3 Resultados con el mecanismo inicial en el experimento H_2S/CH_4 en condiciones oxidantes

4.3 Mecanismo modificado en el presente trabajo

Partiendo del mecanismo mencionado en el apartado 4.2, que, como se ha mencionado anteriormente, da buenos resultados en la simulación de la oxidación de los experimentos de solamente H_2S, se optó primeramente por simular experimentos obtenidos de bibliografía de la combustión de CH_4. Los datos experimentales utilizados se encuentran en el anexo A.

Los resultados de las simulaciones se encuentran en las figuras 4.3.1 a 4.3.3. En estas figuras los resultados experimentales están representados por símbolos, mientras que las simulaciones realizadas se han representado mediante líneas continuas.

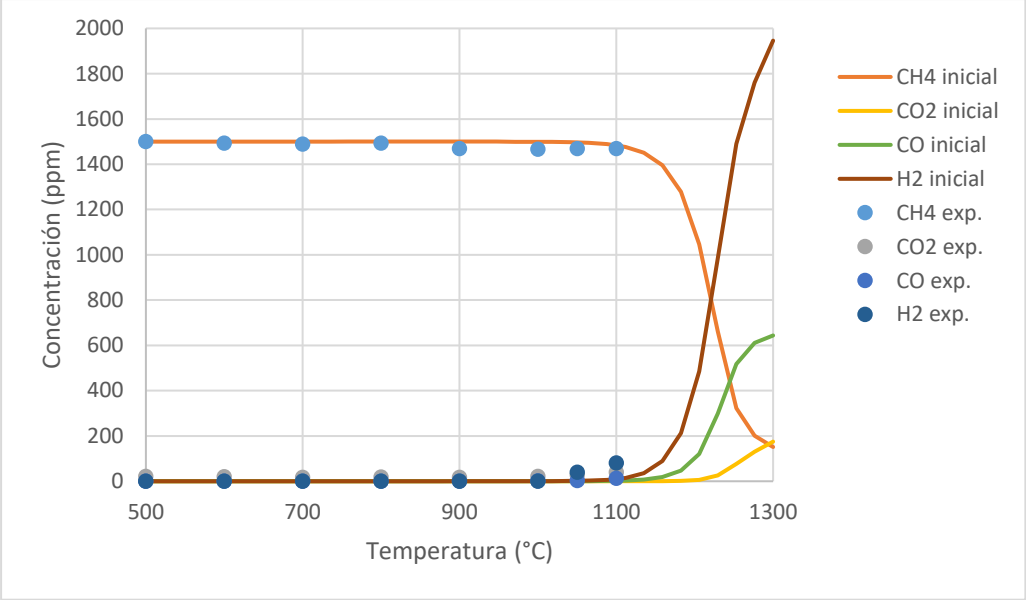


Figura 4.3.1 Resultados con el mecanismo inicial en el experimento CH_4 en condiciones reductoras

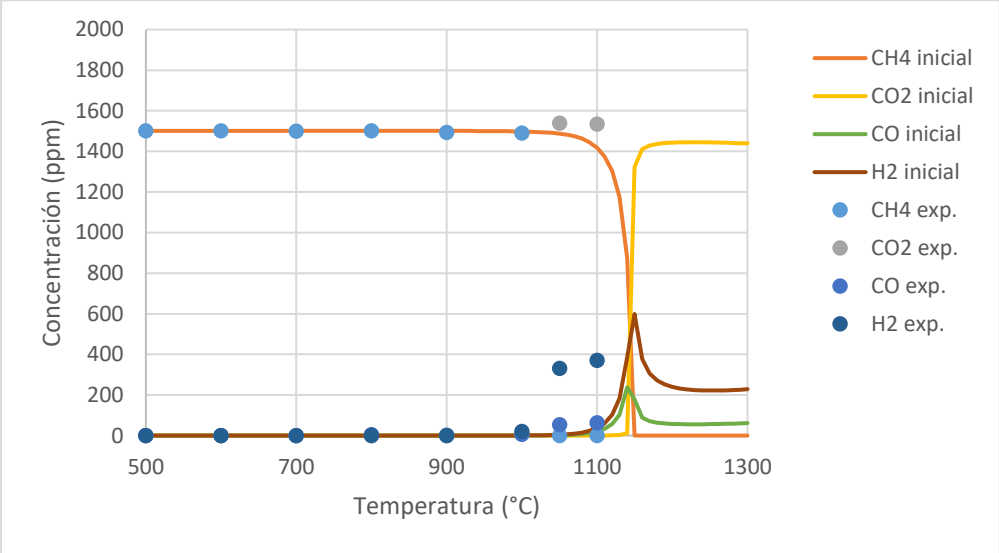


Figura 4.3.2 Resultados con el mecanismo inicial en el experimento CH_4 en condiciones estequiométricas

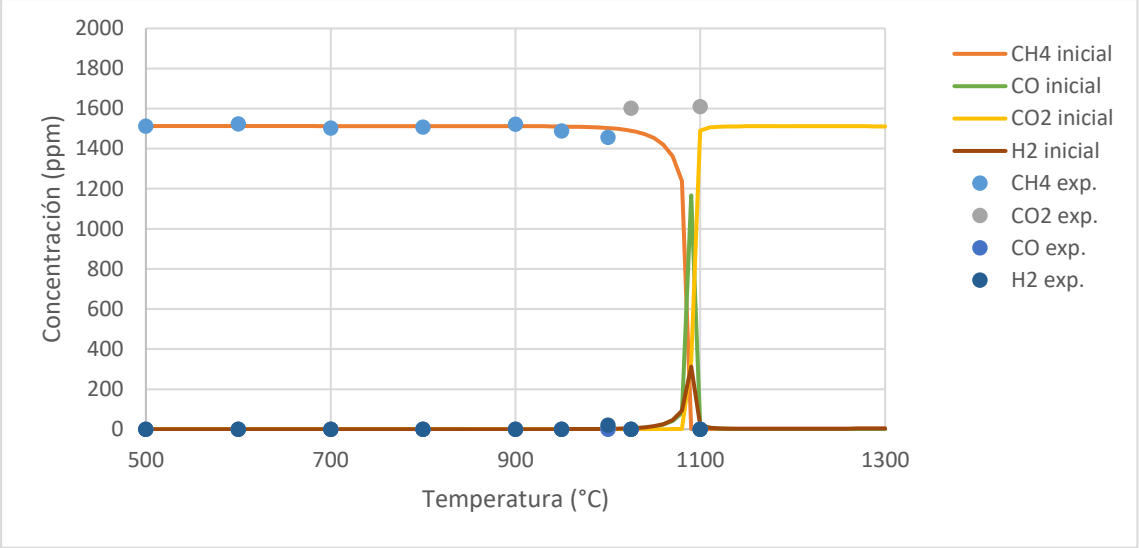


Figura 4.3.3 Resultados con el mecanismo inicial en el experimento CH_4 en condiciones oxidantes

Como se observan en las simulaciones, el proceso de combustión del metano se lleva a cabo a una temperatura menor que la simulada, por lo que habría que buscar el método de reducir la temperatura a la cual se inicia el proceso de combustión. Por ello, se empezó agregando reacciones del mecanismo de Jorge Giménez et al. [12], debido a su extenso trabajo en la oxidación de especies de carbono (CH_4, C_2H_2, C_2H_2, HCN), para mejorar las predicciones, y se actualizaron diferentes reacciones para mejorar el mecanismo.

Las reacciones agregadas del mecanismo de Jorge Giménez et al. [12] se encuentran especificadas en el anexo C.3, en la tabla C.3.1. En la tabla 4.3.1 se encuentran todas las reacciones modificadas con sus nuevos parámetros cinéticos.

Estos cambios conformarán lo que se va a denominar como mecanismo modificado 1, ya que se van a describir varias modificaciones hasta llegar al mecanismo final del presente trabajo.

Tabla 4.3.1 Parámetros cinéticos de las reacciones modificadas en el mecanismo modificado 1. Unidades: mol, cm, s, cal, K.

Reacción	**A**	**β**	**Ea**
$CH_4+OH=CH_3+H_2O$	1E+06	2.183	2300.000
$CH_4+O=CH_3+OH$	4.39E5	2.5	6578.
$CH_3+O_2=CH_2O+OH$	6.38E11	0.0	13515
$CH_3+O_2=CH_3O+O$	2.7E12	0.0	25000
$CH_3+OH=CH_2+H_2O$	7.8E+12	0.000	0.0
$CH_3O+H=CH_3+OH$	1.2E+9	1.010	12000.000
$CH_2OH+H=CH_3+OH$	6.600E+9	1.000	3200.000
$C_2H_6+OH=C_2H_5+H_2O$	6.62E13	0.0	5042
$C_2H_6+H=C_2H_5+H_2$	9.8E013	0.00	9220
$C_2H_6+O=C_2H_5+OH$	1.8E05	2.80	5802
$C_2H_6+HO_2=C_2H_5+H_2O_2$	1.1E5	2.50	16850
$C_2H_6+O_2=C_2H_5+HO_2$	7.29E5	2.5	49160
$C_2H_6+CH_3=C_2H_5+CH_4$ DUP	5.6E10	0.00	9418
$C_2H_6+CH_3=C_2H_5+CH_4$ DUP	8.4E14	0.00	22250
$C_2H_4+H(+M)=C_2H_5(+M)$ Límite de baja presión: Eficiencias de 3er cuerpo:	3.97E9 4.71E18	1.28 0.0	1292. 755.0

H_2/2/ CO/2/ CO_2/3/ H_2O/5/			
C_2H_4+OH=C_2H_3+H_2O	2.23E4	2.745	2216
C_2H_4+H=C_2H_3+H_2	2.35E2	3.62	11266
CH_3+NO=HCN+H_2O	1.50E11	0.0	15000
CH_3+NO=H_2CN+OH	4.50E11	0.0	15000
CH_3+NO(+M)=CH_3NO(+M) Límite de baja presión: Parámetros de TROE: 5.0 1.0E-30 120 1E30	9.0E12 2.5E16	0.0 0.0	192 -2841
CH_2+NO=HCN+OH	3.9E11	0.0	378
CH_2+NO=HCNO+H	3.1E12	0.0	378
HCO+NO=CO+HNO	7.0E21	0.0	0
NH_3+O=NH_2+OH	2.8E2	3.29	4471
NH_2+O=HNO+H	6.6E13	0.0	0
NH_2+O=NH+OH DUP	7.0E12	0.0	0
NH_2+O=NH+OH DUP	8.6E-1	4.01	1673
H_2NO+O = NH_2+O_2	2.6E11	0.4872	29050
NH_2+NO=N_2+H_2O	2.8E20	-2.654	1258
NH_2+NO=NNH+OH	2.3E10	0.425	-814

$NNH=N_2+H$	1.0E9	0.0	0
$NNH+O=N_2+OH$	1.2E13	0.145	-217
$NNH+O=N_2O+H$	1.9E14	-0.274	-22
NNH+O=NH+NO	5.2E11	0.388	-409
$NNH+O_2=N_2+HO_2$	5.6E14	-0.385	13
$NH+NO=N_2O+H$	18E14	-0.351	-244
$NH+NO=N_2+OH$	2.7E12	-0.0721	-512
HCN+O=NCO+H	7.6E10	0.48	7810
HCN+O=NH+CO	4.0E14	-0.65	8514
HCN+O=CN+OH	4.2E10	0.40	20665
$HNCO+OH=NCO+H_2O$	3.3E6	1.5	3597
HNCO+CN=NCO+HCN	5.0E12	0.0	0
$NCO+NCO=N_2+CO+CO$	3.6E13	0.0	0
$HOSO(+M)=H+SO_2(+M)$ Límite de baja presión: Parámetros de TROE: 0.283 272 3995 Eficiencias de 3er cuerpo: CO2/2.5/ SO2/10/ H2O/10/	2.37E8 1.85E37	1.63 -6.14	7339 11075
$HOSO+O_2=HO_2+SO_2$	9.6E1	2.36	-10130

A continuación, se van a presentar las figuras 4.3.4 a 4.3.9, las cuales son una comparativa entre el mecanismo inicial (línea discontinua) y el mecanismo modificado 1 (línea continua), los resultados experimentales se han representado con símbolos.

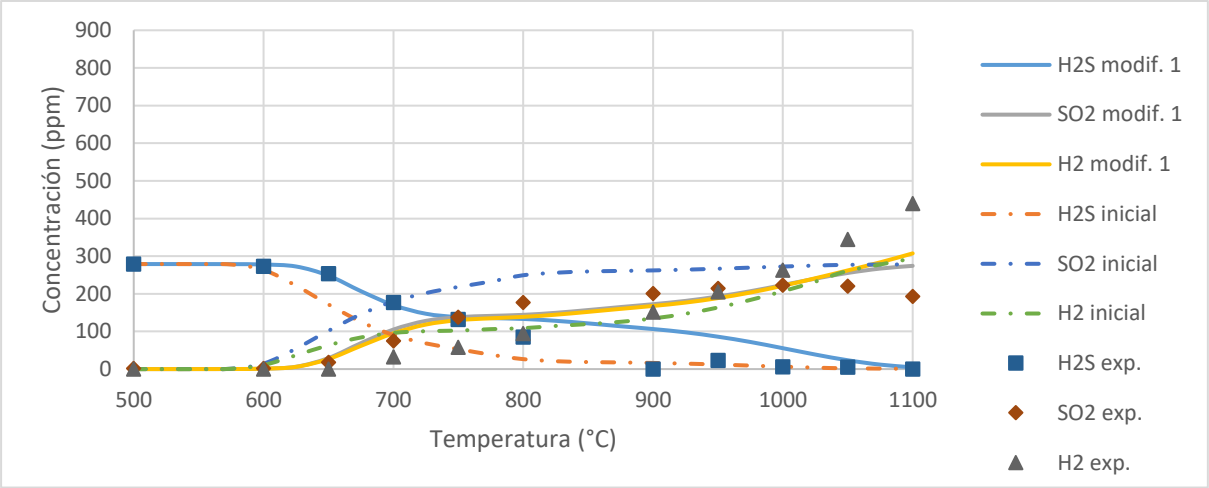


Figura 4.3.4 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 1 en el experimento H_2S/CH_4 en condiciones reductoras

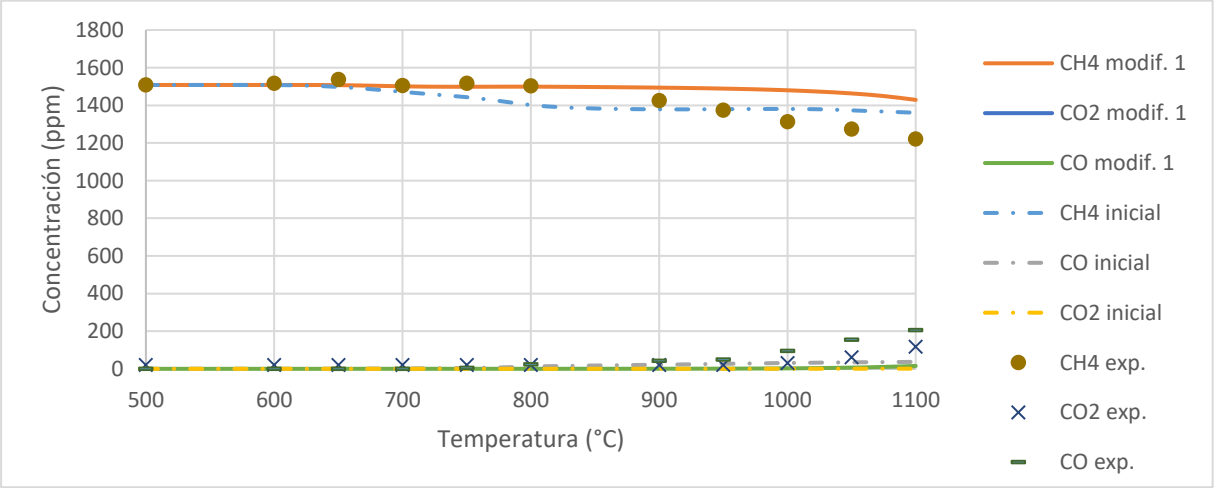


Figura 4.3.5 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 1 en el experimento H_2S/CH_4 en condiciones reductoras

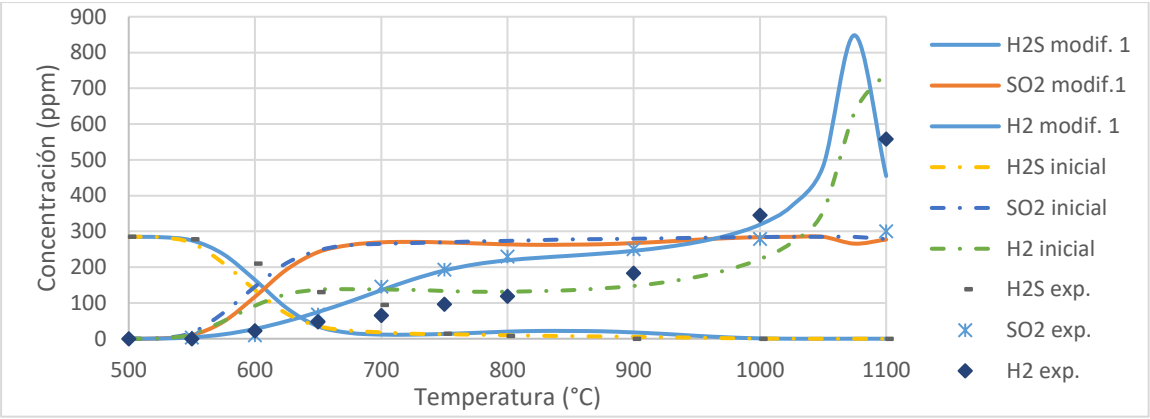


Figura 4.3.6 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 1 en el experimento H_2S/CH_4 en condiciones estequiométricas

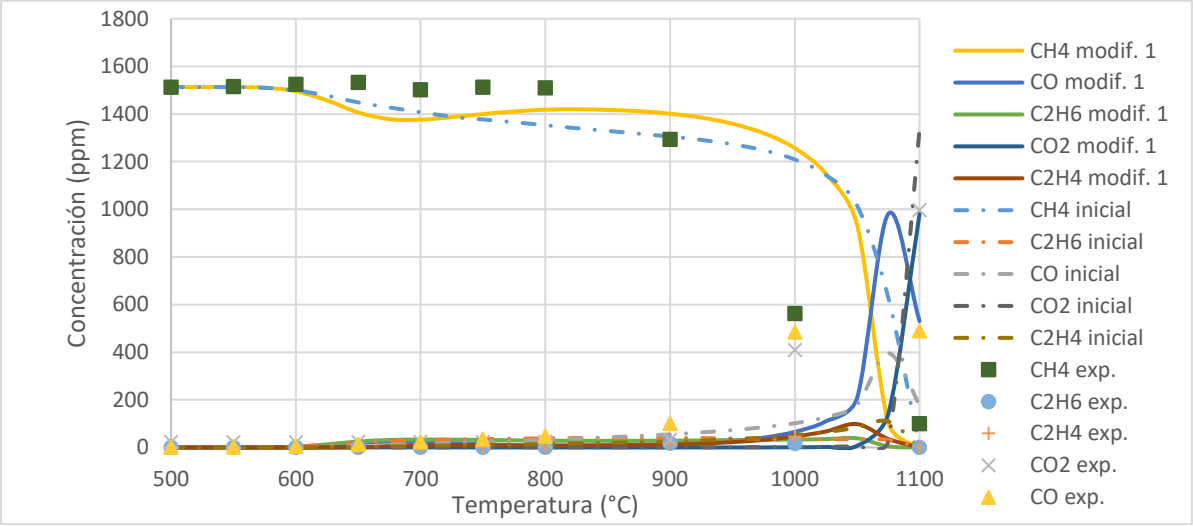


Figura 4.3.7 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 1 en el experimento H_2S/CH_4 en condiciones estequiométricas

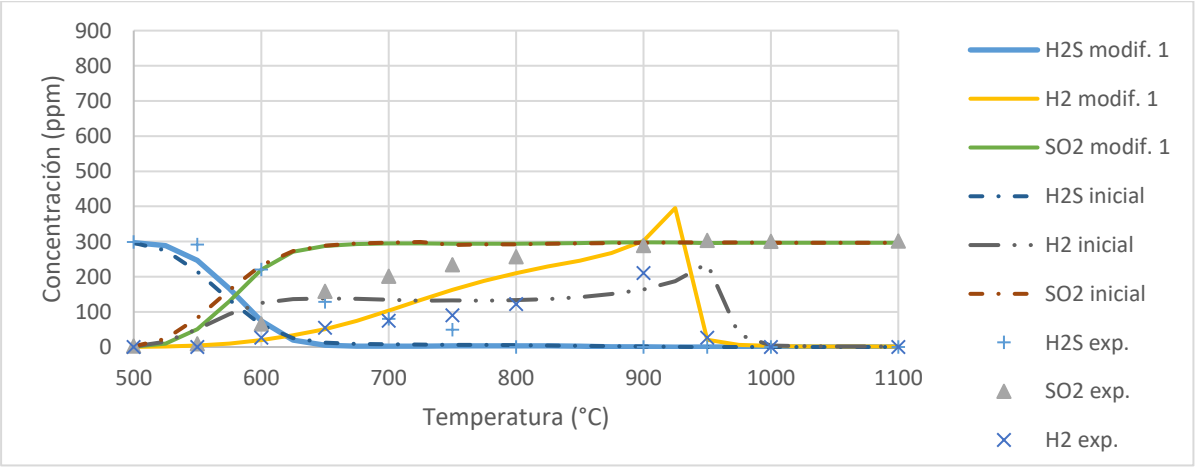


Figura 4.3.8 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 1 en el experimento H_2S/CH_4 en condiciones oxidantes

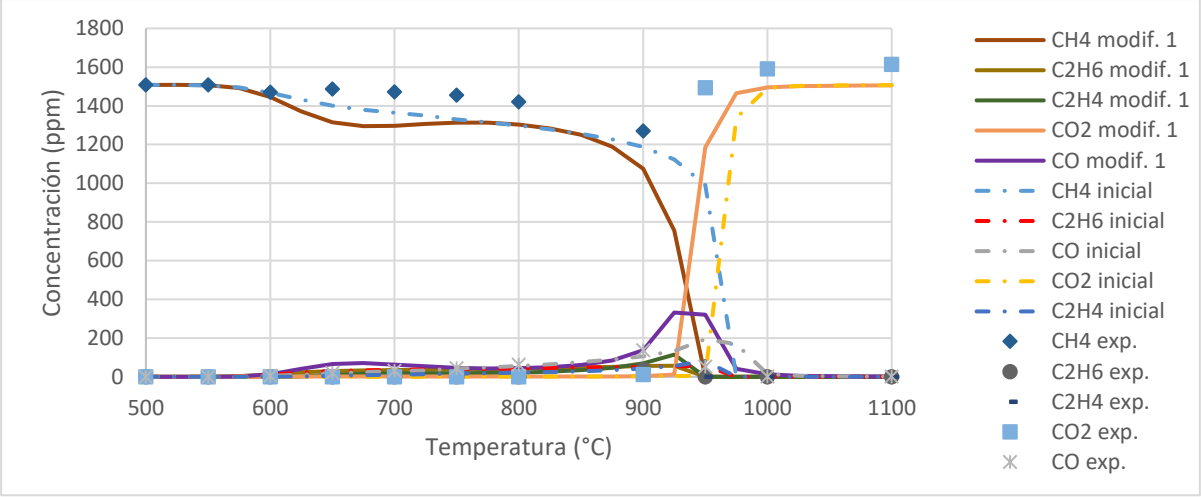


Figura 4.3.9 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 1 en el experimento H_2S/CH_4 en condiciones oxidantes

En las simulaciones de la mezcla CH_4/H_2S, se puede observar cómo para condiciones reductoras se mejora notablemente, a temperaturas bajas, los resultados de H_2S, SO_2 y H_2. Sin embargo, a medida que aumenta la temperatura, existe un cierto desplazamiento a mayores temperaturas del H_2S para consumirse que no encaja con los resultados experimentales. El CH_4 se ve también ligeramente empeorado a temperaturas elevadas ya que también sufre un cierto retardo en consumirse.

En condiciones estequiométricas, el H_2 se ve mejorado ya que concuerda mucho más con los resultados experimentales que el H_2 del mecanismo inicial. En cuanto al CH_4 en las simulaciones del mecanismo modificado vemos una mejora, ya que se acerca más al punto de 1000 ℃, sin embargo, se consume completamente antes de llegar a los 1100 ℃, además, las simulaciones se acercan más a los resultados experimentales en temperaturas intermedias.

En la simulación de condiciones oxidantes se observa que el H_2 se comporta igual que en los resultados experimentales a temperaturas bajas, pero a partir de los 700 ℃ se forma demasiado H_2. Por otra parte, el CH_4 empeora a temperaturas bajas ya que aparece una etapa a 600 ℃ en la que se empieza a consumir y, por tanto, no concordaría con los resultados experimentales. Sin embargo, se consigue que este se acabe consumiendo antes y como resultado se forme antes el CO_2, concordando más con los resultados experimentales.

Debido a que los resultados no fueron los esperados, ya que se había empeorado en ciertas condiciones el mecanismo y mejorado en otras, se utilizó la herramienta de análisis de sensibilidad sobre el CH_4, CO y CO_2 a distintas lambdas y a una conversión del 10%. Se comprobó que existían otras reacciones que no habían sido modificadas por el mecanismo de Giménez-López et al. [12] y que, sin embargo, tenían un impacto importante dentro del mecanismo.

Muchas de las reacciones de especies de carbono reaccionan con radicales libres (OH, H, etc), por lo que las reacciones que forman estos radicales adquieren una gran importancia y por ello aparecen también en los análisis de sensibilidad. Es por ello que se decidió modificarlas también las más importantes junto con las reacciones de CH_4.

Para obtener datos actualizados de las reacciones, se optó por utilizar diversas fuentes bibliográficas. Tanto las reacciones modificadas, como sus parámetros cinéticos y las fuentes consultadas aparecen en la tabla 4.3.2.

Tabla 4.3.2 Parámetros cinéticos de las reacciones modificadas en el mecanismo modificado 2. Unidades: mol, cm, s, cal, K.

Reacción	**A**	**β**	**Ea**	**Fuentes**
HCO(+M)=H+CO(+M) Límite de baja presión: Parámetros de TROE: 0.103 139. 10900. 4550 Eficiencias de 3er cuerpo: N_2/1.5/ O_2/1.5/ CO/1.5/ H_2/2.0/ CH_4/5.0/ CO_2/3. / H_2O/15. /	4.93E+16 7.43E21	-0.9 -2.36	19724 19383	[13]
$CH_2+O_2=CO_2+H+H$	2.1E09	0.9929	-269	[13]

$CH_4+O_2=CH_3+HO_2$	2.03E+05	2.7	51714	[13]
$CH_3+HO_2=CH_3O+OH$	6.8E12	0.0	0.0	[16]
$CH_4+H=CH_3+H_2$	4.1E03	3.156	8755	[17]
$CH_3+H(+M)=CH_4(+M)$ Límite de baja presión: Parámetros de TROE: 0.783 74.0 2941.0 6964.0 Eficiencias de 3er cuerpo: H_2/2.86/ H_2O/8.57/ CH_4/2.86/ CO/2.14/ CO_2/2.86/ C_2H_6/4.29/ N_2/1.43/	5.54E24 1.75E33	-2.17 -4.76	0 2440.0	[18]
$CH_3+CH_3(+M)=C_2H_6(+M)$ Límite de baja presión: Parámetros de TROE: 0.62 73 1180 1E30	9.5E14 1.269E39	-0.538 -7.0	179 2762	[9]
$H+O_2=O+OH$	1.0E14	0.000	15286	[9]
$OH+H_2=H_2O+H$ DUP	2.14E14	0.00	9900	[19]
$OH+H_2=H_2O+H$ DUP	8.31E5	2.34	3500	[19]
$O+H_2=OH+H$ DUP	3.80E+12	0	7948	[13]
$O+H_2=OH+H$ DUP	8.80E+14	0	19175	[13]

HO_2+H=OH+OH	7.10E+13	0	295	[13]
H_2O_2(+M) = OH+OH(+M) Límite de baja presión: Parámetros de TROE: 0.43 1E-30 1E+30 Eficiencias de 3er cuerpo: AR/1.0/ H2O/7.5/ CO2/1.6/ N2/1.5/ O2/1.2/ H2O2/7.7/ H2/3.7/ CO/2.8/	2.00E+12 2.49E+24	0.90 2.30	4.8749E+04 4.8749E+04	[9]

A partir del mecanismo modificado 1, se realizaron las modificaciones de la tabla 4.3.2, dando lugar al mecanismo modificado 2.

Una vez introducidas las modificaciones al mecanismo, se realizaron las simulaciones, y en las figuras 4.3.10 a 4.3.15 se observan los resultados obtenidos de estas. Los resultados del mecanismo inicial se encuentran representados por líneas discontinuas, mientras que los del mecanismo modificado 2 son representados por líneas continuas. Los resultados experimentales se han representado con símbolos.

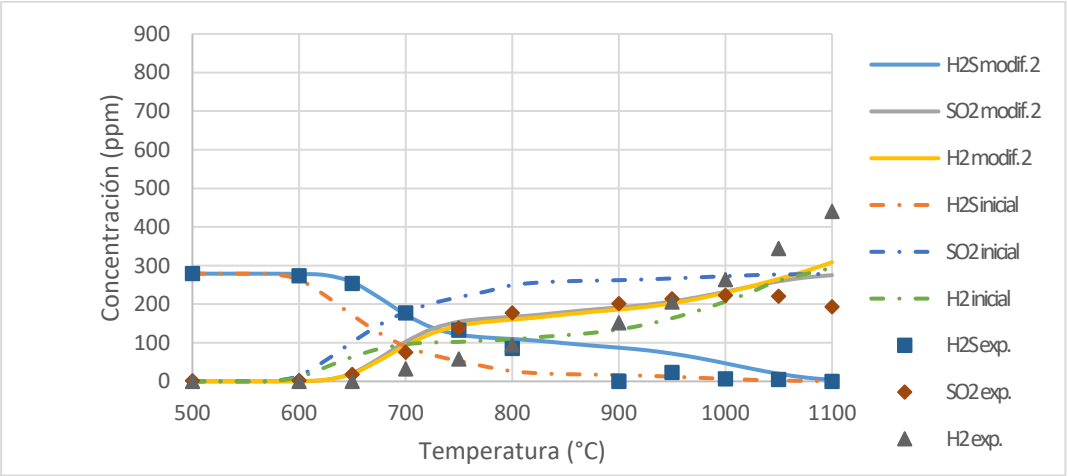


Figura 4.3.10 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 2 en el experimento H_2S/CH_4 en condiciones reductoras.

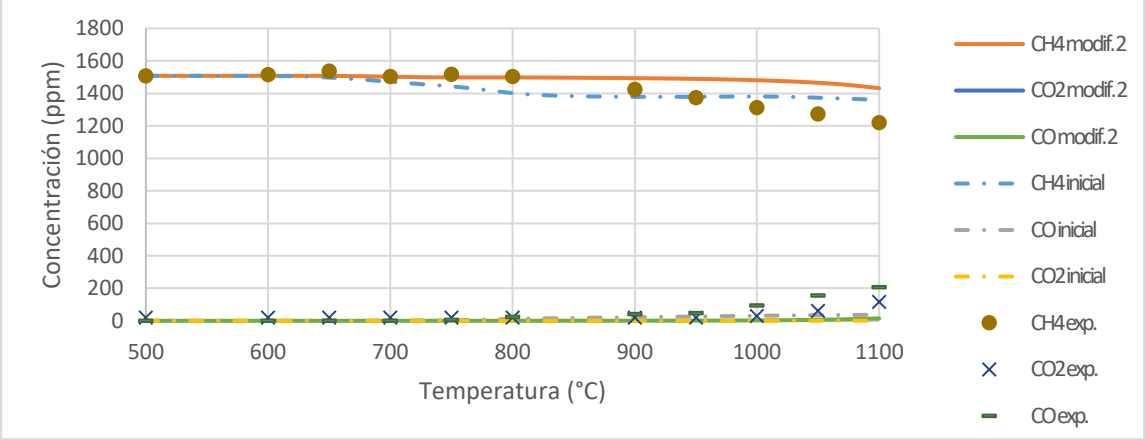


Figura 4.3.11 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 2 en el experimento H_2S/CH_4 en condiciones reductoras.

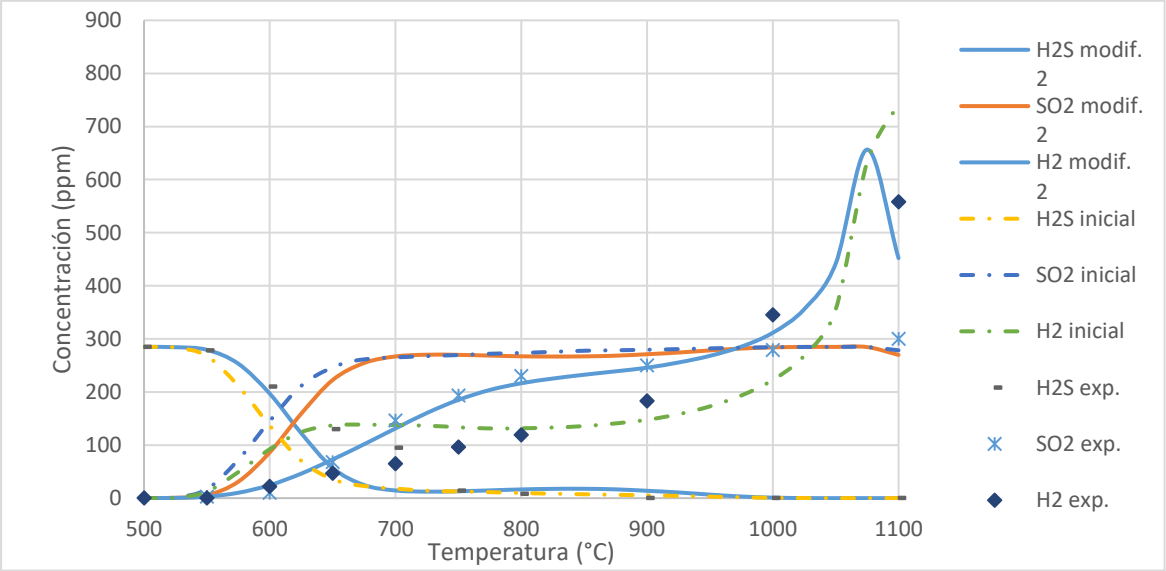


Figura 4.3.12 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 2 en el experimento H_2S/CH_4 en condiciones estequiométricas.

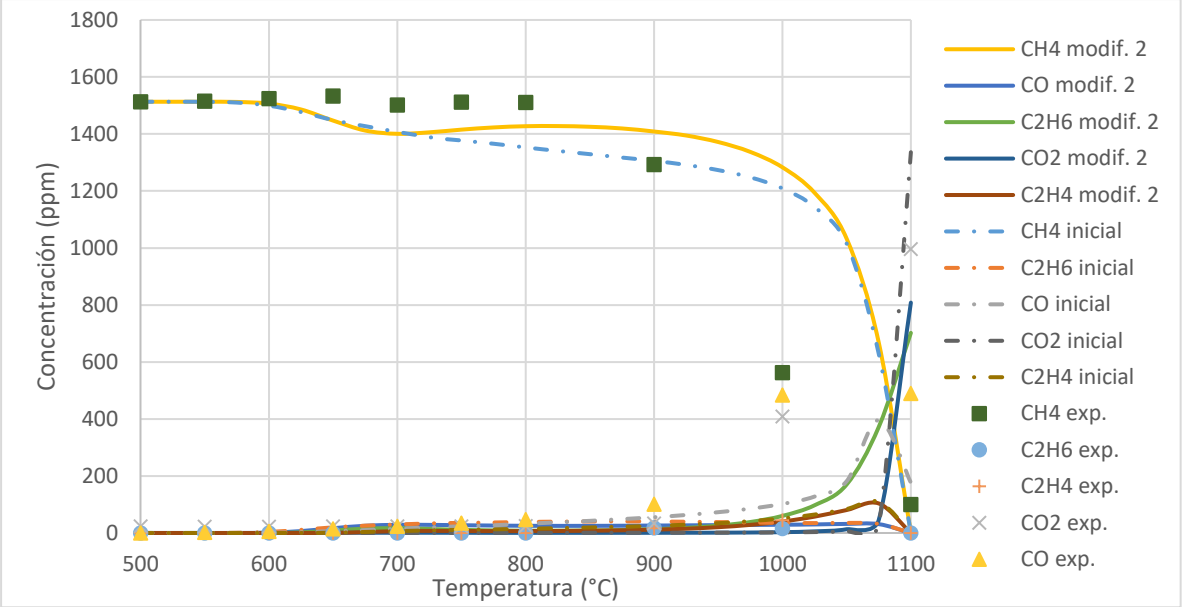


Figura 4.3.13 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 2 en el experimento H_2S/CH_4 en condiciones estequiométricas.

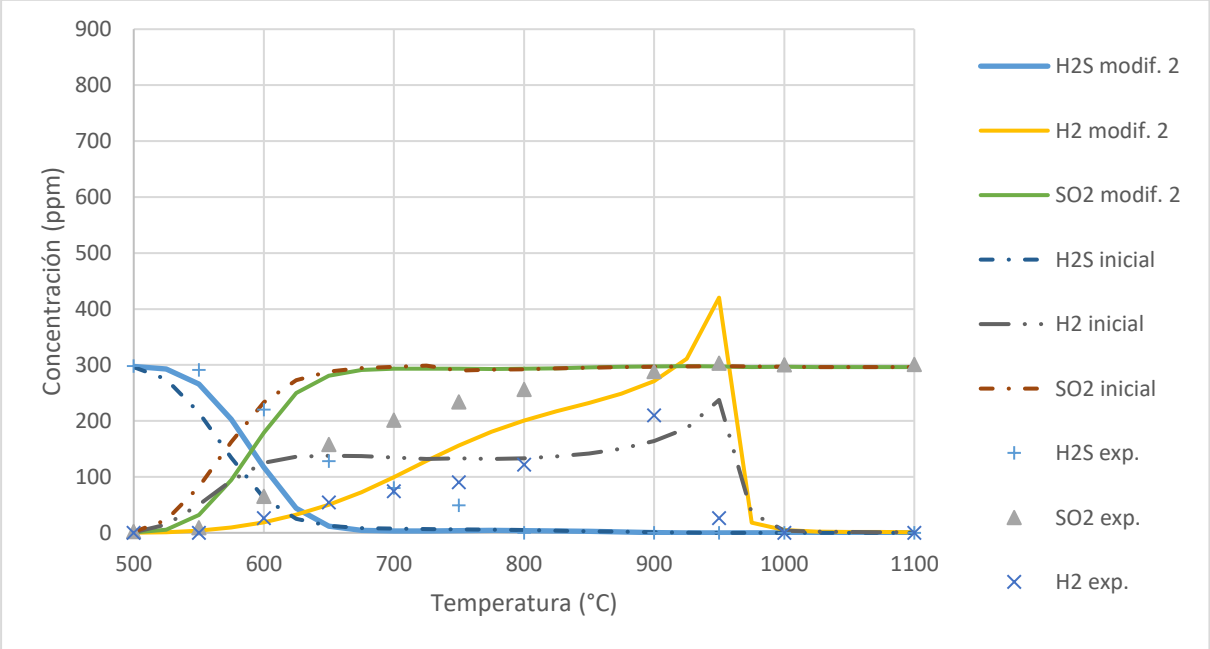


Figura 4.3.14 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 2 en el experimento H_2S/CH_4 en condiciones oxidantes.

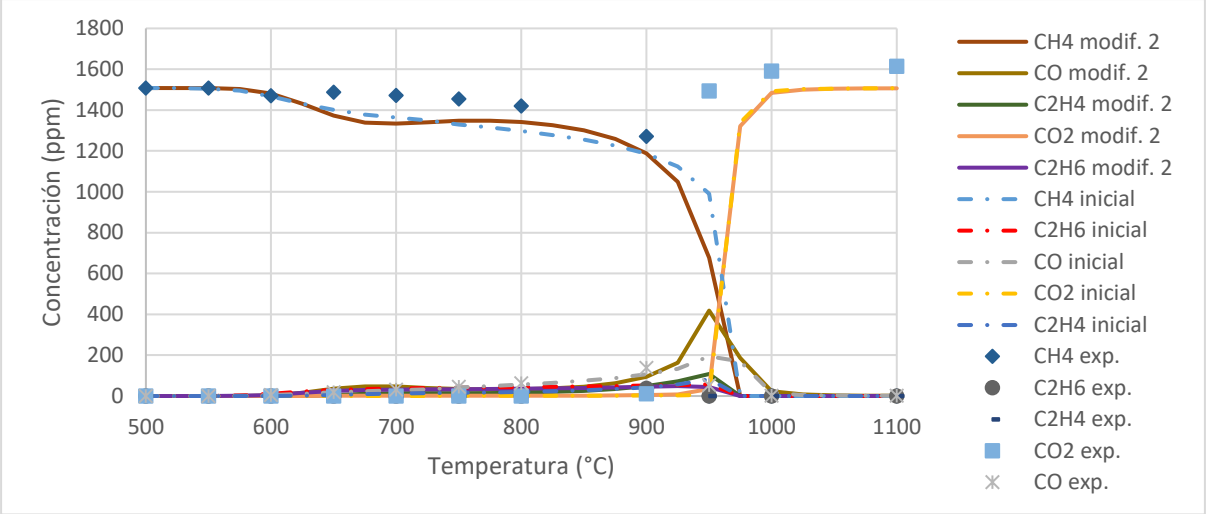


Figura 4.3.15 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 2 en el experimento H_2S/CH_4 en condiciones oxidantes.

En los resultados obtenidos en el mecanismo modificado 2, se observa una ligera mejora del H_2S y del SO_2 respecto al mecanismo anterior en todas las condiciones. Además, el CH_4 en condiciones estequiométricas se acaba consumiendo a 1100 ℃, concordando más con los resultados experimentales. Finalmente, se observa que el CO y el H_2 en condiciones oxidantes se consumen a temperaturas mayores, empeorando las simulaciones con respecto al mecanismo modificado 1.

Posteriormente, se optó por buscar otros mecanismos que estudiaran la combustión de CH_4. Se utilizaron el mecanismo Gri 3.0 [20] debido a que ha sido ampliamente utilizado para simular reacciones de combustión de CH_4 y el de Mulvihill et al.[13] debido a que este mecanismo tiene una gran cantidad de reacciones de compuestos orgánicos que no tiene en cuentra el Gri 3.0 [20] que podrían ser importantes en el mecanismo de combustión de CH_4. Estas reacciones agregadas se encuentran en la tabla C.3.2 y en la tabla C.3.5 respectivamente en el anexo C.3

La inclusión de estas reacciones da lugar a lo que denominaremos como mecanismo modificado 3.

A continuación, se muestran los resultados de las simulaciones en las figuras 4.3.16 a 4.3.21. Los resultados del mecanismo inicial se encuentran representados por líneas discontinuas, mientras que los del mecanismo modificado 3 son representados por líneas continuas. Los resultados experimentales se han representado con símbolos.

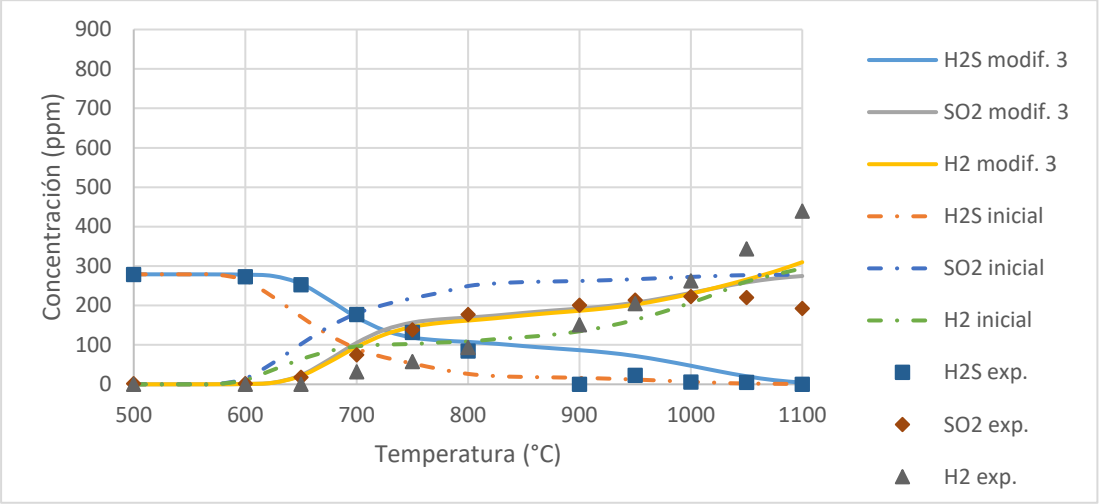


Figura 4.3.16 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 3 en el experimento H_2S/CH_4 en condiciones reductoras.

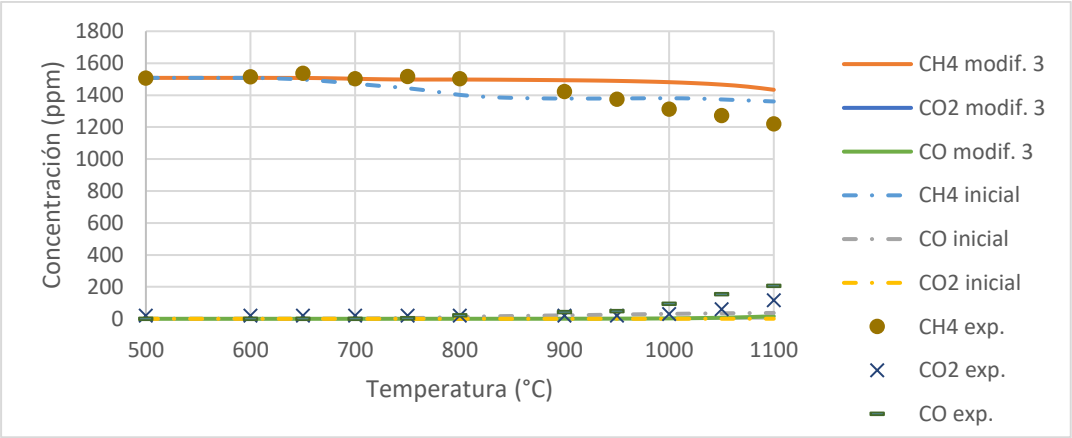


Figura 4.3.17 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 3 en el experimento H_2S/CH_4 en condiciones reductoras

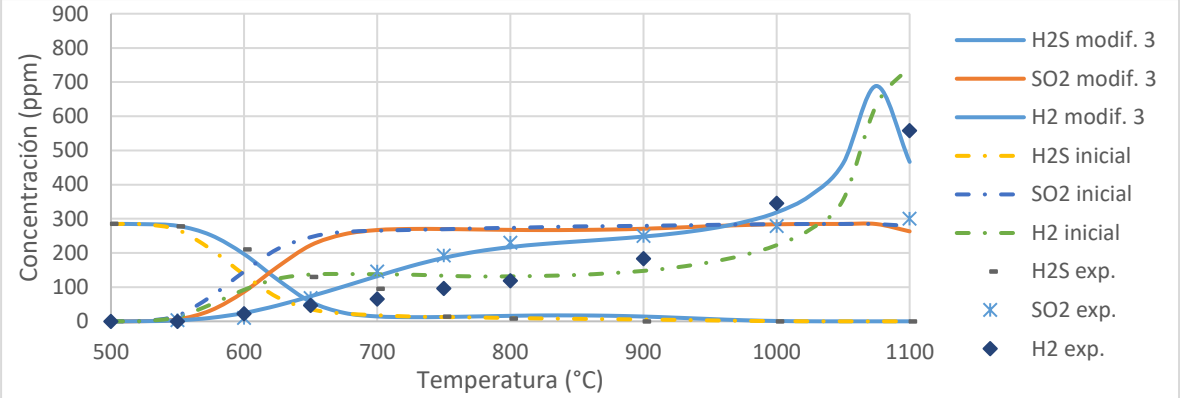


Figura 4.3.18 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 3 en el experimento H_2S/CH_4 en condiciones estequiométricas.

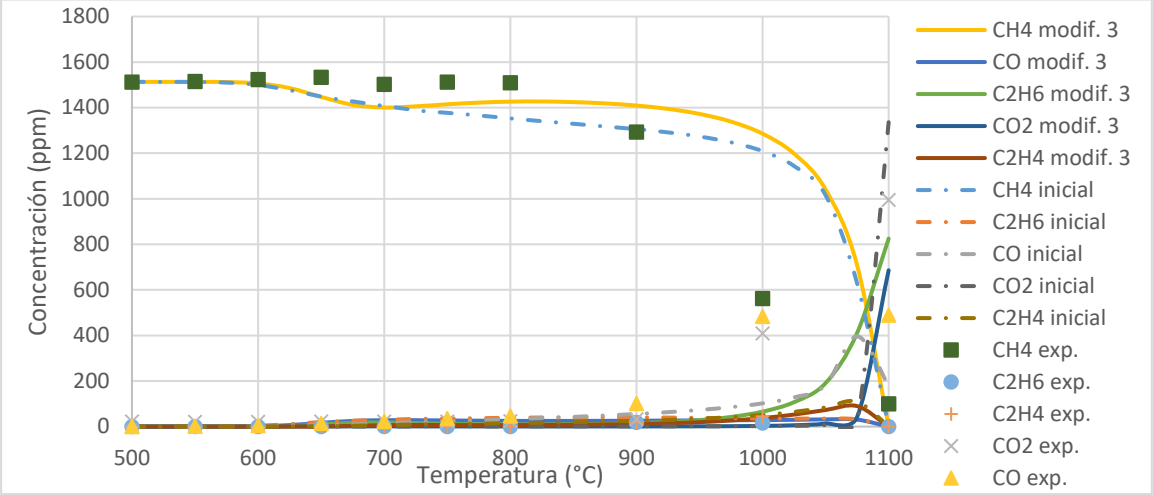


Figura 4.3.19 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 3 en el experimento H_2S/CH_4 en condiciones estequiométricas.

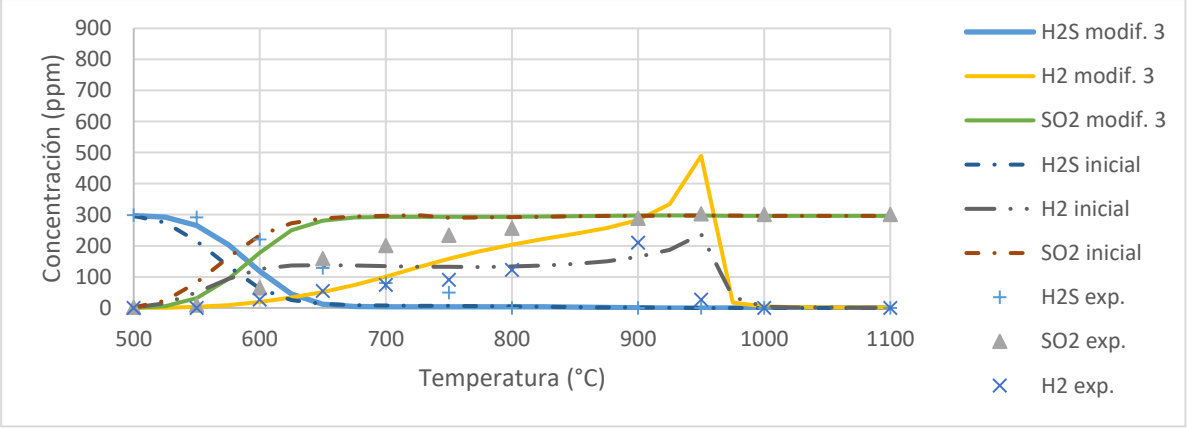


Figura 4.3.20 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 3 en el experimento H_2S/CH_4 en condiciones oxidantes

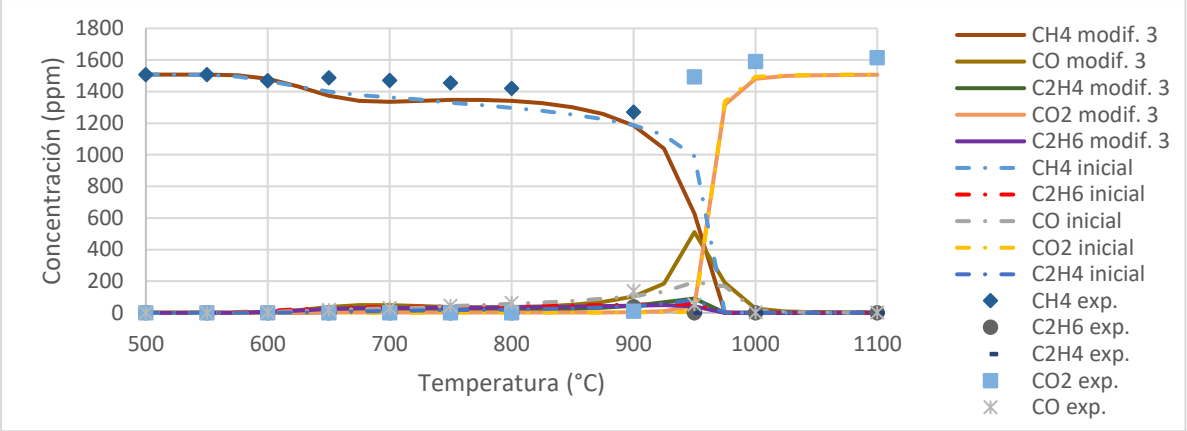


Figura 4.3.21 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 3 en el experimento H_2S/CH_4 en condiciones oxidantes

Como se observa en las figuras 4.3.16 a 4.3.21, no aparece ningún cambio con respecto al mecanismo modificado 2, por lo que se llega a la conclusión que ninguna de las reacciones agregadas en el mecanismo modificado 3 tiene importancia dentro del proceso de combustión de la mezcla CH_4/H_2S.

Como en el mecanismo de Giménez-López [12] se habían modificado dos reacciones de azufre, se revirtieron los cambios para observar claramente si se han mejorado las simulaciones con las modificaciones a las reacciones carbonosas. Por tanto, en el mecanismo modificado 4, se revierten a sus valores originales las siguientes reacciones:

$$HOSO+O_2=HO_2+SO_2 \qquad (R.1)$$

$$HOSO(+M)=H+SO_2(+M) \qquad (R.2)$$

Los resultados de las simulaciones del mecanismo modificado 4 se pueden observar en las figuras 4.3.22 a 4.3.27. Los resultados del mecanismo inicial se encuentran representados por líneas discontinuas, mientras que los del mecanismo modificado 4 son representados por líneas continuas. Los resultados experimentales se han representado con símbolos.

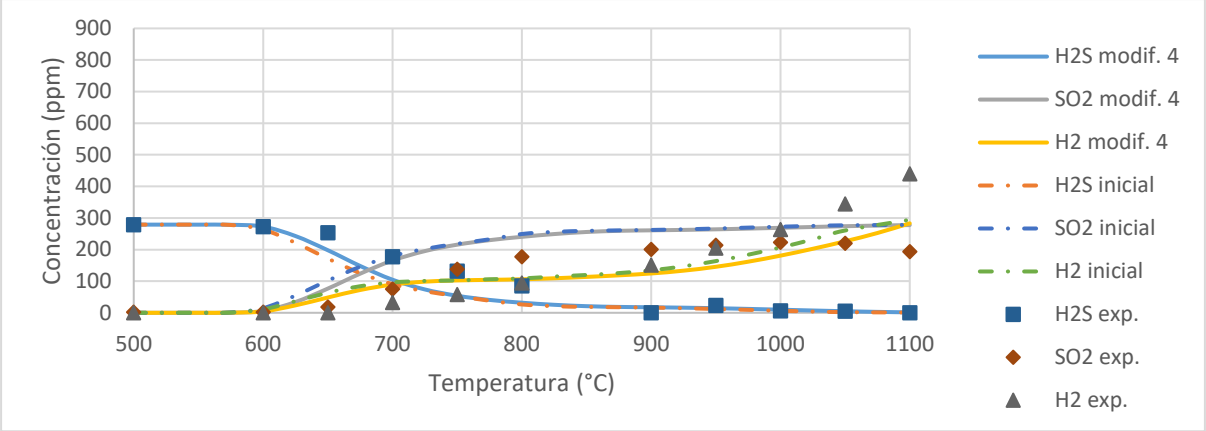


Figura 4.3.22 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 4 en el experimento H_2S/CH_4 en condiciones reductoras.

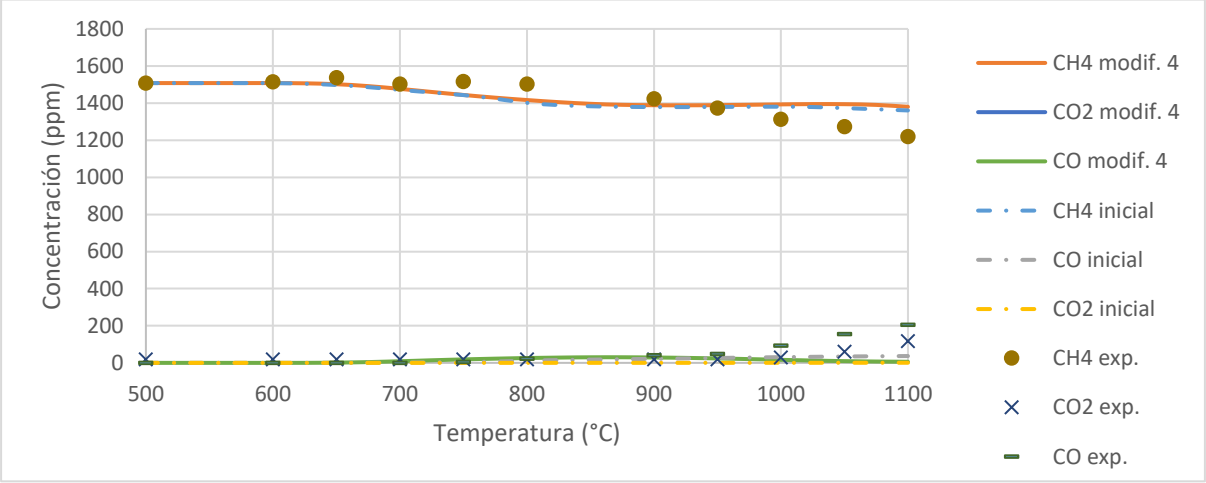


Figura 4.3.23 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 4 en el experimento H_2S/CH_4 en condiciones reductoras.

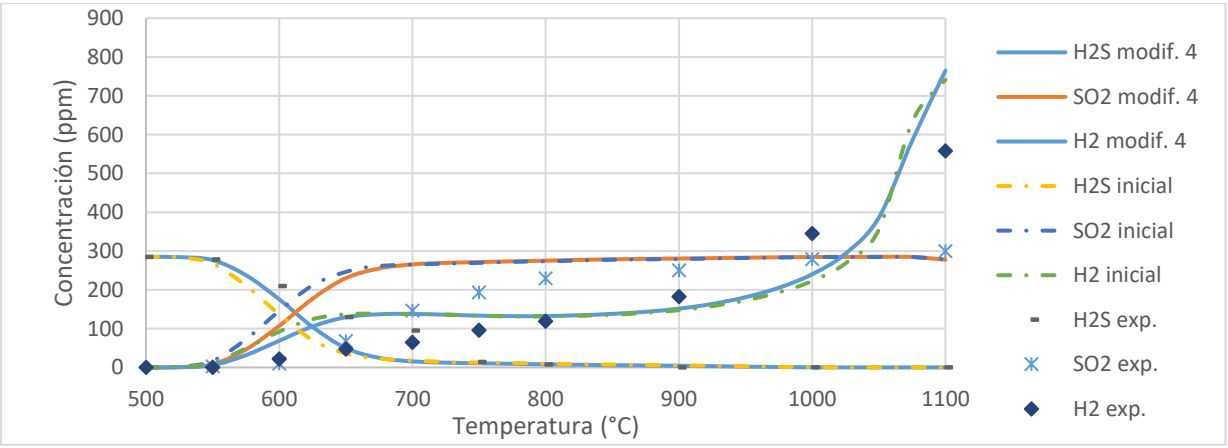


Figura 4.3.24 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 4 en el experimento H_2S/CH_4 en condiciones estequiométricas.

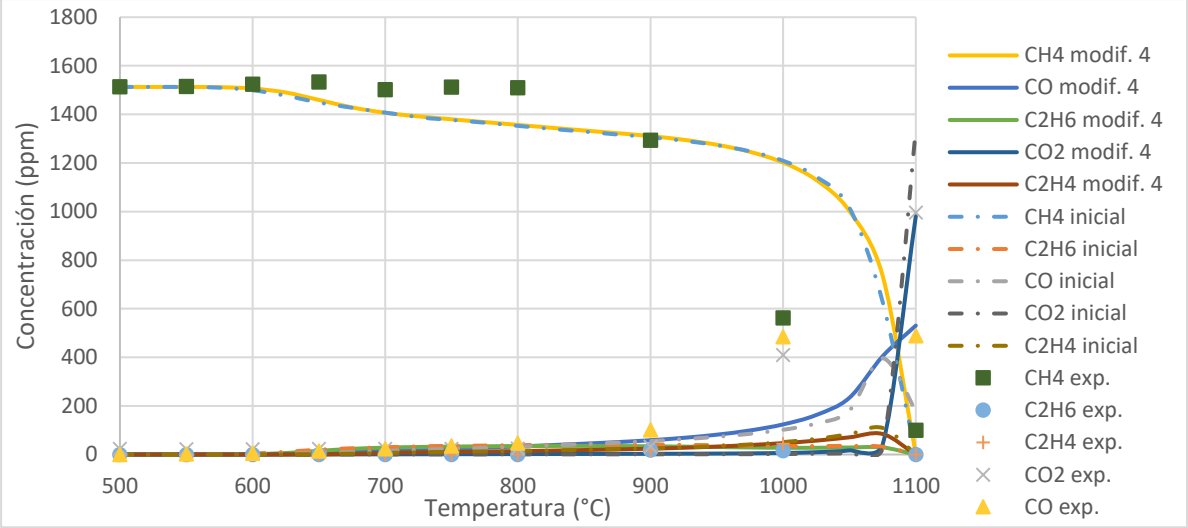


Figura 4.3.25 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 4 en el experimento H_2S/CH_4 en condiciones estequiométricas.

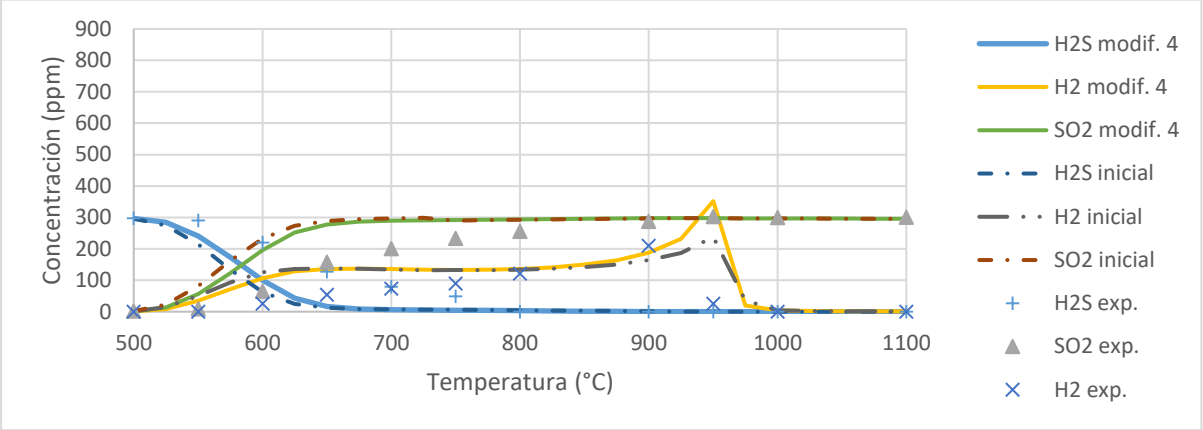


Figura 4.3.26 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 4 en el experimento H_2S/CH_4 en condiciones oxidantes.

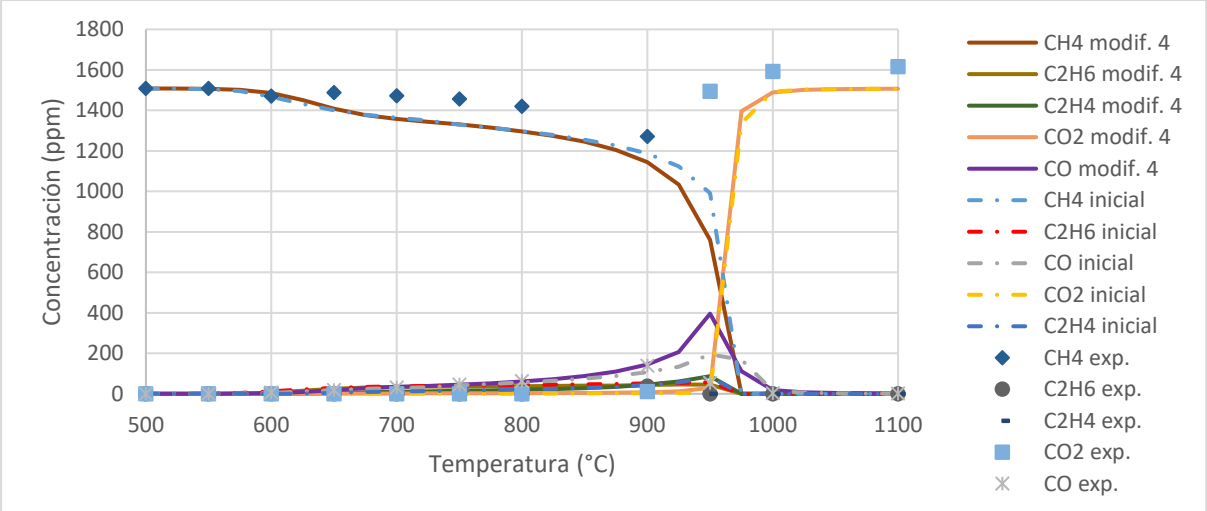


Figura 4.3.27 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 4 en el experimento H_2S/CH_4 en condiciones oxidantes.

Los resultados de las simulaciones muestran una ligera mejora con el mecanismo original en cuanto al H_2S y SO_2 en todas las condiciones. En condiciones estequiométricas se observa cómo el CH_4 requiere una temperatura más alta que en las simulaciones originales para consumirse, sin embargo, esta temperatura es menor a condiciones oxidantes que en el mecanismo original. También se observa un ligero empeoramiento del H_2 a temperaturas elevadas en condiciones reductoras, aunque esta mejora a temperaturas bajas en todas las condiciones.

Debido a que los resultados eran generalmente mejores que los del mecanismo inicial y apenas había un empeoramiento, se decidió mantener esta modificación.

A continuación, se observó que la reacción $CH_3+CH_3(+M)=C_2H_6(+M)$, era muy importante en el mecanismo de CH_4 y se optó por encontrar un valor alternativo que mejorase las simulaciones de CH_4. Sin embargo, debido a que hay muchísima disparidad entre los diferentes valores cinéticos dados en la bibliografía, se optó por modificar los valores cinéticos que utilizaba el mecanismo de Gersen et al. [9]. La modificación se realizó sobre el factor preexponencial (A), el cual, después de varias iteraciones, se llegó a la conclusión de que lo más óptimo era dividirlo por 100. La modificación de esta reacción dará lugar al denominado como mecanismo modificado 5.

En la tabla 4.3.3 se muestran los valores cinéticos de la reacción original y en negrita los de la reacción modificada.

Tabla 4.3.3 Parámetros cinéticos de las reacciones modificadas en el mecanismo modificado 5. Unidades: mol, cm, s, cal, K.

Reacción	**A**	**β**	**Ea**
$CH_3+CH_3(+M)=C_2H_6(+M)$	9.5E14	-0.538	179
Límite de baja presión:	1.269E41	-7.0	2762

Parámetros de TROE: 0.62 73 1180 1E30			
$CH_3+CH_3(+M)=C_2H_6(+M)$ **Límite de baja presión:** **Parámetros de TROE:** **0.62 73 1180 1E30**	**9.5E14** **1.269E39**	**-0.538** **-7.0**	**179** **2762**

Los resultados de las simulaciones del proceso de combustión de la mezcla CH_4/H_2S se pueden observar en las figuras 4.3.28 a 4.3.33. La simulación con el mecanismo inicial aparece en líneas discontinuas, mientras que con el mecanismo modificado en líneas continuas. Los datos experimentales se muestran con puntos.

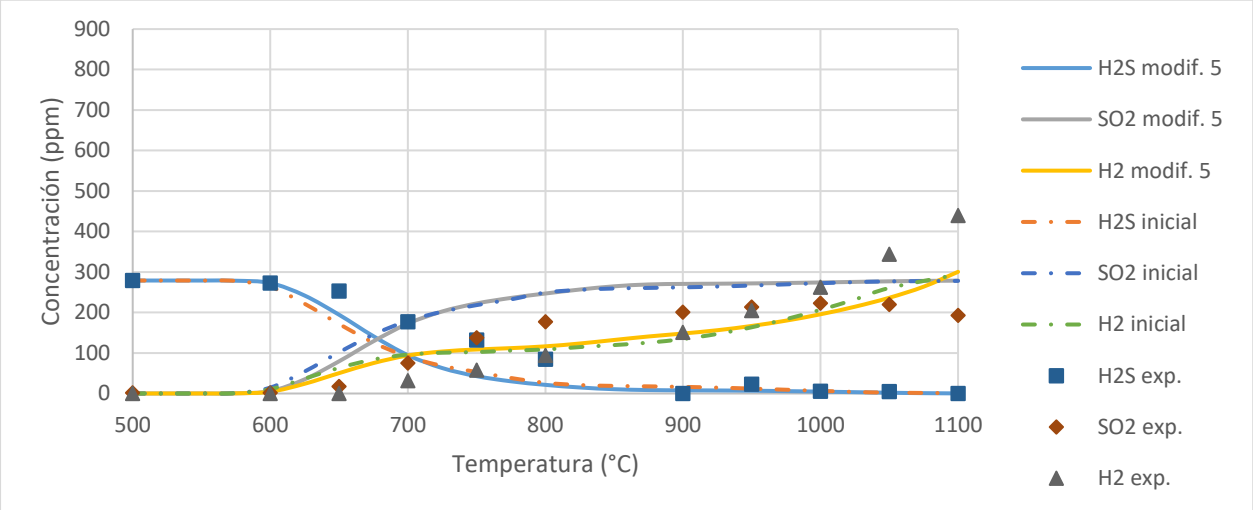


Figura 4.3.28 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 5 en el experimento H_2S/CH_4 en condiciones reductoras.

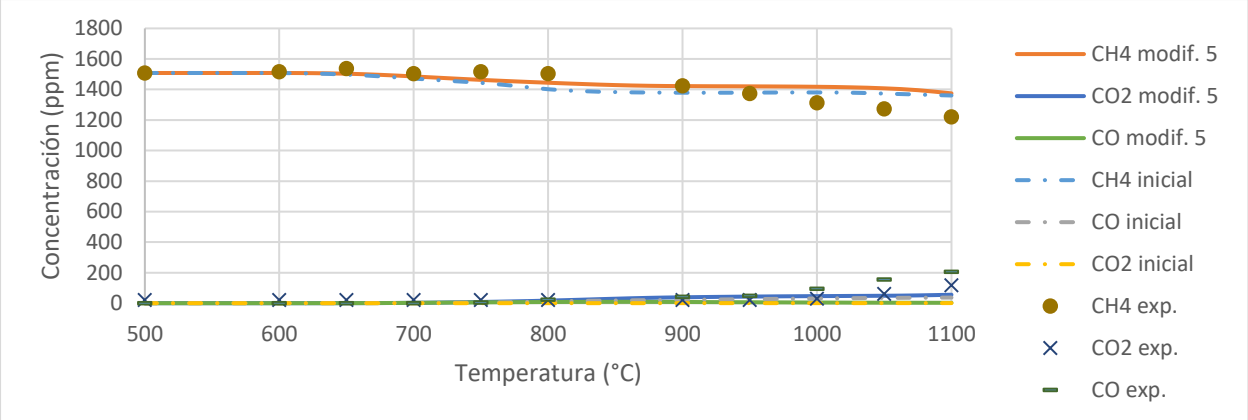


Figura 4.3.29 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 5 en el experimento H_2S/CH_4 en condiciones reductoras.

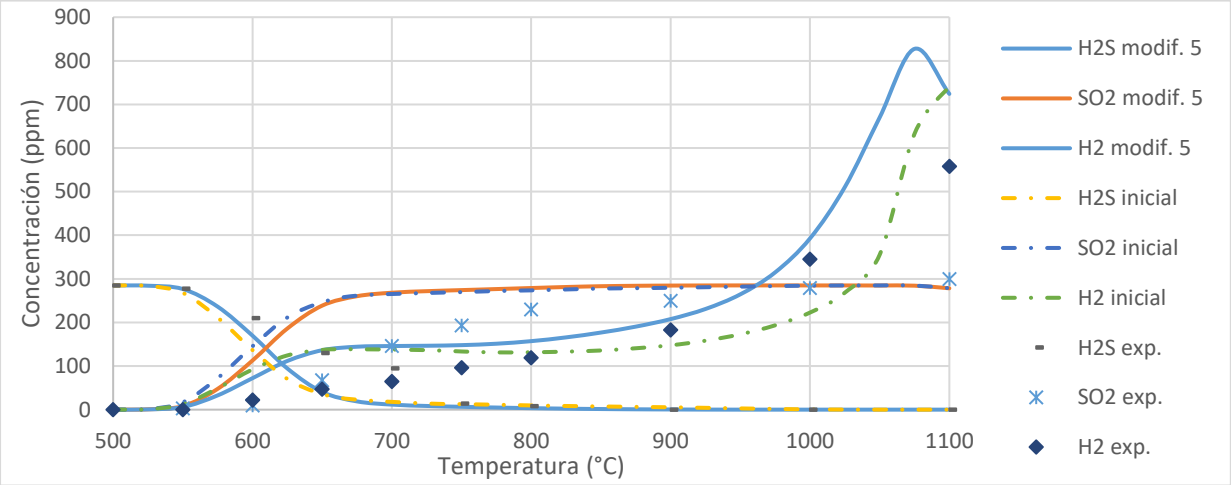


Figura 4.3.30 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 5 en el experimento H_2S/CH_4 en condiciones estequiométricas.

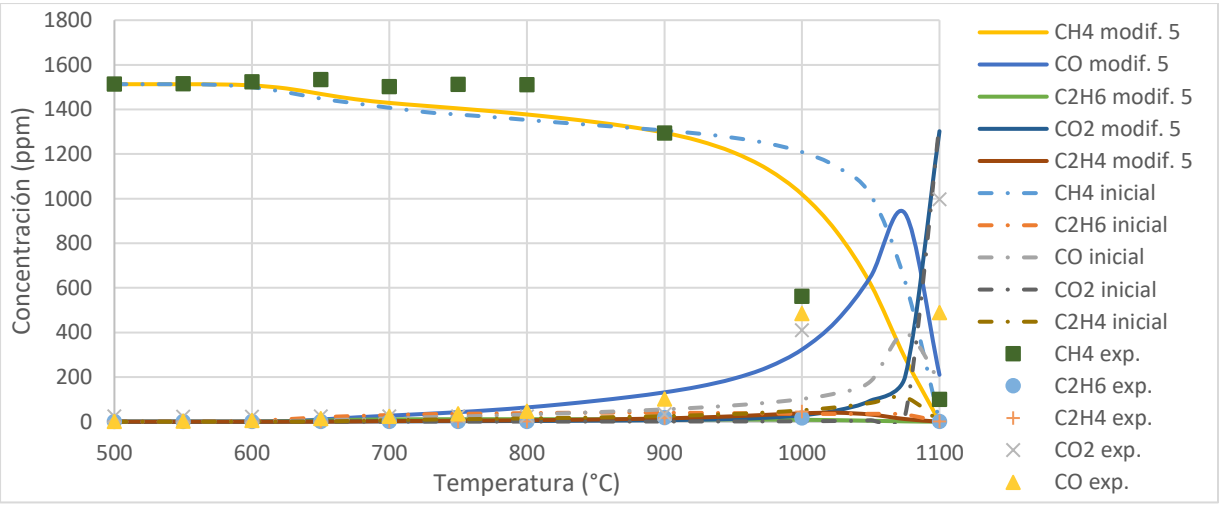


Figura 4.3.31 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 5 en el experimento H_2S/CH_4 en condiciones estequiométricas.

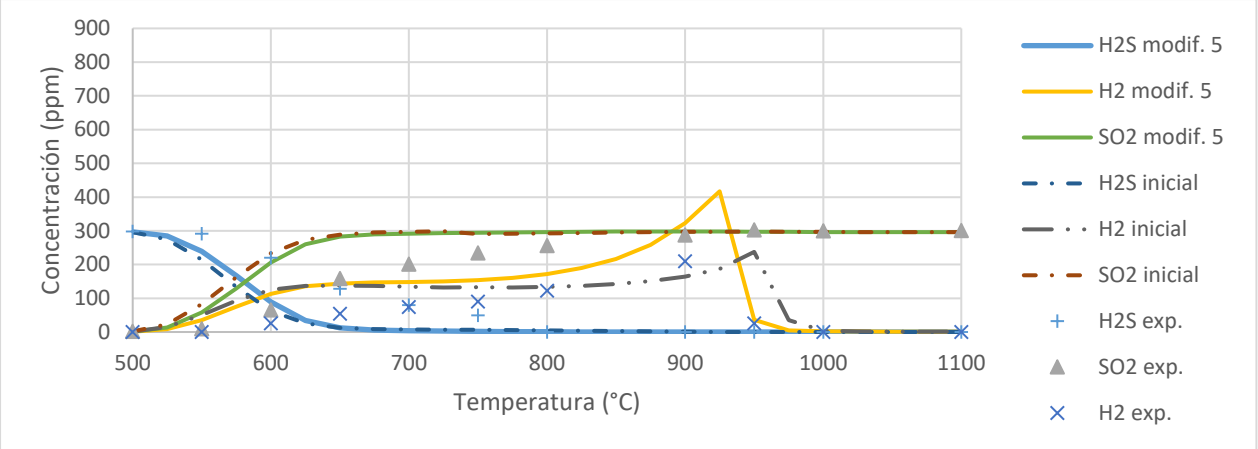


Figura 4.3.32 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 5 en el experimento H_2S/CH_4 en condiciones oxidantes.

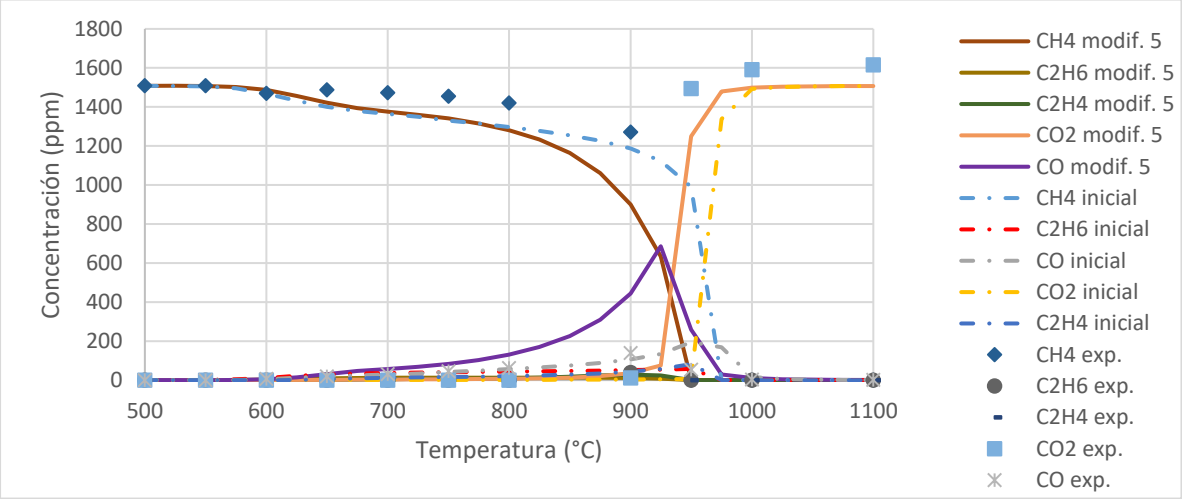


Figura 4.3.33 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 5 en el experimento H_2S/CH_4 en condiciones oxidantes.

Los resultados son positivos en el CH_4 en condiciones estequiométricas ya que se empieza a consumir a temperaturas menores y desaparece a los 1100 ℃, que es un comportamiento más cercano al de los resultados experimentales. El H_2 se observa que mejora bastante a temperaturas intermedias en condiciones estequiométricas.

El CO sufre una gran mejora en condiciones estequiométricas ya que, en el mecanismo inicial, se empieza a formar a temperaturas muy elevadas. Sin embargo, en los resultados experimentales se observa que a 1000 ℃ hay una gran concentración de CO, por lo que el mecanismo modificado 5 estaría más cerca de los resultados experimentales.

En condiciones oxidantes se observa que el metano se consume antes de lo esperado, aunque el CO_2 se forma antes obedeciendo a los resultados experimentales. El CO sin embargo se ve empeorado ya que se forma antes de lo esperado.

En condiciones reductoras se ve que el H_2 a temperaturas elevadas ya no resulta empeorado como pasaba en el mecanismo modificado 4.

Para conocer si esta modificación es correcta o no, se realizaron simulaciones de los experimentos de la combustión de CH_4, cuyos resultados experimentales se muestran en el Anexo A, concretamente en las tablas A.4 a A.6.

Los resultados de las simulaciones se pueden observar en las figuras 4.3.34 a 4.3.36. La simulación con el mecanismo inicial aparece en líneas discontinuas y los resultados del mecanismo modificado en líneas continuas. Los datos experimentales se muestran con puntos.

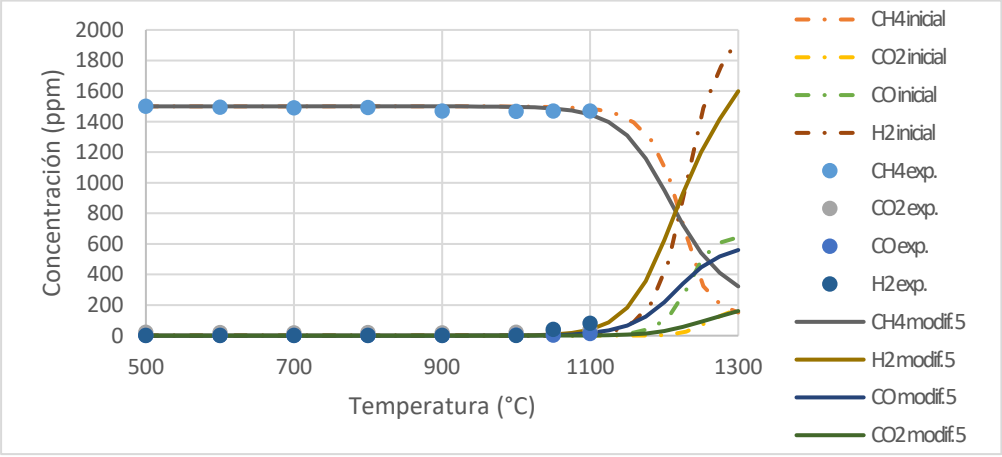


Figura 4.3.34 Comparativa entre el mecanismo original y el modificado 5 para el experimento de combustión de CH_4 en condiciones reductoras.

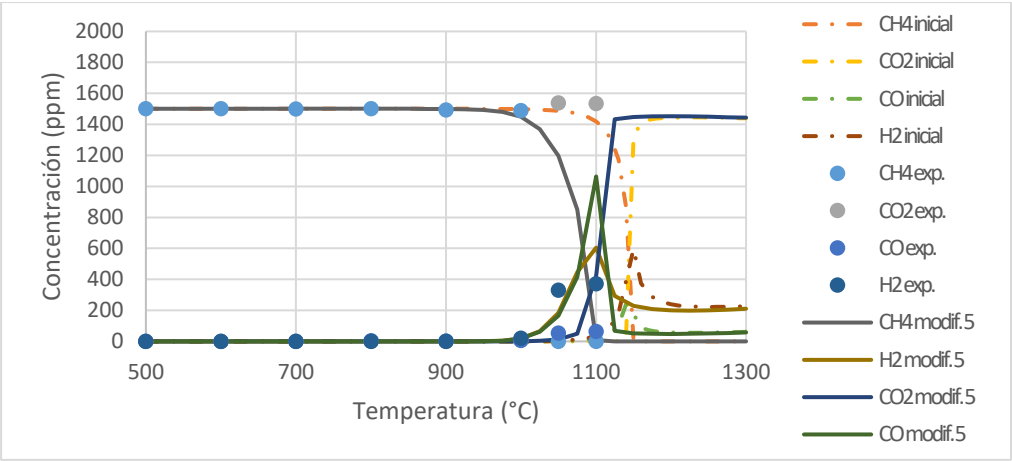
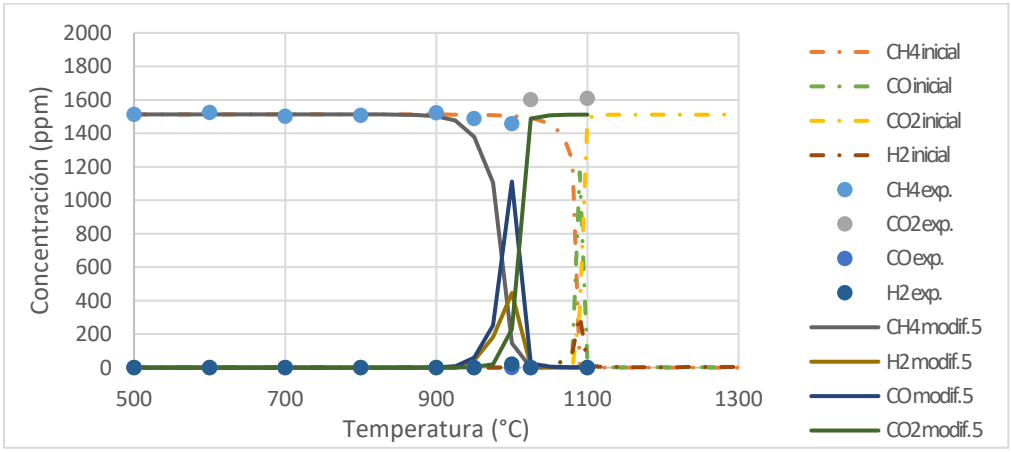


Figura 4.3.35 Comparativa entre el mecanismo original y el modificado 5 para el experimento de combustión de CH_4 en condiciones estequiométricas.



.

Figura 4.3.36 Comparativa entre el mecanismo original y el modificado 5 para el experimento de combustión de CH_4 en condiciones oxidantes.

En el caso de las simulaciones de solo CH_4 vemos una gran mejoría en las 3 condiciones ya que el proceso de combustión aparece a temperaturas menores, coincidiendo con los resultados experimentales. Como conclusión, se aceptará el cambio como válido ya que mejora el mecanismo de combustión de CH_4.

A continuación, se procedió a mejorar los mecanismos de combustión de H_2S y de la mezcla H_2S/CH_4, para ello se agregaron un gran número de reacciones de compuestos de azufre y de interacción entre compuestos de carbono y azufre. Estas se muestran en el Anexo C.3, en las tablas C.3.3, C.3.4 y C.3.6. Estos cambios conforman el mecanismo modificado 6.

Los resultados de las simulaciones se pueden observar en las figuras 4.3.37 a 4.3.42 la simulación con el mecanismo inicial aparece en líneas discontinuas y los resultados del mecanismo modificado en líneas continuas. Los datos experimentales se muestran con símbolos.

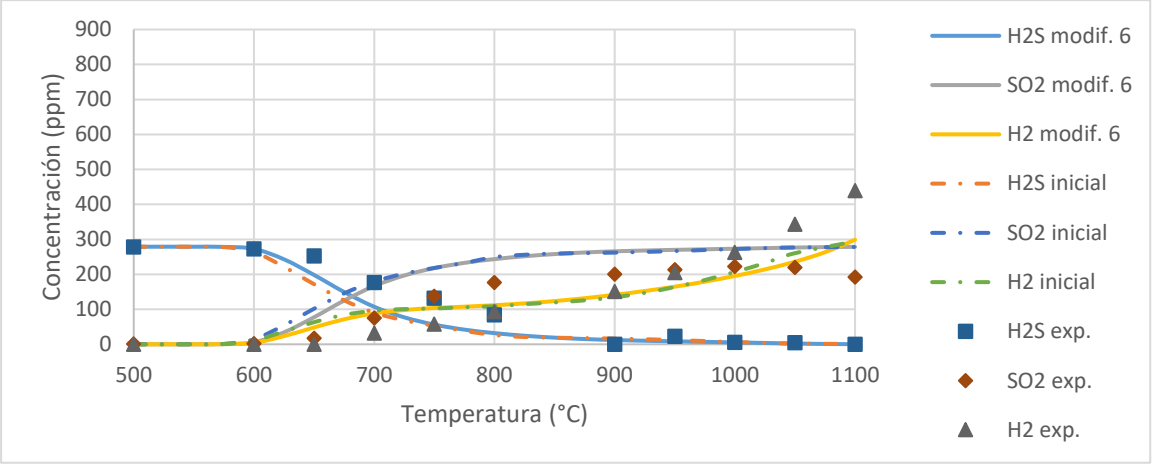


Figura 4.3.37 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 6 en el experimento H_2S/CH_4 en condiciones reductoras

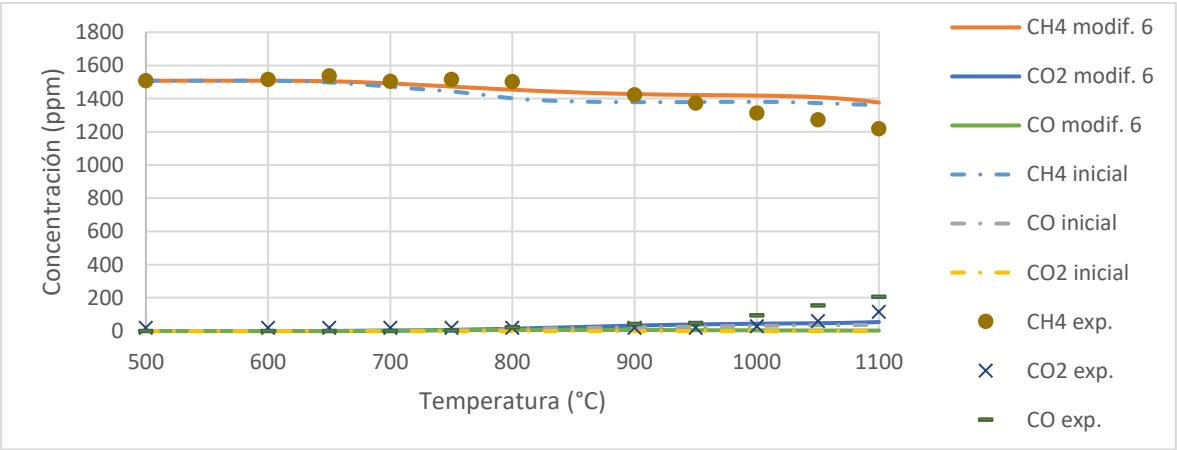


Figura 4.3.38 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 6 en el experimento H_2S/CH_4 en condiciones reductoras

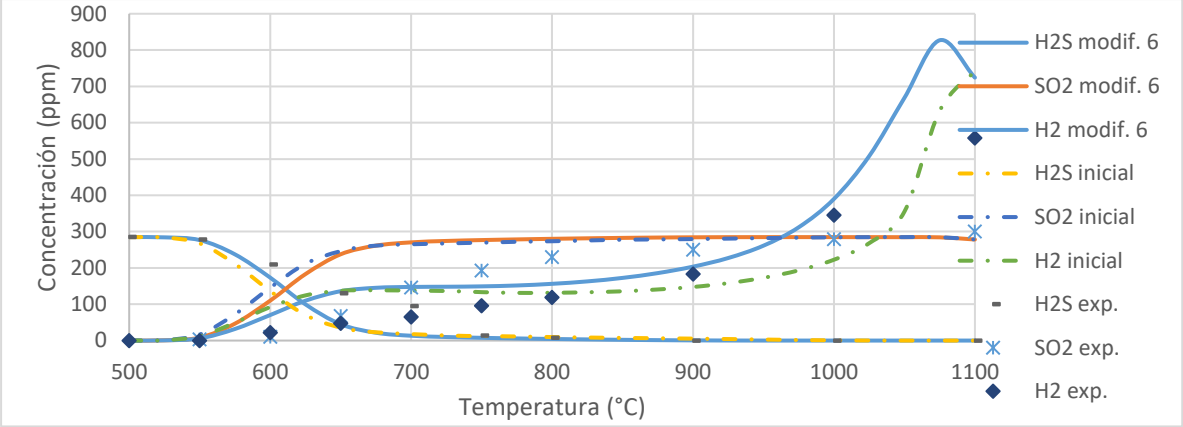


Figura 4.3.39 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 6 en el experimento H_2S/CH_4 en condiciones estequiométricas.

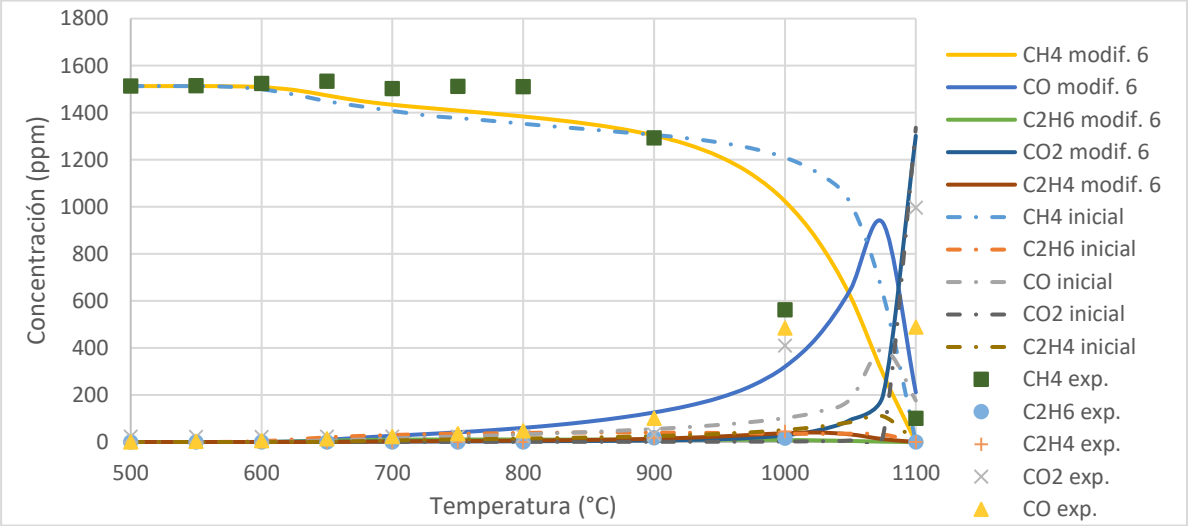


Figura 4.3.40 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 6 en el experimento H_2S/CH_4 en condiciones estequiométricas.

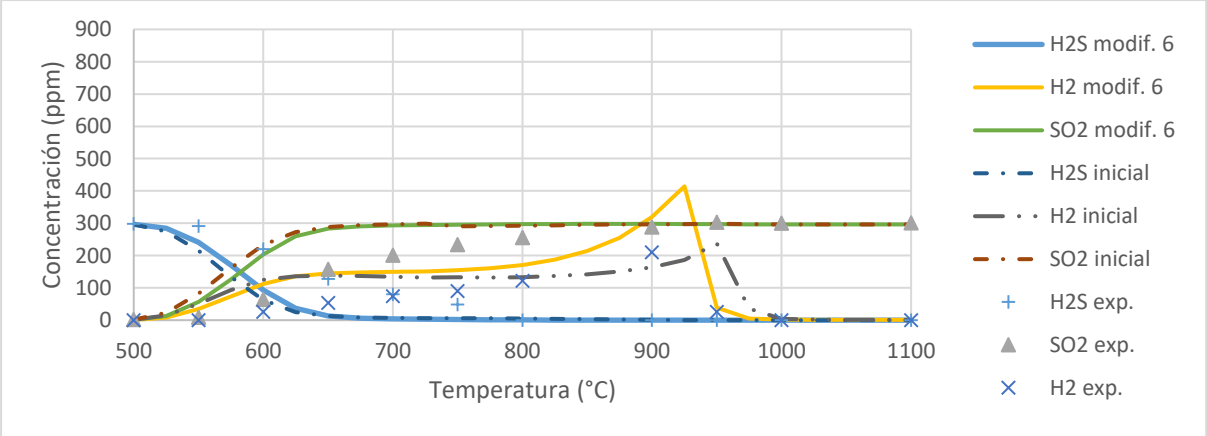


Figura 4.3.41 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 6 en el experimento H_2S/CH_4 en condiciones oxidantes.

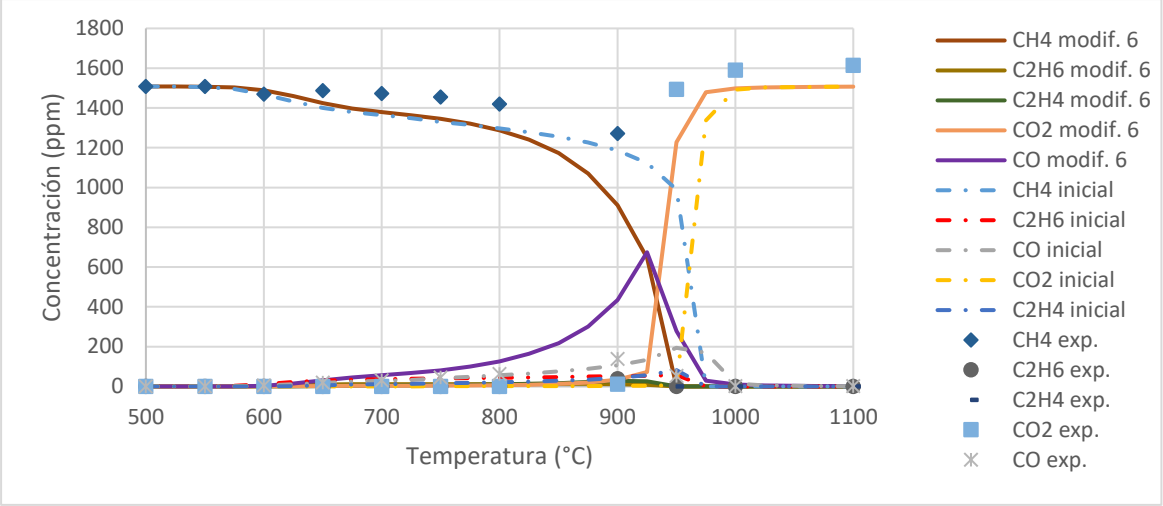


Figura 4.3.42 Resultados de la comparativa entre el mecanismo inicial y el mecanismo modificado 5 en el experimento H_2S/CH_4 en condiciones oxidantes.

Los resultados de las simulaciones son prácticamente idénticos a los del mecanismo modificado 5, por lo que se obtiene como conclusión que ninguna de las reacciones agregadas en el mecanismo modificado 6 es importante dentro del proceso de combustión de la mezcla H_2S/CH_4.

Finalmente, se hicieron análisis de sensibilidad al H_2S y SO_2 a las diferentes condiciones y a una conversión del 10 % de H_2S con el fin de mejorar sus simulaciones. Se descubrió que eran muy sensibles a las reacciones $CH_3+H_2S=CH_4+SH$ y $CH_3+SH=CH_3SH$. Al ser reacciones de interacción entre carbono y azufre, modificar este par de reacciones no va a implicar ningún cambio en los resultados de las simulaciones de los experimentos del proceso de combustión de únicamente CH_4 o de únicamente H_2S. En el mecanismo de Gersen et al. [9] se obtuvieron valores cinéticos más recientes.

Los valores actualizados vienen en la tabla 4.3.4 y formarán el mecanismo modificado 7.

Tabla 4.3.4 Parámetros cinéticos de las reacciones modificadas en el mecanismo modificado 7. Unidades: mol, cm, s, cal, K.

Reacción	A	β	Ea
$CH_3+H_2S=CH_4+SH$	6.8E7	1.2	1434
$CH_3+SH=CH_3SH$	7.3E12	0.230	-139

Los resultados de las simulaciones se pueden observar en las figuras 4.3.43 a 4.3.48. La simulación con el mecanismo inicial aparece en líneas discontinuas y los resultados del mecanismo modificado 7 en líneas continuas. Los datos experimentales se muestran con símbolos.

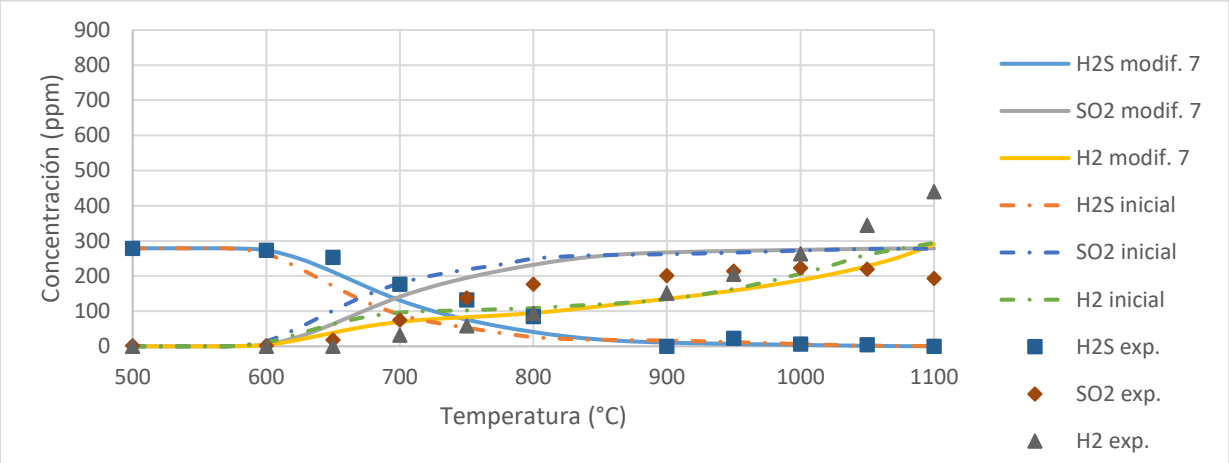


Figura 4.3.43 Comparativa entre el mecanismo original y el modificado 7 para el experimento de combustión de H_2S/CH_4 en condiciones reductoras.

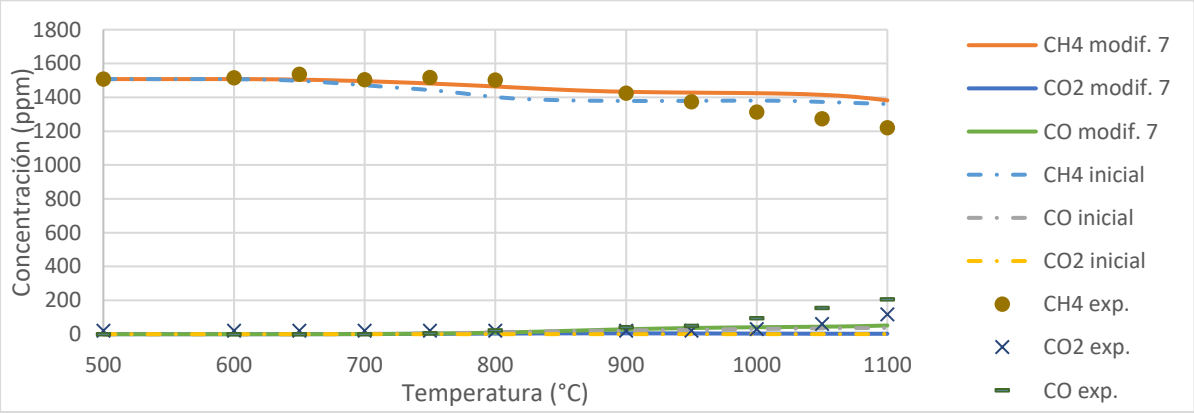


Figura 4.3.44 Comparativa entre el mecanismo original y el modificado 7 para el experimento de combustión de H_2S/CH_4 en condiciones reductoras.

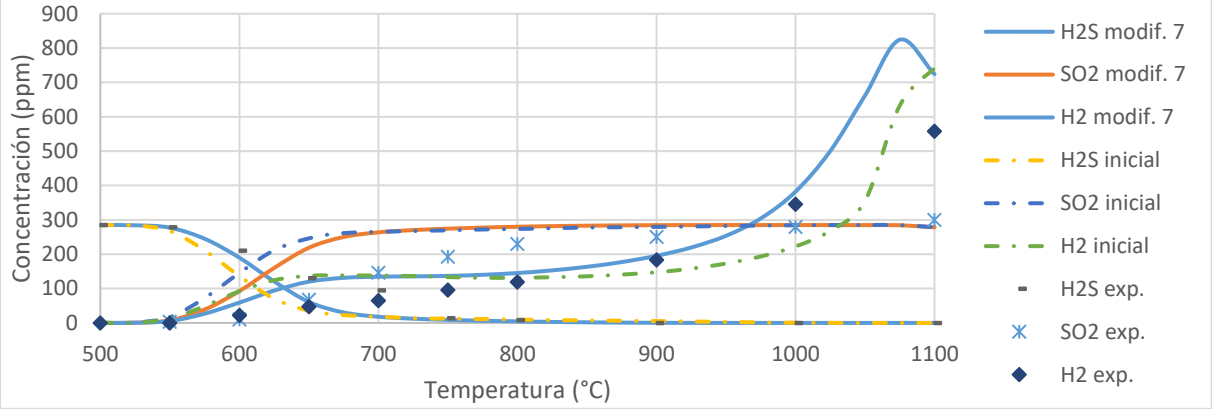


Figura 4.3.45 Comparativa entre el mecanismo original y el modificado 7 para el experimento de combustión de H_2S/CH_4 en condiciones estequométricas.

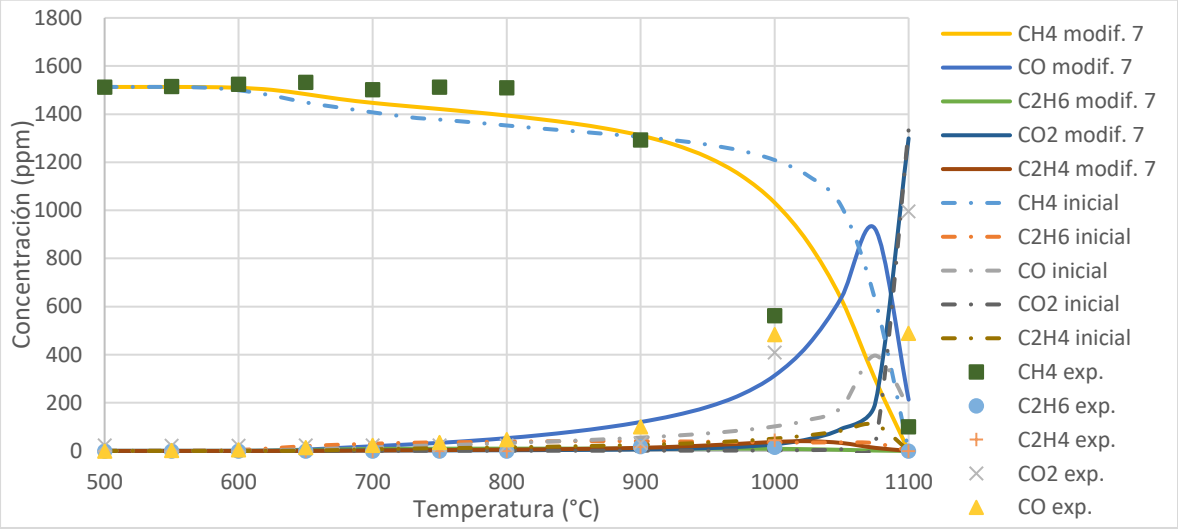


Figura 4.3.46 Comparativa entre el mecanismo original y el modificado 7 para el experimento de combustión de H_2S/CH_4 en condiciones estequiométricas.

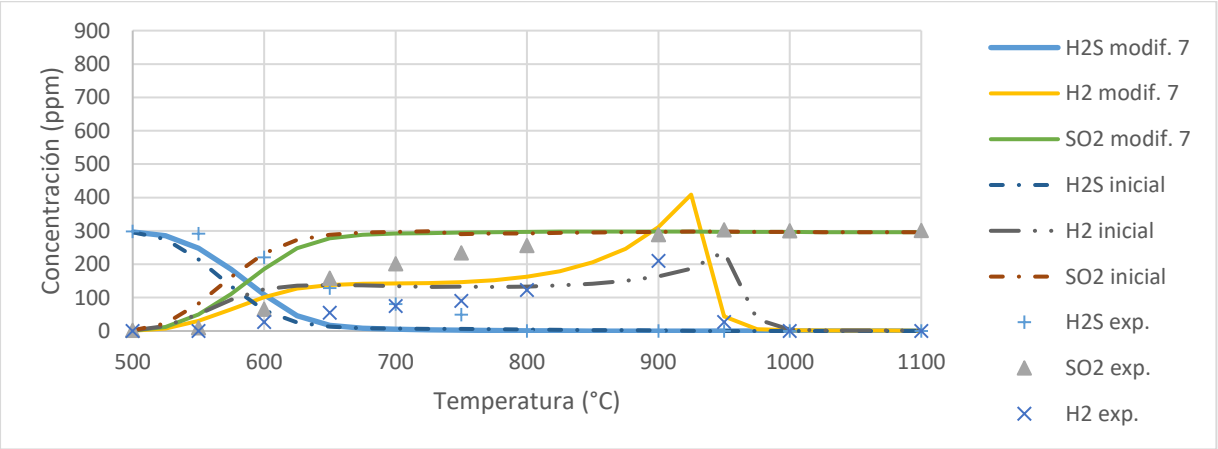


Figura 4.3.47 Comparativa entre el mecanismo original y el modificado 7 para el experimento de combustión de H_2S/CH_4 en condiciones oxidantes.

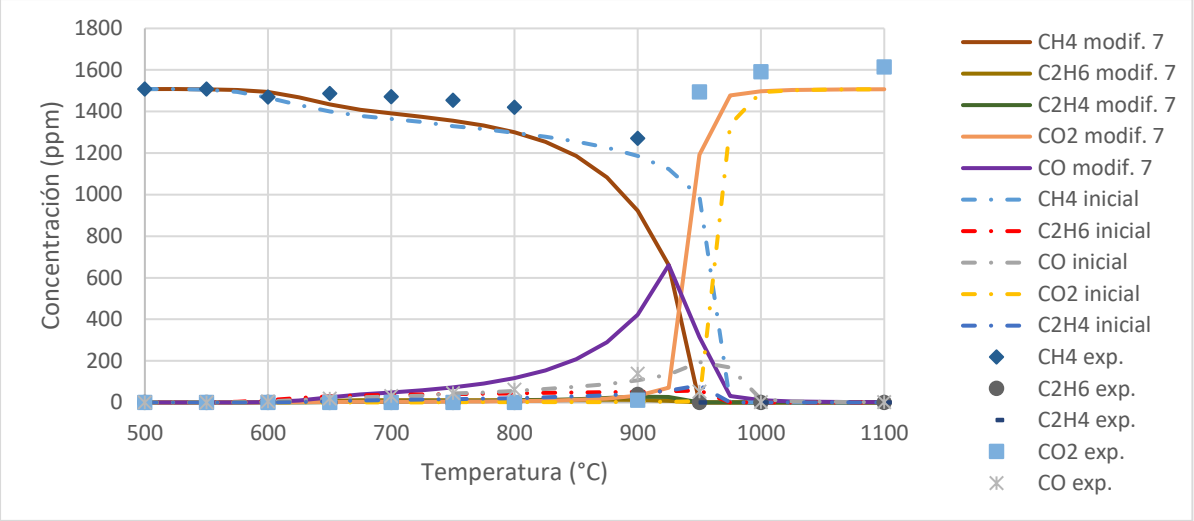


Figura 4.3.48 Comparativa entre el mecanismo original y el modificado 7 para el experimento de combustión de H_2S/CH_4 en condiciones oxidantes.

En los resultados de las simulaciones, se observa que el H_2S se empieza a consumir y el SO_2 a formar a temperaturas mayores y el SO_2 se forma a temperaturas mayores en todas las condiciones, por lo que las modificaciones en el mecanismo acercan las simulaciones a los resultados experimentales.

Como las simulaciones aún no se acercaban lo suficiente a los resultados experimentales y se observó que las modificaciones al mecanismo 7 eran positivas para ambos compuestos, se comprobó qué efecto tenía solo modificar la reacción $CH3+H_2S=CH_4+SH$ y, posteriormente, se revirtió la modificación anterior y se modificó únicamente $CH_3+SH=CH_3SH$. Se vio que la mejor opción era modificar únicamente $CH_3+SH=CH_3SH$. Por tanto, partiendo del mecanismo modificado 7, se revirtieron los valores cinéticos modificados a los del mecanismo inicial de la reacción $CH_3+H_2S=CH_4+SH$ y se mantuvo la reacción $CH_3+SH=CH_3SH$ con sus valores cinéticos modificados. Este cambio dará lugar al mecanismo final del presente trabajo.

A continuación, se presentan los resultados de las simulaciones en las figuras 4.3.43 a 4.3.48. La simulación con el mecanismo inicial aparece en líneas discontinuas y los resultados

del mecanismo modificado final en líneas continuas. Los datos experimentales se muestran con símbolos.

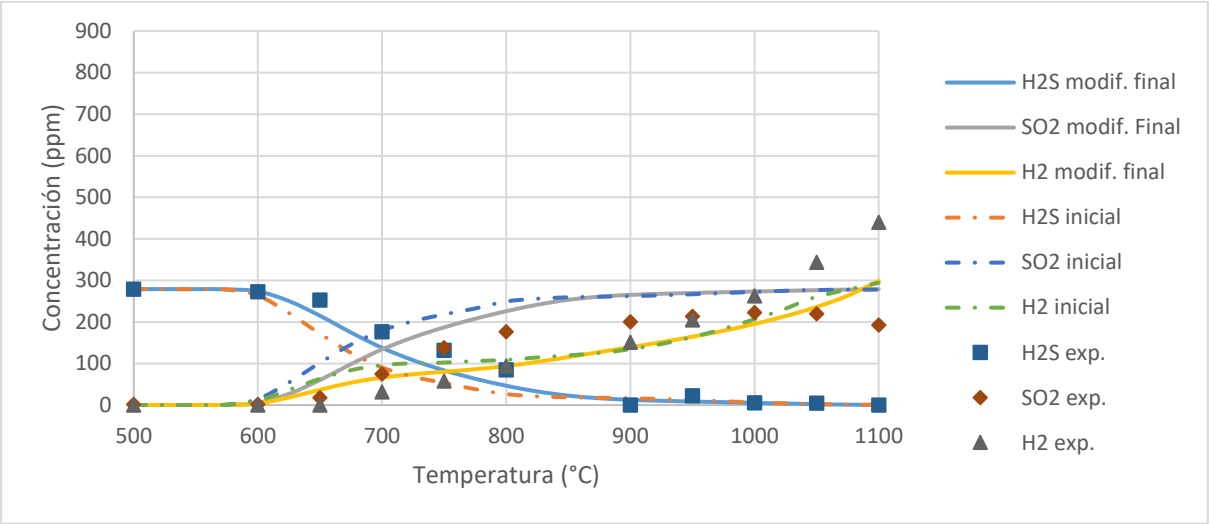


Figura 4.3.49 Comparativa entre el mecanismo original y el mecanismo final del presente trabajo para el experimento de combustión de H_2S/CH_4 en condiciones reductoras.

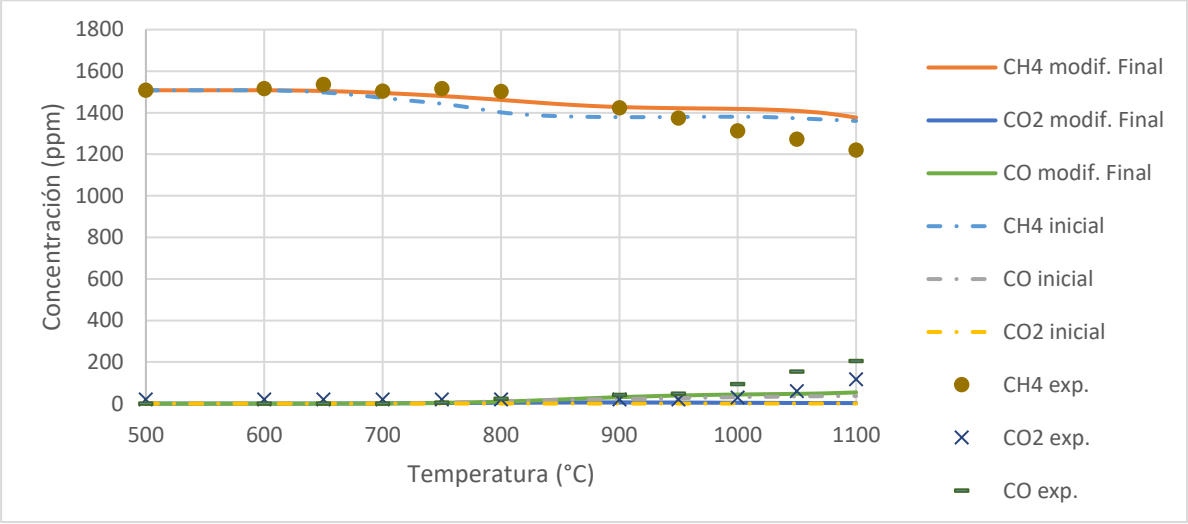


Figura 4.3.50 Comparativa entre el mecanismo original y el mecanismo final del presente trabajo para el experimento de combustión de H_2S/CH_4 en condiciones reductoras.

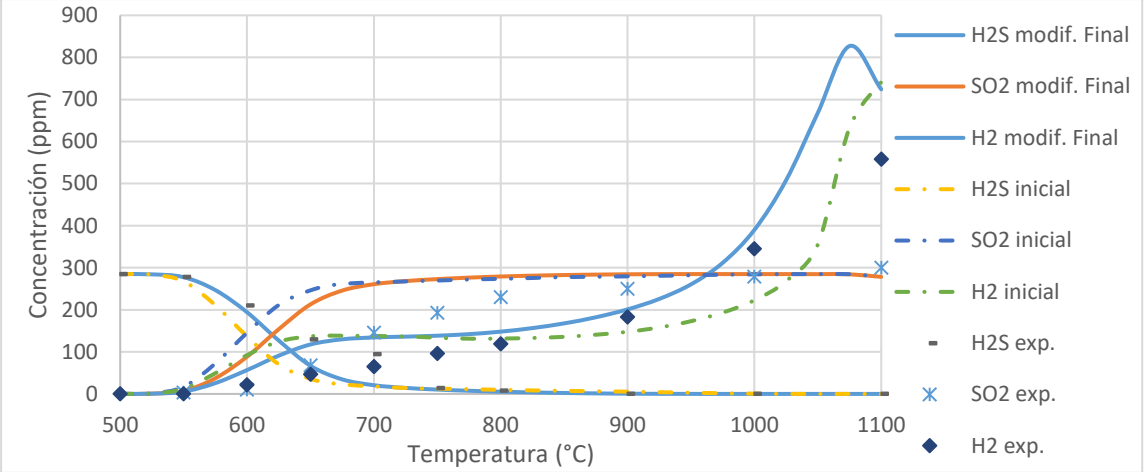


Figura 4.3.51 Comparativa entre el mecanismo original y el mecanismo final del presente trabajo para el experimento de combustión de H_2S/CH_4 en condiciones estequiométricas.

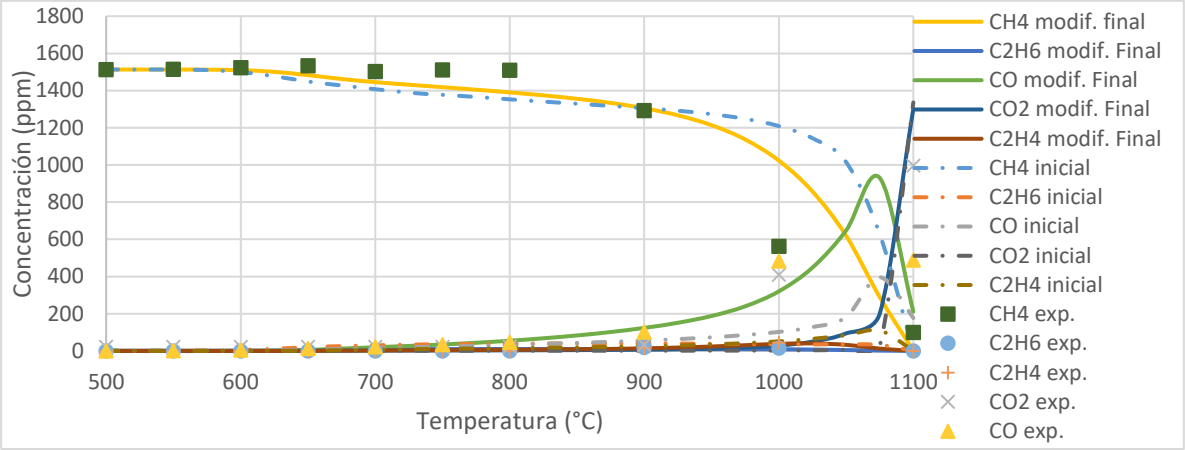


Figura 4.3.52 Comparativa entre el mecanismo original y el mecanismo final del presente trabajo para el experimento de combustión de H_2S/CH_4 en condiciones estequiométricas.

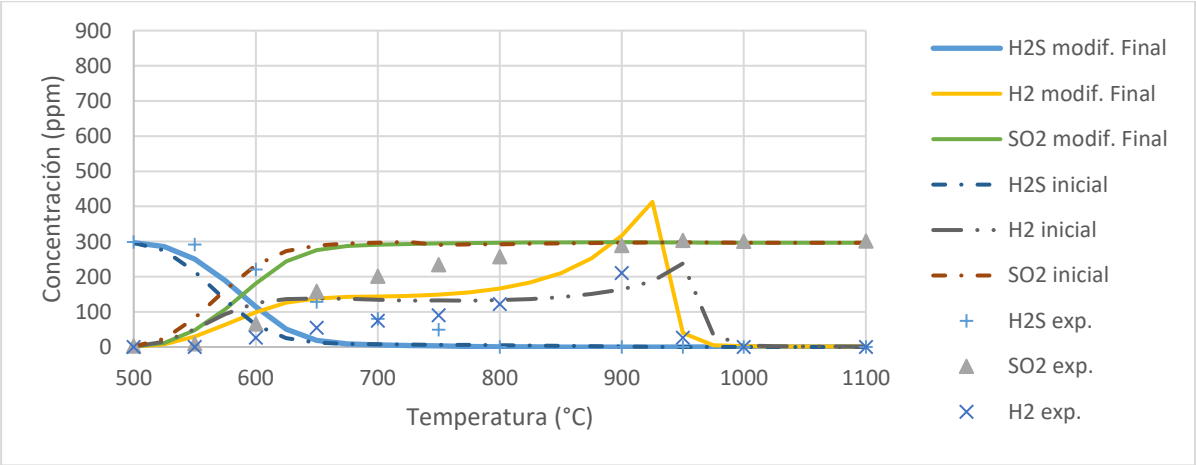


Figura 4.3.53 Comparativa entre el mecanismo original y el mecanismo final del presente trabajo para el experimento de combustión de H_2S/CH_4 en condiciones oxidantes.

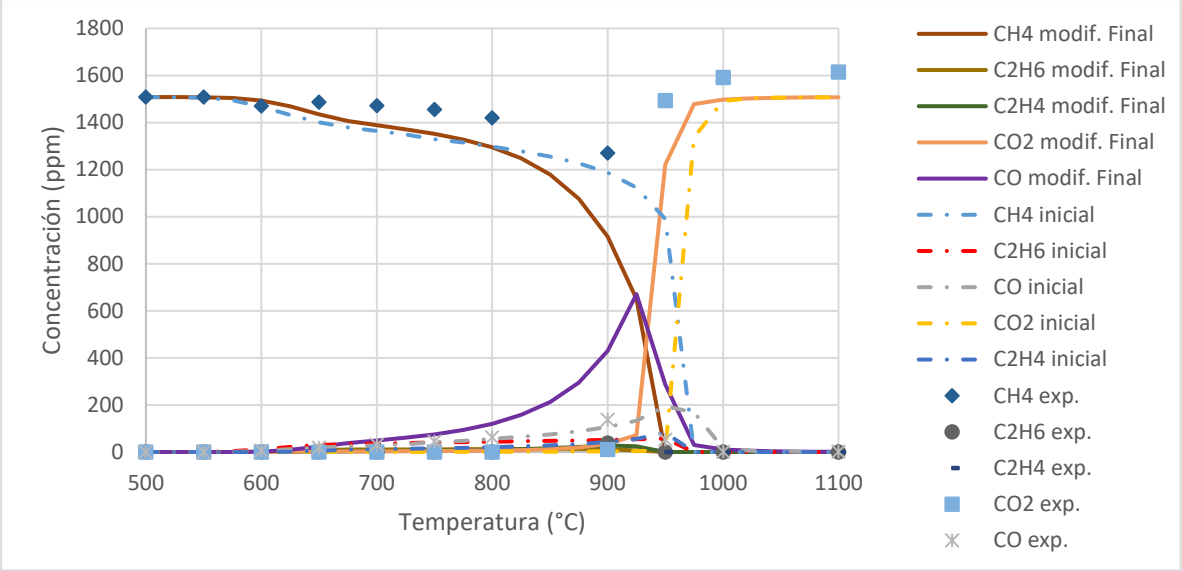


Figura 4.3.54 Comparativa entre el mecanismo original y el mecanismo final del presente trabajo para el experimento de combustión de H_2S/CH_4 en condiciones oxidantes.

Como se observa en los resultados de las simulaciones, las predicciones de H_2S y SO_2 son ligeramente mejores que en el mecanismo modificado 7, ya que se consume el H_2S y se forma el SO_2 a temperaturas mayores.

Como parte final, se realizaron análisis de los caminos preferenciales de reacción para el mecanismo final del presente trabajo, que está detallado en el Anexo C.5, y en el que se indican las reacciones más críticas para el resultado final. Como el mecanismo se ha desarrollado para simular procesos de combustión de la mezcla CH_4/H_2S, se han realizado estos análisis a un 10 % de conversión del reactivo CH_4, y, posteriormente, del H_2S. Estos análisis se realizan para los casos de $\lambda = 2$, $\lambda = 1$, $\lambda = 0.25$. Los resultados de estos análisis se muestran en las figuras 4.3.55 y 4.3.56.

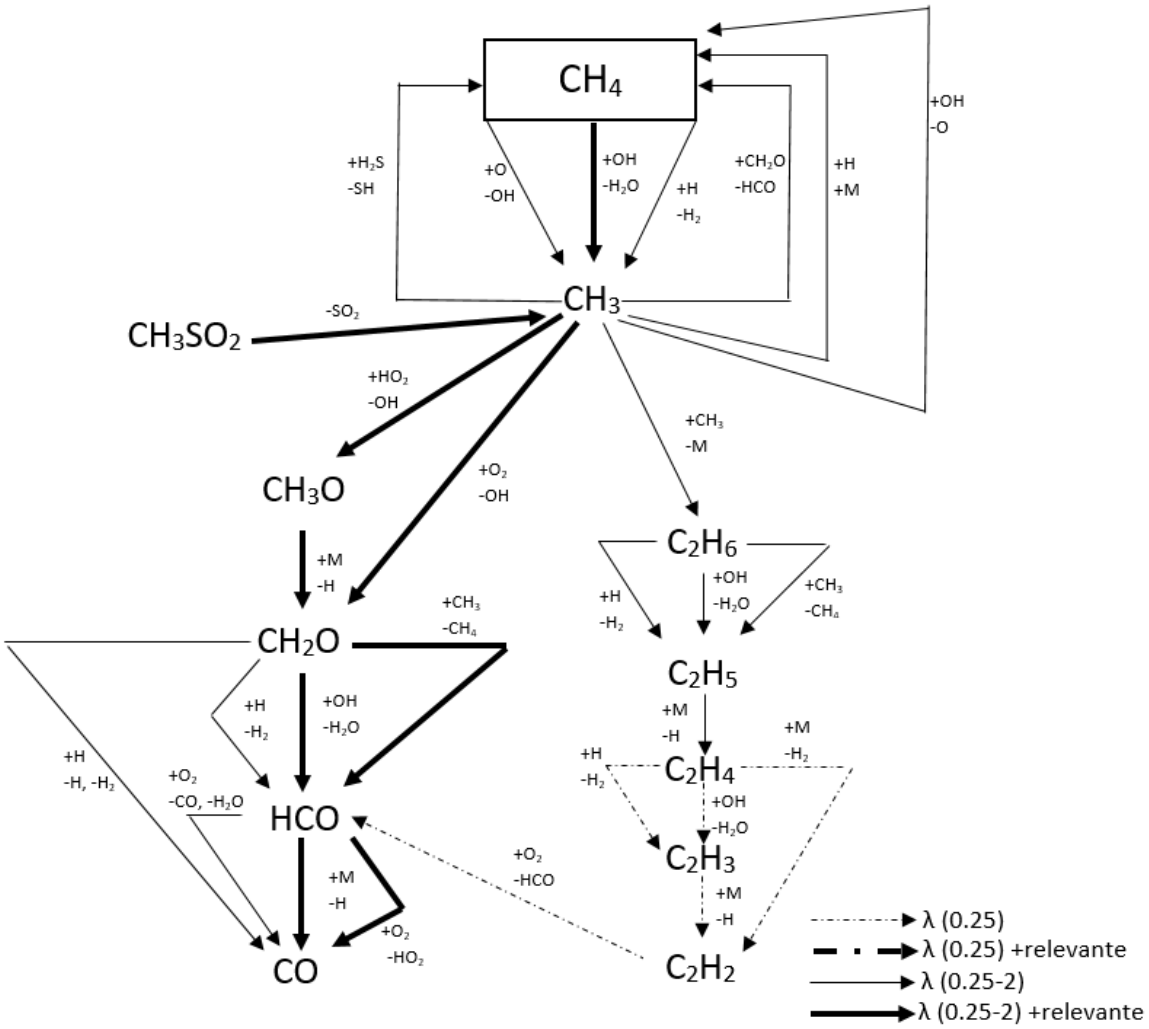


Figura 4.3.55 Caminos de reacción para la oxidación de CH_4 bajo las condiciones estudiadas

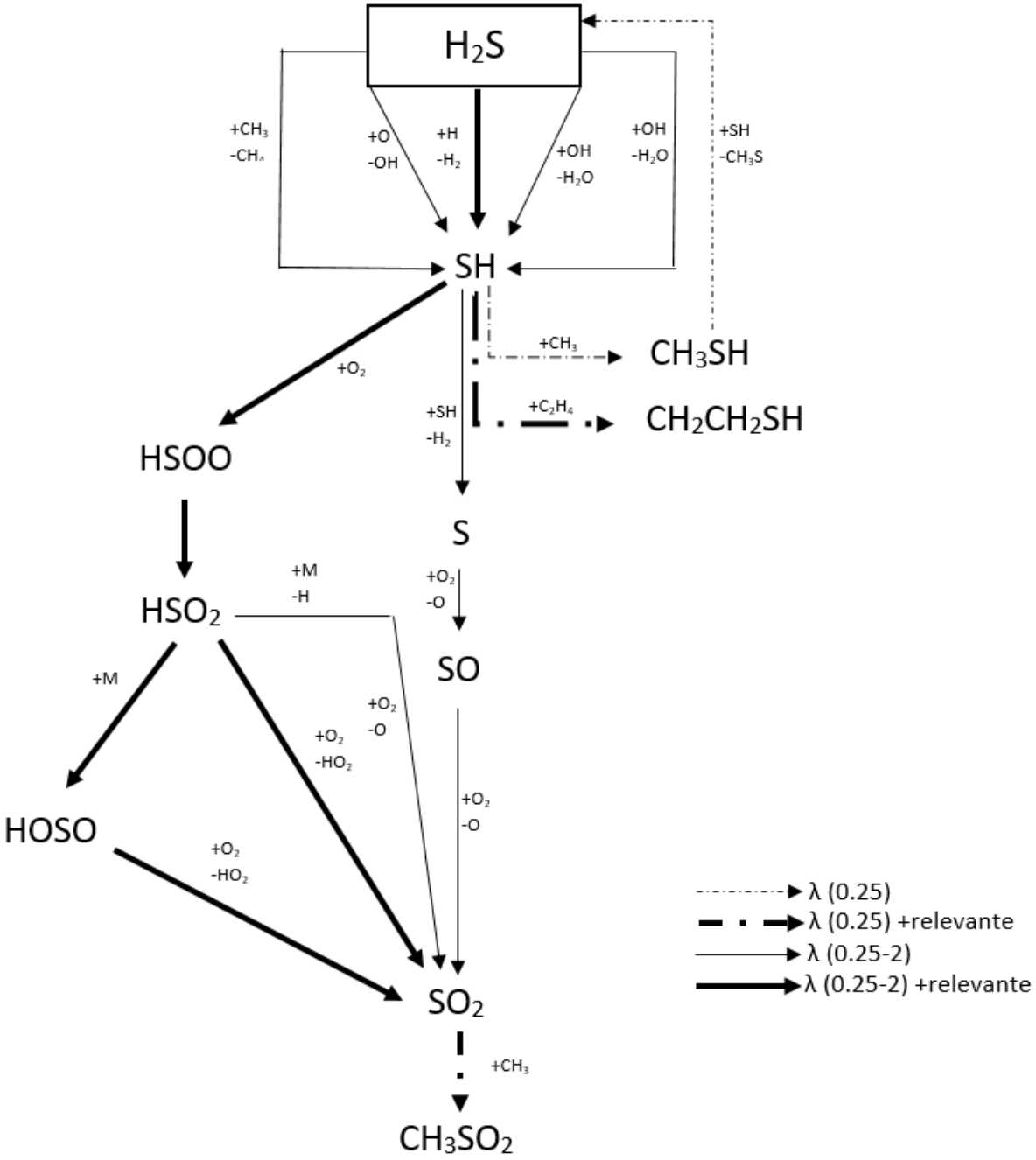


Figura 4.3.56 Caminos de reacción para la oxidación de H_2S bajo las condiciones estudiadas

En cuanto a los resultados de CH_4, se observa en la figura 4.3.55 que el CH_4 reacciona principalmente con el radical OH para formar CH_3 y H_2O, posteriormente el CH_3 reacciona con HO_2 para formar CH_3O y con OH para formar CH_2O. El CH_3O formado se descompondrá en CH_2O y H. El CH_2O formado anteriormente puede reaccionar con radicales OH para formar

HCO y H_2O o con CH_3 para formar HCO y CH_4. Finalmente, este HCO reaccionará con O_2 para formar CO y HO_2 o se descompondrá en H y CO.

En la figura 4.3.56 se observan los caminos de reacción del H_2S. El H_2S reacciona principalmente con H y forma el compuesto SH y H_2. Se observa que el SH puede reaccionar con C_2H_4 para formar CH_2CH_2SH en condiciones reductoras, o formar HSOO en todas las condiciones, por lo que, en condiciones reductoras el SH tendría dos caminos principales de reacción. El HSOO isomeriza formando HSO_2. El HSO_2 se observa que tiene dos caminos de reacción, el primero de estos sería formando HOSO y el segundo reaccionando con O_2 para formar SO_2 y HO_2. El HOSO se observa que también reacciona con O_2 y forma SO_2 y HO_2. Finalmente, en condiciones reductoras aparece un camino de reacción importante en el SO_2, este reacciona con CH_3 y finaliza formando CH_3SO_2.

4.4 Resultados y discusión

A continuación, se muestran los resultados experimentales en las 3 relaciones estequiométricas, así como la comparación entre el mecanismo final del presente trabajo con el mecanismo de partida, de tal manera que se pueda conocer cómo ha mejorado el mecanismo gracias a las reacciones añadidas y a la actualización de los valores cinéticos de reacciones que se utilizaban anteriormente. Los resultados de las simulaciones del mecanismo final se han mostrado anteriormente en las figuras 4.3.49 a 4.3.54.

En condiciones reductoras el mecanismo final da unos resultados mucho más cercanos en general a los resultados experimentales, en comparación con el mecanismo inicial. Se observa cómo en las simulaciones con el mecanismo final del presente trabajo, el H_2S se empieza a consumir más tarde y lo hace más lentamente, igual que el SO_2 se produce a temperaturas mayores y también lo hace más lentamente. Estos resultados se ajustan mucho mejor a los resultados experimentales que el mecanismo inicial. En el caso del H_2, vemos cómo a temperaturas bajas los resultados del mecanismo final se ajustan mucho más que los del

mecanismo inicial, aunque a temperaturas altas ambos son similares. Respecto al CH_4, CO y CO_2 simulados en con el mecanismo final, no se ha conseguido ninguna mejora apreciable en estas condiciones.

En cuanto a las condiciones estequiométricas se observa una ligera mejora en el H_2S ya que se empieza a consumir a temperaturas elevadas y del SO_2 ya que se forma a temperaturas más elevadas si lo comparamos con los resultados del mecanismo inicial. En el caso del H_2 se observa una ligera mejora a temperaturas bajas y medias respecto al mecanismo inicial.

El CH_4 se mejora en las simulaciones del mecanismo final ya que se acerca más a los resultados experimentales en el rango de 500-900 ℃ y se termina de consumir a los 1100 ℃, mientras que en el mecanismo inicial éste se empieza a consumir a temperaturas más altas. El CO se ve mejorado en el mecanismo final ya que se empieza a formar a temperaturas menores acercándose al resultado experimental de 1000 ℃.

Si se observan los resultados obtenidos en condiciones oxidantes, se puede observar una mejora del H_2S y SO_2 respecto al mecanismo inicial, ya que el H_2S se consume a temperaturas más elevadas y el SO_2 se forma a temperaturas más elevadas en el mecanismo final del presente trabajo.

En cuanto al H_2, se observa un empeoramiento respecto al simulado con el mecanismo inicial ya que se forma una gran concentración de H_2 a temperaturas intermedias, sin embargo, ésta se consume antes que la del mecanismo inicial a la misma temperatura que a la de los datos experimentales. En el caso del CH_4, se observa en el mecanismo final del presente trabajo que éste se consume a temperaturas menores que los datos experimentales, consumiéndose totalmente a 950 ℃, coincidiendo con los experimentos. Mientras que, en el mecanismo inicial se consume a temperaturas mayores, aunque este se acerca más al resultado experimental de 900 ℃. El CO_2 se ha mejorado en el mecanismo final debido a que el CH_4 se consume antes en el mecanismo inicial, por lo que el CO_2 simulado con el mecanismo final se acerca mucho más a los datos experimentales que el CO_2 simulado con mecanismo inicial. El CO, sin

embargo, se empeora en el mecanismo final con respecto al inicial debido a que se forma una gran concentración de CO.

5 Conclusiones

En el presente Trabajo de final de grado se ha desarrollado un mecanismo cinético de reacción para el proceso de combustión de CH_4 con H_2S a presión atmosférica, en diferentes atmósferas (reductora, estequiométrica y oxidante) y en un intervalo de temperaturas de 500 a 1100 ℃.

Se ha utilizado como punto de partida el mecanismo para la oxidación de H_2S de Colom-Díaz et al. [5], además de los resultados experimentales obtenidos previamente por Peláez [10], al inicio del TFG para diferentes estequiometrías y temperaturas.

El mecanismo desarrollado se puede considerar válido para presión atmosférica, para el intervalo de temperaturas entre 500-1100 ℃ y en las diferentes concentraciones de oxígeno (atmósfera oxidante, reductora y estequiométrica).

Este supone una mejora en las predicciones en todas las condiciones y, las mejoras más importantes, se pueden observar tanto en CH_4 como en CO_2, mientras que en H_2S y SO_2 se observa una ligera mejora. La condición que más se ha visto mejorada ha sido la estequiométrica mientras que en atmósfera reductora la mejora es muy pequeña si se compara con el mecanismo inicial. En atmósfera oxidante vemos como, en general, las predicciones se han visto mejoradas, sin embargo, en los productos intermedios H_2 y CO se empeora.

Debido a que el mecanismo para la oxidación de sólo CH_4 y sólo H_2S no son del todo precisos, una mejora en ambos mecanismos podría significar una mejora en el mecanismo de CH_4+H_2S. Por tanto, se debería hacer una mayor profundización en las reacciones que intervienen en ambas combustiones y posteriormente profundizar en las reacciones entre carbono y azufre con el fin de mejorar el mecanismo.

Por otra parte, se deberían ajustar las reacciones que producen H_2 y CO en condiciones oxidantes, ya que estos se forman en exceso, afectando negativamente a la simulación de CH_4, H_2S y SO_2.

6 Bibliografía

[1] Wang L.-Y., Xu Y.-L., Li Z.-D., Wei Y.-N., Wei J.-P. *CO_2/CH_4 and H_2S/CO_2 selectivity by ionic liquids in natural gas sweetening.* Energy & Fuels, 2018, 32, 10-23.

[2] Burr B., Lyddon L. *A comparison of physical solvents for acid gas removal,* Bryan Research & Engineering, Inc.

[3] Sassi M., Gupta A. *Sulfur recovery from acid gas using the claus process and high temperature air combustion (HiTAC) technology.* American Journal of Environmental Sciences, 2008, 4, 502-511.

[4] Zhou C., Sendt K., Haynes B.S. *Experimental and kinetic modelling study of H_2S oxidation.* Proceedings of the Combustion Institute, 2013, 34, 625–632.

[5] Colom-Díaz J. M., Abián M., Ballester M.Y., Millera Á., Bilbao R., Alzueta M.U. *H_2S conversion in a tubular flow reactor. Experiments and kinetic modelling.* Proceedings of the Combustion Institute, 2019, 37, in press.

[6] Bongartz D., Goniem A. *Chemical kinetics mechanism for oxy-fuel combustion of mixtures of hydrogen sulfide and methane.* Combustion and Flame, 2015, 162, 544-553.

[7] Giménez-López J., Martínez M., Millera Á., Bilbao R., Alzueta M.U.. *SO_2 effects on CO oxidation in a CO_2 atmosphere, characteristic of oxy-fuel conditions*. Combustion and Flame, 2011, 158, 48-56.

[8] Fleig D., Alzueta M.U., Normann F., Abián M., Andersson K., Johnsson F. *Measurement and modeling of sulfur trioxide formation in a flow reactor under post-flame conditions*. Combustion and Flame, 2013, 160, 1142-1151.

[9] Gersen S., van Essen M., Darmeveil H., Hashemi H., Rasmussen C.-T., Christensen J., Glarborg P., Levinsky H. *Experimental and modeling investigation of the effect of H_2S addition to methane on the ignition and oxidation at high pressures*. Energy & Fuels, 2017, 31, 2175-2182.

[10] Peláez. A, *Estudio de la oxidación de sulfuro de hidrógeno (H_2S) a presión atmosférica en la combustión de gas ácido.* Trabajo fin de grado. Universidad de Zaragoza. Zaragoza, 2017.

[11] Chemkin-Pro. Release 17.2. Reaction Design: San Diego, 2016.

[12] Giménez-López J. *Estudio del proceso de reburning para la reducción de óxidos de nitrógeno en condiciones de oxi-combustión*. Tesis doctoral. Universidad de Zaragoza. Zaragoza, 2015.

[13] Mulvihill C.R., Keesee C.L., Sikes T., Teixeira R.S., Mathieu O., Petersen E.L. *Ignition delay times, laminar flame speeds, and species time-histories in the H_2S/CH_4 system at atmospheric pressure*. Proceedings of the Combustion Institute, 2019, 37, in press.

[14] Abián M., Millera Á., Bilbao R., Alzueta M.U. *Impact of SO_2 on the formation of soot from ethylene pyrolysis*. Fuel, 2015, 159, 550-558.

[15] Song Y., Hashemi H., Christensen J.M., Zou C., Haynes B.S., Marshall P., Glarborg P. *An exploratory flow reactor study of H_2S oxidation at 30–100 bar*, International Journal of Chemical Kinetics, 2017, 49, 37–52.

[16] Hong Z.K., Davidson D.F., Lam K.Y., Hanson R.K. *A shock tube study of the rate constants of HO_2 and CH_3 reactions*. Combustion and Flame, 2012, 159, 3007-3013.

[17] Sutherland J.W., Su M.-C., Michael J.V. *Rate constants for $H + CH_4$, $CH_3 + H_2$, and CH_4 dissociation at high temperature*. International Journal of Chemical Kinetics, 2001, 33, 669-684.

[18] Golden D.M. *Yet another look at the reaction $CH_3+H+M=CH_4+M$.* International Journal of Chemical Kinetics, 2008, 40, 310-319.

[19] Haworth N.L., Bacskay G.B., Mackie J.C. *The role of phosphorus dioxide in the H+OH recombination reaction: ab initio quantum chemical computation of thermochemical and rate parameters*. Journal of Physical Chemistry A, 2002, 106, 1533-1541.

[20] Smith G.P., Golden D.M., Frenklach M., Moriarty N.W., Eiteneer B., Goldenberg M., Bowman C.T., Hanson R.K., Song S., Gardiner W.C., Lissianski V.V., Qin Z., GRI-Mech 3.0, <http://www.me.berkeley.edu/gri-mech/

[21] Petherbridge J.R., May P.W., Shallcross D.E., Harvey J.N., Fuge G.M., Rosser K.N., Ashfold M.N.R., *Simulation of H–C–S containing gas mixtures relevant to diamond chemical vapour deposition.* Diamond and Related Materials, 2003, 12, 2178–2185.

Anexo A. Resultados experimentales

En las tablas A.1 a A.6 se exponen los resultados experimentales de los experimentos cuyo proceso se encuentra descrito en el apartado 3 del presente trabajo de final de grado. Los experimentos fueron realizados en atmósfera de nitrógeno, para que los datos experimentales no fuesen afectados por el calor de reacción y la temperatura pudiera considerarse homogénea en todo momento.

El proceso experimental fue llevado a cabo por Peláez A. [10].

En las simulaciones la temperatura ha sido considerada constante y homogénea.

Tabla A.1 Experimento H_2S/CH_4 en condiciones reductoras (λ=0.25), O_2=754 ppm, H_2O=14470 ppm

Tª (°C)	H_2S (ppm)	SO_2 (ppm)	H_2 (ppm)	CH_4 (ppm)	CO_2 (ppm)	CO (ppm)
500	279	1,6	0	1508	20	0
600	273	1,9	0	1516	20	0
650	253	18	0	1537	20	0
700	177	75	32	1504	20	0
750	132	138	58	1517	20	5
800	85	177	94	1503	20	23
900	0	201	151	1424	20	42
950	23	214	205	1374	20	48
1000	6	223	263	1313	30	94
1050	5	220	344	1273	61	155
1100	0	193	440	1220	117	206

Tabla A.2 Experimento H_2S/CH_4 en condiciones estequiométricas ($\lambda=1$), O_2=3000 ppm, H_2O=14470 ppm

Tª (°C)	H_2S (ppm)	SO_2 (ppm)	H_2 (ppm)	CH_4 (ppm)	C_2H_6 (ppm)	C_2H_4 (ppm)	CO_2 (ppm)	CO (ppm)
500	285	3	0	1513	0	0	23	0
550	278	10	0	1515	0	0	22	2
600	210	68	22	1524	0	0	22	5
650	130	146	47	1533	0	0	23	14
700	95	193	65	1502	0	0	23	23
750	14	230	96	1512	0	0	23	35
800	8	250	119	1510	0	0	24	47
900	0	279	183	1293	18	17	33	101
1000	0	300	345	562	16	45	409	484
1100	0	300	558	100	0	0	996	489

Tabla A.3 Experimento H_2S/CH_4 en condiciones oxidantes ($\lambda=2$), O_2=6000 ppm, H_2O=10294 ppm

Tª (°C)	H_2S (ppm)	SO_2 (ppm)	H_2 (ppm)	CH_4 (ppm)	C_2H_6 (ppm)	C_2H_4 (ppm)	CO_2 (ppm)	CO (ppm)
500	298	2	0	1508	0	0	0	0
550	291	9	0	1508	0	0	0	0
600	220	65	26	1470	0	0	0	5
650	128	158	54	1487	0	0	0	19
700	80	201	74	1472	0	0	0	31
750	49	234	90	1455	0	0	0	45
800	0	256	122	1420	0	0	0	62
900	0	288	210	1271	38	36	11	138
950	0	303	26	0	0	0	1494	53
1000	0	300	0	0	0	0	1591	2

1100	0	301	0	0	0	0	1615	1

Tabla A.4 Experimento CH_4 en condiciones reductoras (λ=0.25), O_2=750 ppm, H_2O=13215 ppm

Tª (°C)	CH_4 (ppm)	CO_2 (ppm)	CO (ppm)	H_2 (ppm)
500	1500	21	0	0
600	1494	20	0	0
700	1489	17	0	0
800	1493	19	0	0
900	1469	17	1	0
1000	1467	21	2	0
1050	1470	28	3	40
1100	1470	40	13	81

Tabla A.5 Experimento CH_4 en condiciones estequiométricas (λ=1), O_2=3000 ppm, H_2O=13215 ppm

Tª (°C)	CH_4 (ppm)	CO_2 (ppm)	CO (ppm)	H_2 (ppm)
500	1501	0	0	0
600	1502	0	0	0
700	1499	0	0	0
800	1502	0	4	0
900	1493	0	2	0
1000	1490	8	6	21
1050	0	1539	53	331
1100	0	1535	63	371

Tabla A.6 Experimento CH_4 en condiciones oxidantes (λ=2), O_2=6000 ppm, H_2O=10294 ppm

Tª (°C)	CH_4 (ppm)	CO_2 (ppm)	CO (ppm)	H_2 (ppm)
500	1513	0	0	0
600	1524	0	0	0
700	1502	0	0	0
800	1507	0	0	0
900	1522	0	0	0
950	1488	0	0	0
1000	1457	8	0	21
1025	0	1601	0	0
1100	0	1609	0	0

Anexo B. Software Chemkin-Pro

B.1 Introducción

Para realizar la simulación del de todos los procesos de combustión que se han requerido en este Trabajo de final de Grado, se ha utilizado el software CHEMKIN-PRO. Este software es capaz de resolver problemas que involucren modelos químicos complejos con cinéticas que pueden estar compuestas por muchas reacciones y especies químicas. CHEMKIN facilita la formulación, solución e interpretación de problemas en fase homogénea. En este trabajo se ha utilizado la versión comercial CHEMKIN-Pro [11], de la compañía Reaction Design.

B.2 Estructura del programa

GAS-PHASE KINETICS Pre-processor es un programa que lee una descripción simbólica del mecanismo de reacción en fase gas y extrae los datos termodinámicos necesarios de cada especie involucrada en el mecanismo. Para la ejecución del programa se necesitan dos ficheros:

Fichero Gas Phase Chemistry: En él se introducen las reacciones que componen el mecanismo de reacción. Este fichero debe incluir los elementos y especies que intervienen en el mecanismo de reacción y la descripción del mismo. En la descripción de las reacciones, se deben incluir los tres coeficientes de la ecuación de Arrhenius modificada para el cálculo de la constante cinética de la reacción.

Fichero Thermodynamic Data: Base de datos que incluye toda la información termodinámica de las especies involucradas en el mecanismo de reacción. La base de datos debe contener una serie de datos para cada especie química en un formato específico.

Cuando el mecanismo cinético y los datos termodinámicos se han introducido en el formato adecuado, se ejecuta el Pre-processor para producir el GAS-PHASE KINETICS Linking File, que contiene toda la información química requerida respecto a la cinética en fase gas del problema (elementos, especies y reacciones). Este fichero tiene que crearse para cualquier tipo de aplicación o modelo de reactor de Chemkin-Pro que se quiera realizar.

El software CHEMKIN-Pro permite simular multitud de modelos de reactor (CHEMKIN Application): reactores de flujo-pistón (PFR), de mezcla perfecta (CSTR), motores de combustión interna (MACI) entre otros. Para este trabajo se utiliza el modelo de reactor de flujo pistón. Según el modelo de reactor elegido, el usuario debe especificar unas condiciones del proceso determinadas (Application Input). En este estudio se considera un modelo de presión y temperatura constantes, por lo que para cada simulación se requiere especificar las siguientes condiciones de operación del proceso: temperatura, presión, concentración y caudal de gases reactantes, así como dimensiones del reactor (longitud y diámetro). El análisis de temperaturas puede hacerse según dos modelos distintos:

Con perfil de temperaturas. Para cada temperatura de análisis, se introduce el perfil de temperaturas completo a lo largo de la longitud del reactor.

Con temperatura constante. Se establece que la zona de reacción es isoterma, suponiendo que las zonas anterior y posterior se encuentran a una temperatura muy baja a la que no se produce reacción.

El modelo de temperatura constante requiere menos coste computacional ya que en una única resolución se puede realizar toda la simulación mientras que para el modelo de perfil de temperaturas se debe resolver para cada temperatura por separado.

El tratamiento de datos (Text Output), una vez realizado el cálculo de cada caso particular, el software CHEMKIN-Pro permite analizar los resultados a través del propio programa, ya que dispone de un post-procesador para representar los datos de forma gráfica o bien mediante un post-procesador externo (como puede ser Microsoft Excel), donde se obtendrán todos los datos del proceso que se deseen de una forma numérica, que requerirán un posterior tratamiento. La opción elegida fue la de un post-procesador externo, concretamente Microsoft Excel 2010 ya que el resto de los datos del trabajo se encontraban en dicho formato.

El software también ofrece otras herramientas, como el análisis de la velocidad de reacción (Reaction Path Analyzer Tool), que permite comparar la importancia de cada reacción con respecto al conjunto de reacciones en que interviene una especie determinada y todo ello con respecto al mecanismo global de reacción planteado en el modelo. Esto permite identificar los caminos preferenciales por los que transcurre un mecanismo de reacción para unas condiciones determinadas.

Anexo C. Mecanismo de reacción

C.1 Mecanismo de reacción

El mecanismo cinético químico utilizado se desarrolló en el Grupo de Procesos Termoquímicos (GTP) del Instituto de Investigación de Ingeniería de Aragón (I3A) por Colom-Díaz et al. [5].

En el apartado C.3, se muestran todas las reacciones añadidas al mecanismo de Colom-Díaz et al. [5] con los valores de los parámetros de la ecuación de Arrhenius modificada (Ec. C.1) que se utiliza para el cálculo de la constante de velocidad de reacción:

$$k = AT^{\beta}\exp(\frac{-E_A}{RT}) \qquad \text{Ec.C.1}$$

Donde:

A = Factor pre-exponencial [mol, cm, s, K].

β = Exponente de temperatura.

Ea = Energía de activación [cal/mol].

T = Temperatura [K].

R = Constante universal de los gases (1,987 cal/mol K).

C.2 Mecanismo inicial

En este apartado se va a insertar el mecanismo inicial desarrollado por Colom-D

íaz et al. [5].

```
!                                                    !
!      MSR MODIFIED M1A MECHANISM FROM POPE AND MILLER              !
!                                                    !
!=====================================================================
=======!  !
!Modified and updtated: Abián M., Millera A., Bilbao R., Alzueta M.U.,
!                       Impact of SO2 on the formation of soot from ethylene pyrolysis.
!                       FUEL 159 (2015) 550-558
!
!*****************************************************
!
! *** 8 November 2017: Mmo preparado por Juan Manuel Colom.
!
!*****************************************************
!
!
ELEMENTS
H O C N S AR
END
SPECIES
!!!ordenadas en el mec
H2S
CH2SH
SO2
SH
H
OH
O
H2              ! m=    2
S2
O3
CO
CO2
COS
CS2
CS
```

SO
C2H4
C2H2
CH4
!
!!!CO ! m= 28
!!!CO2 ! m= 44
!!!!C2H4 ! m= 28
!!!!CH4 ! m= 16
C2H6 ! m= 30
!!!!C2H2 ! m= 26
CH2O ! m= 30
CH ! m= 13
CH2 ! m= 14
CH2(S) ! m= 14
CH3 ! m= 15
H2O ! m= 18
C2 ! m= 24
C2H ! m= 25
C2H3 ! m= 27
HCO ! m= 29
N2 ! m= 28
C2H5 ! m= 29
CH2OH ! m= 31
CH3O ! m= 31
O2 ! m= 32
CH3OH ! m= 32
HO2 ! m= 33
H2O2 ! m= 34
C3H2 ! m= 38
H2CCCH ! m= 39
C2H2OH
AR ! m= 40
C2O ! m= 40
HCCO ! m= 41
CH2CHCH2 ! m= 41

CH3CCH2 ! m= 41
CH3CHCH ! m= 41
CH2CO ! m= 42
HCCOH ! m= 42
OCHCHO ! m= 58
CH2HCO
!
! ESPECIES INCLUIDAS EN EL MECANISMO DE ETANOL
!
C2H5OH
C2H4OH
CH3CH2O
CH3HCO
CH3CO
C2H5CHO
C2H5CO
HCOO
NO
HCN
C
NO2
NO3
HNO
HONO
H2NO
HNOH
NH3
NH2
NH
N
N2H2
NNH
N2O
CN
NCO
HNCO

HOCN

HCNO

C2N2

NCN

CH3CN

CH2CN

H2CN

CH3NO

HONO2

CH3CHOH

!

!Nuevas especies incluidas

!

CH3O2

CH2CHCHCH2

CH2CHCHCH

C4H2

HCCHCCH

CH2CHCCH

CH2CHCCH2

H2CCCCH

C4H

H2CCCCCH

HCCCHCCH

C6H2 ! m= 74

C5H2 ! m= 62

C5H5 ! m= 65

H2C4O ! m= 66

!

!S Species:

!!!SO2

SO2* SO3

!SO

SO(S) HSO HOS HOSO HSO2 HOSO2 HOSOH HOSHO H2SO HSOH S HSOO OSSO SSO2 HS2O

!S2

HS2 H2S2 HSSO2 H2S3O HSSSOH H2S2O2 VDW1 S4 S5 S6 S7 S8

!COS CS2 CS

CH3S CH3SH CH2S CH3CHO CH3SO2 CH3OSO S2O S3 H2SO4 CH3SO HCS

CH3CH2S CH3SCH3 CH2CH2SH CS2OH

!!!COS2

!

END

!

!

THERMO

300.000 1000.000 5000.000

C2H4 121286C 2H 4 G 0300.00 5000.00 1000.00 1

0.03528418E+02 0.11485185E-01-0.04418385E-04 0.07844600E-08-0.05266848E-12 2

0.04428288E+05 0.02230389E+02-0.08614880E+01 0.02796162E+00-0.03388677E-03 3

0.02785152E-06-0.09737879E-10 0.05573046E+05 0.02421148E+03 4

CO 121286C 1O 1 G 0300.00 5000.00 1000.00 1

0.03025078E+02 0.14426885E-02-0.05630827E-05 0.10185813E-09-0.06910951E-13 2

-0.14268350E+05 0.06108217E+02 0.03262451E+02 0.15119409E-02-0.03881755E-04 3

0.05581944E-07-0.02474951E-10-0.14310539E+05 0.04848897E+02 4

CO2 121286C 1O 2 G 0300.00 5000.00 1000.00 1

0.04453623E+02 0.03140168E-01-0.12784105E-05 0.02393996E-08-0.16690333E-13 2

-0.04896696E+06-0.09553959E+01 0.02275724E+02 0.09922072E-01-0.10409113E-04 3

0.06866686E-07-0.02117280E-10-0.04837314E+06 0.10188488E+02 4

CH4 121286C 1H 4 G 0300.00 5000.00 1000.00 1

0.01683478E+02 0.10237236E-01-0.03875128E-04 0.06785585E-08-0.04503423E-12 2

-0.10080787E+05 0.09623395E+02 0.07787415E+01 0.01747668E+00-0.02783409E-03 3

0.03049708E-06-0.12239307E-10-0.09825229E+05 0.13722195E+02 4

CH2O 121286C 1H 2O 1 G 0300.00 5000.00 1000.00 1

0.02995606E+02 0.06681321E-01-0.02628954E-04 0.04737153E-08-0.03212517E-12 2

-0.15320369E+05 0.06912572E+02 0.16527311E+01 0.12631439E-01-0.01888168E-03 3

0.02050031E-06-0.08413237E-10-0.14865404E+05 0.13784820E+02 4

H 120186H 1 G 0300.00 5000.00 1000.00 1

0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2

0.02547162E+06-0.04601176E+01 0.02500000E+02 0.00000000E+00 0.00000000E+00 3

0.00000000E+00 0.00000000E+00 0.02547162E+06-0.04601176E+01 4

H2 121286H 2 G 0300.00 5000.00 1000.00 1

0.02991423E+02 0.07000644E-02-0.05633828E-06-0.09231578E-10 0.15827519E-14 2
-0.08350340E+04-0.13551101E+01 0.03298124E+02 0.08249441E-02-0.08143015E-05 3
-0.09475434E-09 0.04134872E-11-0.10125209E+04-0.03294094E+02 4
C 121086C 1 G 0300.00 5000.00 1000.00 1
0.02602087E+02-0.01787081E-02 0.09087041E-06-0.11499333E-10 0.03310844E-14 2
0.08542154E+06 0.04195177E+02 0.02498584E+02 0.08085776E-03-0.02697697E-05 3
0.03040729E-08-0.11066518E-12 0.08545878E+06 0.04753459E+02 4
CH 121286C 1H 1 G 0300.00 5000.00 1000.00 1
0.02196223E+02 0.02340381E-01-0.07058201E-05 0.09007582E-09-0.03855040E-13 2
0.07086723E+06 0.09178373E+02 0.03200202E+02 0.02072875E-01-0.05134431E-04 3
0.05733890E-07-0.01955533E-10 0.07045259E+06 0.03331587E+02 4
CH2(S) 83194H 2C 1 0 0G 300.000 4000.000 1400.00 0 1
0.40752106E+01 0.15779120E-02-0.10806129E-06-0.84592437E-10 0.14033284E-13 2
0.50007492E+05-0.15480316E+01 0.35932946E+01 0.13151238E-02 0.30756846E-06 3
0.42637904E-09-0.34178712E-12 0.50451547E+05 0.17780241E+01 4
CH2 83194H 2C 1 0 0G 300.000 4000.000 1400.00 0 1
0.39737520E+01 0.16097502E-02-0.10785119E-06-0.86399922E-10 0.14301196E-13 2
0.45608973E+05 0.75549729E-01 0.36872995E+01 0.15066403E-02 0.69679857E-07 3
0.23537297E-09-0.19397147E-12 0.45863672E+05 0.20267601E+01 4
CH3 121286C 1H 3 G 0300.00 5000.00 1000.00 1
0.02844051E+02 0.06137974E-01-0.02230345E-04 0.03785161E-08-0.02452159E-12 2
0.16437809E+05 0.05452697E+02 0.02430442E+02 0.11124099E-01-0.01680220E-03 3
0.16218288E-07-0.05864952E-10 0.16423781E+05 0.06789794E+02 4
O 120186O 1 G 0300.00 5000.00 1000.00 1
0.02542059E+02-0.02755061E-03-0.03102803E-07 0.04551067E-10-0.04368051E-14 2
0.02923080E+06 0.04920308E+02 0.02946428E+02-0.16381665E-02 0.02421031E-04 3
-0.16028431E-08 0.03890696E-11 0.02914764E+06 0.02963995E+02 4
CH4 121286C 1H 4 G 0300.00 5000.00 1000.00 1
0.01683478E+02 0.10237236E-01-0.03875128E-04 0.06785585E-08-0.04503423E-12 2
-0.10080787E+05 0.09623395E+02 0.07787415E+01 0.01747668E+00-0.02783409E-03 3
0.03049708E-06-0.12239307E-10-0.09825229E+05 0.13722195E+02 4
OH 121286O 1H 1 G 0300.00 5000.00 1000.00 1
0.02882730E+02 0.10139743E-02-0.02276877E-05 0.02174683E-09-0.05126305E-14 2
0.03886888E+05 0.05595712E+02 0.03637266E+02 0.01850910E-02-0.16761646E-05 3
0.02387202E-07-0.08431442E-11 0.03606781E+05 0.13588605E+01 4
H2O 20387H 2O 1 G 0300.00 5000.00 1000.00 1

0.02672145E+02 0.03056293E-01-0.08730260E-05 0.12009964E-09-0.06391618E-13 2
-0.02989921E+06 0.06862817E+02 0.03386842E+02 0.03474982E-01-0.06354696E-04 3
0.06968581E-07-0.02506588E-10-0.03020811E+06 0.02590232E+02 4
C2 121286C 2 G 0300.00 5000.00 1000.00 1
0.04135978E+02 0.06531618E-03 0.01837099E-05-0.05295085E-09 0.04712137E-13 2
0.09967272E+06 0.07472923E+01 0.06996045E+02-0.07400601E-01 0.03234703E-04 3
0.04802535E-07-0.03295917E-10 0.09897487E+06-0.13862268E+02 4
C2H 83194H 1C 2 0 0G 300.000 4000.000 1400.00 0 1
0.52086663E+01 0.12875765E-02-0.10398387E-06-0.67526325E-10 0.11751871E-13 2
0.64697773E+05-0.53721781E+01 0.39396334E+01 0.32114412E-02-0.39412765E-06 3
-0.74782530E-09 0.27493521E-12 0.65224684E+05 0.17814000E+01 4
C2H2 121386C 2H 2 G 0300.00 5000.00 1000.00 1
0.04436770E+02 0.05376039E-01-0.01912816E-04 0.03286379E-08-0.02156709E-12 2
0.02566766E+06-0.02800338E+02 0.02013562E+02 0.15190446E-01-0.16163189E-04 3
0.09078992E-07-0.01912746E-10 0.02612444E+06 0.08805378E+02 4
C2H3 83194H 3C 2 0 0G 300.000 4000.000 1400.00 0 1
0.71861677E+01 0.34552682E-02-0.29435373E-06-0.20681942E-09 0.36797774E-13 2
0.32229627E+05-0.15977573E+02 0.24955740E+01 0.10269993E-01-0.10226917E-05 3
-0.27594382E-08 0.96919825E-12 0.34232813E+05 0.10614626E+02 4
CO 121286C 1O 1 G 0300.00 5000.00 1000.00 1
0.03025078E+02 0.14426885E-02-0.05630827E-05 0.10185813E-09-0.06910951E-13 2
-0.14268350E+05 0.06108217E+02 0.03262451E+02 0.15119409E-02-0.03881755E-04 3
0.05581944E-07-0.02474951E-10-0.14310539E+05 0.04848897E+02 4
C2H4 121286C 2H 4 G 0300.00 5000.00 1000.00 1
0.03528418E+02 0.11485185E-01-0.04418385E-04 0.07844600E-08-0.05266848E-12 2
0.04428288E+05 0.02230389E+02-0.08614880E+01 0.02796162E+00-0.03388677E-03 3
0.02785152E-06-0.09737879E-10 0.05573046E+05 0.02421148E+03 4
HCO 121286H 1C 1O 1 G 0300.00 5000.00 1000.00 1
0.03557271E+02 0.03345572E-01-0.13350060E-05 0.02470572E-08-0.01713850E-12 2
0.03916324E+05 0.05552299E+02 0.02898329E+02 0.06199146E-01-0.09623084E-04 3
0.10898249E-07-0.04574885E-10 0.04159922E+05 0.08983614E+02 4
N2 121286N 2 G 0300.00 5000.00 1000.00 1
0.02926640E+02 0.14879768E-02-0.05684760E-05 0.10097038E-09-0.06753351E-13 2
-0.09227977E+04 0.05980528E+02 0.03298677E+02 0.14082404E-02-0.03963222E-04 3
0.05641515E-07-0.02444854E-10-0.10208999E+04 0.03950372E+02 4
C2H5 83194H 5C 2 0 0G 300.000 4000.000 1400.00 0 1

0.87349157E+01 0.54537677E-02-0.37647177E-06-0.31297920E-09 0.52844000E-13 2
0.10265269E+05-0.23104086E+02 0.24398923E+01 0.13747212E-01-0.85500653E-06 3
-0.31469924E-08 0.93754355E-12 0.13158588E+05 0.13099146E+02 4
CH2O 121286C 1H 2O 1 G 0300.00 5000.00 1000.00 1
0.02995606E+02 0.06681321E-01-0.02628954E-04 0.04737153E-08-0.03212517E-12 2
-0.15320369E+05 0.06912572E+02 0.16527311E+01 0.12631439E-01-0.01888168E-03 3
0.02050031E-06-0.08413237E-10-0.14865404E+05 0.13784820E+02 4
C2H6 121686C 2H 6 G 0300.00 4000.00 1000.00 1
0.04825938E+02 0.13840429E-01-0.04557258E-04 0.06724967E-08-0.03598161E-12 2
-0.12717793E+05-0.05239506E+02 0.14625388E+01 0.15494667E-01 0.05780507E-04 3
-0.12578319E-07 0.04586267E-10-0.11239176E+05 0.14432295E+02 4
CH2OH 120186H 3C 1O 1 G 0250.00 4000.00 1000.00 1
0.06327520E+02 0.03608270E-01-0.03201547E-05-0.01938750E-08 0.03509704E-12 2
-0.04474509E+05-0.08329365E+02 0.02862628E+02 0.10015273E-01-0.05285435E-05 3
-0.05138539E-07 0.02246041E-10-0.03349678E+05 0.10397938E+02 4
CH3O 121686C 1H 3O 1 G 0300.00 3000.00 1000.00 1
0.03770799E+02 0.07871497E-01-0.02656384E-04 0.03944431E-08-0.02112616E-12 2
0.12783252E+03 0.02929575E+02 0.02106204E+02 0.07216595E-01 0.05338472E-04 3
-0.07377636E-07 0.02075610E-10 0.09786011E+04 0.13152177E+02 4
O2 121386O 2 G 0300.00 5000.00 1000.00 1
0.03697578E+02 0.06135197E-02-0.12588420E-06 0.01775281E-09-0.11364354E-14 2
-0.12339301E+04 0.03189165E+02 0.03212936E+02 0.11274864E-02-0.05756150E-05 3
0.13138773E-08-0.08768554E-11-0.10052490E+04 0.06034737E+02 4
CH3OH 121686C 1H 4O 1 G 0300.00 5000.00 1000.00 1
0.04029061E+02 0.09376593E-01-0.03050254E-04 0.04358793E-08-0.02224723E-12 2
-0.02615791E+06 0.02378195E+02 0.02660115E+02 0.07341508E-01 0.07170050E-04 3
-0.08793194E-07 0.02390570E-10-0.02535348E+06 0.11232631E+02 4
HO2 20387H 1O 2 G 0300.00 5000.00 1000.00 1
0.04072191E+02 0.02131296E-01-0.05308145E-05 0.06112269E-09-0.02841164E-13 2
-0.15797270E+03 0.03476029E+02 0.02979963E+02 0.04996697E-01-0.03790997E-04 3
0.02354192E-07-0.08089024E-11 0.01762273E+04 0.09222724E+02 4
H2O2 120186H 2O 2 G 0300.00 5000.00 1000.00 1
0.04573167E+02 0.04336136E-01-0.14746888E-05 0.02348903E-08-0.14316536E-13 2
-0.01800696E+06 0.05011369E+01 0.03388753E+02 0.06569226E-01-0.14850125E-06 3
-0.04625805E-07 0.02471514E-10-0.01766314E+06 0.06785363E+02 4
C3H2 102193H 2C 3 G 0150.00 4000.00 1000.00 1

0.07670981E+02 0.02748749E-01-0.04370942E-05-0.06455599E-09 0.16638874E-13 2
0.06259722E+06-0.12368903E+02 0.03166713E+02 0.02482571E+00-0.04591637E-03 3
0.04268019E-06-0.14821524E-10 0.06350421E+06 0.08869446E+02 4
H2CCCH 032599C 3H 3 G 0300.00 4000.00 1000.00 1
0.08831047E+02 0.04357194E-01-0.04109066E-05-0.02368723E-08 0.04376520E-12 2
0.39983875E+05-0.22559194E+02 0.04754199E+02 0.11080277E-01 0.02793323E-05 3
-0.05479212E-07 0.01949629E-10 0.41398515E+05-1.94548824E-01 4
AR 120186AR 1 G 0300.00 5000.00 1000.00 1
0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2
-0.07453750E+04 0.04366000E+02 0.02500000E+02 0.00000000E+00 0.00000000E+00 3
0.00000000E+00 0.00000000E+00-0.07453750E+04 0.04366000E+02 4
C2O 121286C 2O 1 G 0300.00 5000.00 1000.00 1
0.04849809E+02 0.02947585E-01-0.10907286E-05 0.01792562E-08-0.11157585E-13 2
0.03282055E+06-0.06453225E+01 0.03368850E+02 0.08241803E-01-0.08765145E-04 3
0.05569262E-07-0.15400086E-11 0.03317081E+06 0.06713314E+02 4
C3H4 101993H 4C 3 G 0300.00 4000.00 1400.00 1
0.09776256E+02 0.05302137E-01-0.03701117E-05-0.03026385E-08 0.05089581E-12 2
0.01954972E+06-0.03077061E+03 0.02539830E+02 0.16334371E-01-0.01764950E-04 3
-0.04647365E-07 0.01729130E-10 0.02251242E+06 0.09935702E+02 4
C3H4P 101993H 4C 3 G 0300.00 4000.00 1400.00 1
0.09768102E+02 0.05219151E-01-0.03753140E-05-0.02992191E-08 0.05107878E-12 2
0.01860277E+06-0.03020678E+03 0.03029730E+02 0.14989613E-01-0.13985000E-05 3
-0.03969619E-07 0.13882165E-11 0.02148408E+06 0.08004594E+02 4
HCCO 32387H 1C 2O 1 G 0300.00 4000.00 1000.00 1
0.06758073E+02 0.02000400E-01-0.02027607E-05-0.10411318E-09 0.01965164E-12 2
0.01901513E+06-0.09071262E+02 0.05047965E+02 0.04453478E-01 0.02268282E-05 3
-0.14820945E-08 0.02250741E-11 0.01965891E+06 0.04818439E+01 4
CH2CHCH2 82489C 3H 5 G 0300.00 4000.00 1000.00 1
0.09651539E+02 0.08075596E-01-0.07965424E-05-0.04650696E-08 0.08603281E-12 2
0.15300955E+05-0.02686773E+03 0.02276486E+02 0.01985564E+00 0.11238421E-05 3
-0.10145757E-07 0.03441342E-10 0.01789496E+06 0.13725151E+02 4
CH3CCH2 82489C 3H 5 G 0300.00 4000.00 1000.00 1
0.09101018E+02 0.07964167E-01-0.07884945E-05-0.04562036E-08 0.08529212E-12 2
0.02670680E+06-0.02150559E+03 0.03385811E+02 0.14045337E-01 0.03204127E-04 3
-0.03824120E-07-0.09053742E-11 0.02909066E+06 0.11266487E+02 4
CH3CHCH 82489C 3H 5 G 0300.00 4000.00 1000.00 1

0.09209764E+02 0.07871412E-01-0.07724522E-05-0.04497357E-08 0.08377272E-12 2
0.02853967E+06-0.02232369E+03 0.03161863E+02 0.15180997E-01 0.02722659E-04 3
-0.05177112E-07 0.05435286E-12 0.03095547E+06 0.11979733E+02 4
CH2CO 121686C 2H 2O 1 G 0300.00 5000.00 1000.00 1
0.06038817E+02 0.05804840E-01-0.01920953E-04 0.02794484E-08-0.14588676E-13 2
-0.08583402E+05-0.07657581E+02 0.02974970E+02 0.12118712E-01-0.02345045E-04 3
-0.06466685E-07 0.03905649E-10-0.07632636E+05 0.08673553E+02 4
HCCOH 32387H 2C 2O 1 G 0300.00 4000.00 1000.00 1
0.07328324E+02 0.03336416E-01-0.03024705E-05-0.01781106E-08 0.03245168E-12 2
0.07598258E+05-0.14012140E+02 0.03899465E+02 0.09701075E-01-0.03119309E-05 3
-0.05537732E-07 0.02465732E-10 0.08701190E+05 0.04491874E+02 4
C3H6 120186C 3H 6 G 0300.00 5000.00 1000.00 1
0.06732257E+02 0.14908336E-01-0.04949899E-04 0.07212022E-08-0.03766204E-12 2
-0.09235703E+04-0.13313348E+02 0.14933071E+01 0.02092517E+00 0.04486794E-04 3
-0.16689121E-07 0.07158146E-10 0.10748264E+04 0.16145340E+02 4
C2H2OH HCCO TRAN 121196H 3C 2O 1 0G 300.000 3000.000 1000.00 0 1
0.57206843E+01 0.10704185E-01-0.50358494E-05 0.11324499E-08-0.10086621E-12 2
0.12849424E+05-0.47081776E+01 0.81498282E-01 0.31640644E-01-0.34085361E-04 3
0.18978838E-07-0.41950165E-11 0.14060783E+05 0.22908977E+02 4
CH2HCO 110393O 1H 3C 2 G 0300.00 5000.00 1000.00 1
0.05975670E+02 0.08130591E-01-0.02743624E-04 0.04070304E-08-0.02176017E-12 2
0.04903218E+04-0.05045251E+02 0.03409062E+02 0.10738574E-01 0.01891492E-04 3
-0.07158583E-07 0.02867385E-10 0.15214766E+04 0.09558290E+02 4
CH3CO 120186C 2H 3O 1 G 0300.00 5000.00 1000.00 1
0.05612279E+02 0.08449886E-01-0.02854147E-04 0.04238376E-08-0.02268403E-12 2
-0.05187863E+05-0.03274949E+02 0.03125278E+02 0.09778220E-01 0.04521448E-04 3
-0.09009462E-07 0.03193717E-10-0.04108507E+05 0.11228854E+02 4
CO2 121286C 1O 2 G 0300.00 5000.00 1000.00 1
0.04453623E+02 0.03140168E-01-0.12784105E-05 0.02393996E-08-0.16690333E-13 2
-0.04896696E+06-0.09553959E+01 0.02275724E+02 0.09922072E-01-0.10409113E-04 3
0.06866686E-07-0.02117280E-10-0.04837314E+06 0.10188488E+02 4
CH3HCO 120186C 2O 1H 4 G 0300.00 5000.00 1000.00 1
0.05868650E+02 0.10794241E-01-0.03645530E-04 0.05412912E-08-0.02896844E-12 2
-0.02264568E+06-0.06012946E+02 0.02505695E+02 0.13369907E-01 0.04671953E-04 3
-0.11281401E-07 0.04263566E-10-0.02124588E+06 0.13350887E+02 4
CH3O2 BUR95 H 3C 1O 2 0G 200.000 6000.000 1000.000 0 1

0.66812963E 01 0.80057271E-02-0.27188507E-05 0.40631365E-09-0.21927725E-13 2
0.52621851E 03-0.99423847E 01 0.20986490E 01 0.15786357E-01 0.75683261E-07 3
-0.11274587E-07 0.56665133E-11 0.20695879E 04 0.15007068E 02 0.33715510E+04 4
CH3OOH BUR95 H 4C 1O 2 00G 200.000 6000.000 1000.000 1
0.61600316E+01 0.10239957E-01-0.36101507E-05 0.57550301E-09-0.34178147E-13 2
-0.17654526E+05-0.61911544E+01 0.49652507E+01 0.92343510E-03 0.34455956E-04 3
-0.44469600E-07 0.17456120E-10-0.16726970E+05 0.29880275E+01-0.14980760E+05 4
C4H 121686C 4H 1 G 0300.00 5000.00 1000.00 1
0.06242882E+02 0.06193682E-01-0.02085931E-04 0.03082203E-08-0.16364826E-13 2
0.07568019E+06-0.07210806E+02 0.05023247E+02 0.07092375E-01-0.06073762E-07 3
-0.02275752E-07 0.08086994E-11 0.07623812E+06-0.06942594E+00 4
C4H2 121686C 4H 2 G 0300.00 5000.00 1000.00 1
0.09031407E+02 0.06047252E-01-0.01948788E-04 0.02754863E-08-0.13856080E-13 2
0.05294735E+06-0.02385067E+03 0.04005191E+02 0.01981000E+00-0.09865877E-04 3
-0.06635158E-07 0.06077413E-10 0.05424065E+06 0.01845736E+02 4
H2CCCCH 82489C 4H 3 G 0300.00 4000.00 1000.00 1
0.11314095E+02 0.05014414E-01-0.05350444E-05-0.02825309E-08 0.05403279E-12 2
0.05181211E+06-0.03062434E+03 0.06545799E+02 0.12424768E-01 0.05603226E-05 3
-0.05631141E-07 0.16652183E-11 0.05352502E+06-0.04264082E+02 4
HCCHCCH 82489C 4H 3 G 0300.00 4000.00 1000.00 1
0.10752738E+02 0.05381153E-01-0.05549637E-05-0.03052266E-08 0.05761740E-12 2
0.06121419E+06-0.02973025E+03 0.04153881E+02 0.01726287E+00-0.02389374E-05 3
-0.10187000E-07 0.04340504E-10 0.06338070E+06 0.06036506E+02 4
CH2CHCCH 82489C 4H 4 G 0300.00 4000.00 1000.00 1
0.10697773E+02 0.06982014E-01-0.06567747E-05-0.03884517E-08 0.07200946E-12 2
0.03034803E+06-0.03128430E+03 0.03233893E+02 0.01865634E+00 0.12703205E-05 3
-0.09410096E-07 0.02956110E-10 0.03301097E+06 0.09922676E+02 4
CH2CHCCH2 82489C 4H 5 G 0300.00 4000.00 1000.00 1
0.11997762E+02 0.07990580E-01-0.08098172E-05-0.04568733E-08 0.08636911E-12 2
0.03228493E+06-0.03528494E+03 0.03879443E+02 0.01997663E+00 0.01872777E-04 3
-0.09306953E-07 0.02386116E-10 0.03526859E+06 0.09842152E+02 4
CH2CHCHCH 82489C 4H 5 G 0300.00 4000.00 1000.00 1
0.12865971E+02 0.07943369E-01-0.08626466E-05-0.04655635E-08 0.08951131E-12 2
0.03783552E+06-0.04182502E+03 0.02995240E+02 0.02288456E+00 0.01975471E-04 3
-0.11482454E-07 0.03197823E-10 0.04142218E+06 0.12894539E+02 4
CH2CHCHCH2 120189C 4H 6 G 0300.00 4000.00 1000.00 1

0.12544366E+02 0.09596525E-01-0.09187012E-05-0.05429640E-08 0.10053636E-12 2
0.08597330E+05-0.04217450E+03 0.01931624E+02 0.02479030E+00 0.03018071E-04 3
-0.11546856E-07 0.02586623E-10 0.12554682E+05 0.01701999E+03 4
OCHCHO 120596H 2C 2O 2 0G 300.000 3000.000 1000.00 0 1
0.49087462E+01 0.13182673E-01-0.71416730E-05 0.18461316E-08-0.18525858E-12 2
-0.27116386E+05 0.59148768E+00 0.25068862E+01 0.18899139E-01-0.10302623E-04 3
0.62607508E-09 0.88114253E-12-0.26427374E+05 0.13187043E+02 4
C5H2 20587C 5H 2 G 0300.00 5000.00 1000.00 1
0.11329175E+02 0.07424056E-01-0.02628188E-04 0.04082541E-08-0.02301332E-12 2
0.07878706E+06-0.03617117E+03 0.03062321E+02 0.02709998E+00-0.10091697E-04 3
-0.12727451E-07 0.09167219E-10 0.08114969E+06 0.07071078E+02 4
H2CCCCCH 101993H 3C 5 G 0300.00 4000.00 1400.00 1
0.14407361E+02 0.04424058E-01-0.03618244E-05-0.02456408E-08 0.04327859E-12 2
0.05896103E+06-0.04775144E+03 0.07441420E+02 0.15851654E-01-0.02219895E-04 3
-0.04928037E-07 0.01984559E-10 0.06162266E+06-0.09047891E+02 4
HCCCHCCH 101993H 3C 5 G 0300.00 4000.00 1400.00 1
0.14122474E+02 0.04593411E-01-0.03738175E-05-0.02574328E-08 0.04539160E-12 2
0.06249257E+06-0.04722335E+03 0.06854796E+02 0.01699404E+00-0.02582284E-04 3
-0.05488764E-07 0.02281480E-10 0.06515364E+06-0.07133854E+02 4
C5H5 101993H 5C 5 G 0300.00 4000.00 1400.00 1
0.15310937E+02 0.07473806E-01-0.05837457E-05-0.04386651E-08 0.07696839E-12 2
0.02525889E+06-0.05951593E+03 0.10073161E+01 0.03189880E+00-0.04748189E-04 3
-0.11023903E-07 0.04584680E-10 0.03047390E+06 0.01934167E+03 4
H2C4O 120189H 2C 4O 1 G 0300.00 4000.00 1000.00 1
0.10268878E+02 0.04896164E-01-0.04885080E-05-0.02708566E-08 0.05107013E-12 2
0.02346902E+06-0.02815985E+03 0.04810971E+02 0.13139988E-01 0.09865073E-05 3
-0.06120720E-07 0.16400028E-11 0.02545803E+06 0.02113424E+02 4
C6H2 121686C 6H 2 G 0300.00 5000.00 1000.00 1
0.12756519E+02 0.08034381E-01-0.02618215E-04 0.03725060E-08-0.01878850E-12 2
0.08075469E+06-0.04041262E+03 0.05751085E+02 0.02636719E+00-0.11667596E-04 3
-0.10714498E-07 0.08790297E-10 0.08262012E+06-0.04335532E+02 4
C6H4 111293H 4C 6 G 0300.00 4000.00 1000.00 1
0.14016253E+02 0.08242769E-01-0.08099663E-05-0.04654132E-08 0.08748122E-12 2
0.04410395E+06-0.05139376E+03 0.15200236E+01 0.02876611E+00 0.14177245E-05 3
-0.16505889E-07 0.05873156E-10 0.04844894E+06 0.01719033E+03 4
C6H5 82489C 6H 5 G 0300.00 4000.00 1000.00 1

0.15775887E+02 0.09651109E-01-0.09429416E-05-0.05469111E-08 0.10265216E-12 2
0.03302698E+06-0.06176280E+03 0.11435567E+00 0.03627324E+00 0.11582856E-05 3
-0.02196964E-06 0.08463556E-10 0.03836054E+06 0.02380117E+03 4
C6H6 20387C 6H 6 G 0300.00 5000.00 1000.00 1
0.12910740E+02 0.01723296E+00-0.05024210E-04 0.05893497E-08-0.01947521E-12 2
0.03664511E+05-0.05002699E+03-0.03138012E+02 0.04723103E+00-0.02962207E-04 3
-0.03262819E-06 0.01718691E-09 0.08890031E+05 0.03657573E+03 4
CH3CN 111596H 3C 2N 1 0G 300.000 3000.000 1000.00 0 1
0.23924046E+01 0.15618873E-01-0.79120497E-05 0.19372333E-08-0.18611956E-12 2
0.84999377E+04 0.11145236E+02 0.25197531E+01 0.13567523E-01-0.25764077E-05 3
-0.30893967E-08 0.14288692E-11 0.85533762E+04 0.10920868E+02 4
CH2CN 111596H 2C 2N 1 0G 300.000 3000.000 1000.00 0 1
0.46058146E+01 0.94485160E-02-0.47116329E-05 0.11389957E-08-0.10828942E-12 2
0.29171486E+05 0.10084415E+01 0.25296724E+01 0.18114138E-01-0.18960575E-04 3
0.11944583E-07-0.32544142E-11 0.29592293E+05 0.10993441E+02 4
HNO pg9601H 1N 1O 1 G 0300.00 5000.00 1000.00 1
0.03615144E+02 0.03212486E-01-0.01260337E-04 0.02267298E-08-0.01536236E-12 2
0.11769108E+05 0.04810264E+02 0.02784403E+02 0.06609646E-01-0.09300223E-04 3
0.09437980E-07-0.03753146E-10 0.12025976E+05 0.09035629E+02 4
HCN 110193H 1C 1N 1 G 0300.00 4000.00 1000.00 1
0.03426457E+02 0.03924190E-01-0.01601138E-04 0.03161966E-08-0.02432850E-12 2
0.01485552E+06 0.03607795E+02 0.02417787E+02 0.09031856E-01-0.01107727E-03 3
0.07980141E-07-0.02311141E-10 0.01501044E+06 0.08222891E+02 4
HNCO 110193H 1C 1N 1O 1G 0300.00 4000.00 1400.00 1
0.06545307E+02 0.01965760E-01-0.01562664E-05-0.01074318E-08 0.01874680E-12 2
-0.01664773E+06-0.01003880E+03 0.03858467E+02 0.06390342E-01-0.09016628E-05 3
-0.01898224E-07 0.07651380E-11-0.01562343E+06 0.04882493E+02 4
HOCN 110193H 1C 1N 1O 1G 0300.00 4000.00 1400.00 1
0.06022112E+02 0.01929530E-01-0.01455029E-05-0.01045811E-08 0.01794814E-12 2
-0.04040321E+05-0.05866433E+02 0.03789424E+02 0.05387981E-01-0.06518270E-05 3
-0.01420164E-07 0.05367969E-11-0.03135335E+05 0.06667052E+02 4
NCO 110193C 1N 1O 1 G 0300.00 4000.00 1400.00 1
0.06072346E+02 0.09227829E-02-0.09845574E-06-0.04764123E-09 0.09090445E-13 2
0.01359820E+06-0.08507293E+02 0.03359593E+02 0.05393239E-01-0.08144585E-05 3
-0.01912868E-07 0.07836794E-11 0.01462809E+06 0.06549694E+02 4
NO* dummy O 1N 1 0 G 0300.00 4000.00 1400.00 1

0.06072346E+02 0.09227829E-02-0.09845574E-06-0.04764123E-09 0.09090445E-13 2
0.01359820E+06-0.08507293E+02 0.03359593E+02 0.05393239E-01-0.08144585E-05 3
-0.01912868E-07 0.07836794E-11 0.01462809E+06 0.06549694E+02 4
!
!VALORES TERMODINAMICOS DEL MECANISMO DE ETANOL
!
C2H5OH BUR 8/88C 2H 6O 1 G 200.000 6000.000 1000.00 1
0.65624365E+01 0.15204222E-01-0.53896795E-05 0.86225011E-09-0.51289787E-13 2
-0.31525621E+05-0.94730202E+01 0.48586957E+01-0.37401726E-02 0.69555378E-04 3
-0.88654796E-07 0.35168835E-10-0.29996132E+05 0.48018545E+01-0.28257829E+05 4
C2H4OH MARI99C 2H 5O 1 0G 200.000 4000.000 1000.00 1
0.74564000E+00 0.02930200E-00-2.18510000E-05 8.85746000E-09-1.38170000E-12 2
-0.54736000E+04 0.22235000E+02 0.74564000E+00 0.02930200E-00-2.18510000E-05 3
8.85746000E-09-1.38170000E-12-0.54736000E+04 0.22235000E+02 4
C2H5CHO BURC92C 3H 6O 1 0G 273.150 5000.000 1000.00 1
0.33137982E+01 0.26619606E-01-0.10475596E-04 0.18815334E-08-0.12761310E-12 2
-0.25459603E+05 0.96608447E+01 0.76044596E+01-0.86403564E-02 0.73930097E-04 3
-0.79687398E-07 0.28004927E-10-0.25489789E+05-0.67643691E+01-0.23097645E+05 4
C2H5CO BURC92C 3H 5O 1 0G 298.150 5000.000 1000.00 1
0.30445698E+01 0.23236429E-01-0.86317936E-05 0.14799550E-08-0.96860829E-13 2
-0.61787211E+04 0.13122302E+02 0.67368294E+01-0.26945299E-02 0.49927017E-04 3
-0.50025808E-07 0.15011503E-10-0.65703366E+04-0.23398732E+01-0.43321855E+04 4
HCOO BOZELLI C 1H 1O 2 0G 300.000 5000.000 1453.000 01
6.40920688E+00 3.28189026E-03-1.18710674E-06 1.91323635E-10-1.13932748E-14 2
-2.20542060E+04-1.04575060E+01 1.52482282E+00 1.26249843E-02-6.61406757E-06 3
7.72750880E-10 2.09088864E-13-2.02040511E+04 1.64205770E+01 4
CH2SH BUR 8/88C 1H 3S 1 G 300.000 5000.000 1000.00 1
0.02560000E+02 0.19780000E-01-0.26780000E-04 2.17600000E-08-0.73490000E-13 2
0.17539000E+05 1.17400000E+01 0.02560000E+02 0.19780000E-01-0.26780000E-04 3
2.17600000E-08-0.73490000E-13 0.17539000E+05 1.17400000E+01 4
!
!
!VALORES TERMODINAMICOS DEL MECANISMO DEL S
!
!SO2 121286S 1O 2 G 0300.00 5000.00 1000.00 1
! 0.05254498E+02 0.01978545E-01-0.08204226E-05 0.01576383E-08-0.01120451E-12 2

!-0.03756886E+06-0.01146056E+02 0.02911439E+02 0.08103022E-01-0.06906710E-04 3
! 0.03329016E-07-0.08777121E-11-0.03687882E+06 0.01111740E+03 4
SO2 tpis89S 1.O 2. 0. 0.G 200.000 6000.000 1000. 1 ! -70.95 59.29
5.38423482E+00 1.67930560E-03-6.32062944E-07 1.08465348E-10-6.66890336E-15 2
-3.76067022E+04-1.83130517E+00 3.67480752E+00 2.28302107E-03 8.46893049E-06 3
-1.36562039E-08 5.76271873E-12-3.69455073E+04 7.96866430E+00-3.56978343E+04 4
! GBR1509
SO2* pg00 S 1O 2 G 0300.00 5000.00 1000.00 1
0.05254498E+02 0.01978545E-01-0.08204226E-05 0.01576383E-08-0.01120451E-12 2
-0.08300578E+04-0.01146056E+02 0.02911439E+02 0.08103022E-01-0.06906710E-04 3
0.03329016E-07-0.08777121E-11-0.01400178E+04 0.01111740E+03 4
!SO3 121286S 1O 3 G 0300.00 5000.00 1000.00 1
! 0.07050668E+02 0.03246560E-01-0.01408897E-04 0.02721535E-08-0.01942365E-12 2
!-0.05020668E+06-0.01106443E+03 0.02575283E+02 0.01515092E+00-0.01229872E-03 3
! 0.04240257E-07-0.05266812E-11-0.04894411E+06 0.01219512E+03 4
SO3 tpis89S 1.O 3. 0. 0.G 200.000 6000.000 1000. 1 ! -94.61 61.30
7.29677572E+00 2.73576437E-03-1.06377755E-06 1.80776031E-10-1.12077527E-14 2
-5.03096739E+04-1.24246659E+01 2.37461122E+00 1.59543297E-02-1.26322543E-05 3
2.81827264E-09 6.23371547E-13-4.89269231E+04 1.31043046E+01-4.76155540E+04 4
! GBR 1509
!SO 121286S 1O 1 G 0300.00 5000.00 1000.00 1
! 0.04021078E+02 0.02584856E-02 0.08948142E-06-0.03580145E-09 0.03228430E-13 2
!-0.07119620E+04 0.03452523E+02 0.03080401E+02 0.01803106E-01 0.06705022E-05 3
!-0.02069005E-07 0.08514657E-11-0.03986163E+04 0.08581028E+02 4
SO tpis89S 1.O 1. 0. 0.G 200.000 6000.000 1000. 1 ! 1.14 53.04
3.96894225E+00 3.77296831E-04 7.67102696E-09-1.37544433E-11 1.37139416E-15 2
-7.28571725E+02 3.73493087E+00 3.61859514E+00-2.32173768E-03 1.16462669E-05 3
-1.42092510E-08 5.60765370E-12-4.80621641E+02 6.36504115E+00 5.72529951E+02 4
! GBR 1509
SO(S) est09 S 1O 1 G 0300.00 5000.00 1000.00 1
0.04309940E+02-0.12150870E-02 2.75383045E-06-2.07106108E-09 5.55106589E-13 2
1.07760928E+04 0.01311757E+02 0.04309940E+02-0.12150870E-02 2.75383045E-06 3
-2.07106108E-09 5.55106589E-13 1.07760928E+04 0.01311757E+02 4
!HSO BOZ/PGH 1O 1S 1 0G 300.000 1500.000 1500.00 0 1
! 0.25807593E+01 0.79910902E-02-0.51535972E-05 0.74202801E-09 0.24445691E-12 2
!-0.37976678E+04 0.12226703E+02 0.25807593E+01 0.79910902E-02-0.51535972E-05 3

! 0.74202801E-09 0.24445691E-12-0.37976678E+04 0.12226703E+02 4

HSO T04/07H 1.S 1.O 1. 0.G 200.000 6000.000 1000. 1! -5.20 57.75

4.34724125E+00 2.53372236E-03-9.51430950E-07 1.58095446E-10-9.65294637E-15 2

-4.20893834E+03 3.15887502E+00 4.13565093E+00-3.69243127E-03 2.05169784E-05 3

-2.40530656E-08 9.17084270E-12-3.82371653E+03 5.88770120E+00-2.61672666E+03 4

! GBR 1509

!HOS BOZ/PGH 1O 1S 1 0G 300.000 1500.000 1500.00 0 1

! 0.26373673E+01 0.78911909E-02-0.81172603E-05 0.42483382E-08-0.85790116E-12 2

!-0.10726887E+04 0.11709682E+02 0.26373673E+01 0.78911909E-02-0.81172603E-05 3

! 0.42483382E-08-0.85790116E-12-0.10726887E+04 0.11709682E+02 4

HOS T04/07S 1.O 1.H 1. 0.G 200.000 6000.000 1000. 1 ! -1.60/57.31

4.37246017E+00 2.01398865E-03-6.50854476E-07 9.74413078E-11-5.52225169E-15 2

-2.28578181E+03 3.13657231E+00 3.69440567E+00 3.94327613E-04 1.10155102E-05 3

-1.63102588E-08 7.03352877E-12-1.99257018E+03 7.31635620E+00-8.05146665E+02 4

! GBR 1509

!HOSO Whe09 H 1O 2S 1 0G 300.000 1500.000 1500.00 0 1

! 0.16711716E+01 0.20882497E-01-0.26138676E-04 0.15816303E-07-0.36463525E-11 2

!-0.30422867E+05 0.19201855E+02 0.16711716E+01 0.20882497E-01-0.26138676E-04 3

! 0.15816303E-07-0.36463525E-11-0.30422867E+05 0.19201855E+02 4

HOSO DAGGLA03 GOUMAR99 H 1O 2S 1 0G 300.000 1500.000 1500.00 0 1 ! -57.70 67.47

0.16184697E+01 0.21164061E-01-0.26690482E-04 0.16272216E-07-0.37779005E-11 2

-0.30255641E+05 0.19477260E+02 0.16184697E+01 0.21164061E-01-0.26690482E-04 3

0.16272216E-07-0.37779005E-11-0.30255641E+05 0.19477260E+02 4

DAG/GLA03 GOU/MAR99

!HSO2 PG00 H 1O 2S 1 0G 300.000 1500.000 1500.00 0 1

! 0.15627374E+01 0.20691389E-01-0.23112073E-04 0.12670203E-07-0.27274176E-11 2

!-0.18214824E+05 0.17556820E+02 0.15627374E+01 0.20691389E-01-0.23112073E-04 3

! 0.12670203E-07-0.27274176E-11-0.18214824E+05 0.17556820E+02 4

HSO2 H 1O 2S 1 0G 300.00 2000.00 1000.00 1 ! -33.80 63.00

0.15627374E+01 0.20691389E-01-0.23112073E-04 0.12670203E-07-0.27274176E-11 2

-0.18214824E+05 0.17556820E+02 0.15627374E+01 0.20691389E-01-0.23112073E-04 3

0.12670203E-07-0.27274176E-11-0.18214824E+05 0.17556820E+02 4

ALZ/GLA01 GOU/MAR99

HOSO2 BOZ/R H 1O 3S 1 0G 300.000 1500.000 1500.00 0 1

0.24358474E+01 0.29991941E-01-0.40650871E-04 0.26047603E-07-0.62778546E-11 2

-0.48803251E+05 0.14364072E+02 0.24358474E+01 0.29991941E-01-0.40650871E-04 3
0.26047603E-07-0.62778546E-11-0.48803251E+05 0.14364072E+02 4
HOSOH BOZ/R H 2O 2S 1 0G 300.000 1500.000 1500.00 0 1
0.17225311E+01 0.25308046E-01-0.30864965E-04 0.18614741E-07-0.42872813E-11 2
-0.39295778E+05 0.16536892E+02 0.17225311E+01 0.25308046E-01-0.30864965E-04 3
0.18614741E-07-0.42872813E-11-0.39295778E+05 0.16536892E+02 4
HOSHO BOZ/R H 2O 2S 1 0G 300.000 1500.000 1500.00 0 1
0.11903822E+01 0.25644735E-01-0.26622842E-04 0.13479665E-07-0.26474629E-11 2
-0.33744886E+05 0.19095494E+02 0.11903822E+01 0.25644735E-01-0.26622842E-04 3
0.13479665E-07-0.26474629E-11-0.33744886E+05 0.19095494E+02 4
H2SO BOZ/R H 2O 1S 1 0G 300.000 1500.000 1500.00 0 1
0.19580519E+01 0.97265201E-02 0.68413170E-06-0.62343720E-08 0.24166577E-11 2
-0.66770889E+04 0.14783451E+02 0.19580519E+01 0.97265201E-02 0.68413170E-06 3
-0.62343720E-08 0.24166577E-11-0.66770889E+04 0.14783451E+02 4
!HSOH BOZ/R H 2O 1S 1 0G 300.000 1500.000 1500.00 0 1
! 0.25676441E+01 0.11380521E-01-0.58667324E-05-0.59470041E-09 0.87438329E-12 2
!-0.15571256E+05 0.11766399E+02 0.25676441E+01 0.11380521E-01-0.58667324E-05 3
!-0.59470041E-09 0.87438329E-12-0.15571256E+05 0.11766399E+02 4
HSOH H 2O 1S 1 0G 300.00 5000.00 1388.00 1 ! -28.52 58.66
0.25676441E+01 0.11380521E-01-0.58667324E-05-0.59470041E-09 0.87438329E-12 2
-0.15571256E+05 0.11766399E+02 0.25676441E+01 0.11380521E-01-0.58667324E-05 3
-0.59470041E-09 0.87438329E-12-0.15571256E+05 0.11766399E+02 4
! GLABOZ96
! Zhou - Leeds University
!S 121286S 1 G 0300.00 5000.00 1000.00 1
! 0.02902148E+02-0.05484546E-02 0.02764576E-05-0.05017115E-09 0.03150685E-13 2
! 0.03249423E+06 0.03838471E+02 0.03187329E+02-0.01595776E-01 0.02005531E-04 3
!-0.01507081E-07 0.04931282E-11 0.03242259E+06 0.02414441E+02 4
S J 9/82S 1. 0. 0. 0.G 200.000 6000.000 1000. 1 ! 66.19/40.11
2.87936498E+00-5.11050388E-04 2.53806719E-07-4.45455458E-11 2.66717362E-15 2
3.25013791E+04 3.98140647E+00 2.31725616E+00 4.78018342E-03-1.42082674E-05 3
1.56569538E-08-5.96588299E-12 3.25068976E+04 6.06242434E+00 3.33128471E+04 4
! GBR 1509
!SH 121286S 1H 1 G 0300.00 5000.00 1000.00 1
! 0.03053810E+02 0.01258884E-01-0.04249169E-05 0.06929591E-09-0.04281691E-13 2
! 0.01588225E+06 0.05973551E+02 0.04133327E+02-0.03787893E-02-0.02777854E-04 3

! 0.05370112E-07-0.02394006E-10 0.01555862E+06 0.01611535E+01 4
SH H 1S 1 0 0G 300.00 5000.00 1000.00 1 ! 34.23 46.73
3.05381000E+00 1.25888400E-03-4.24916900E-07 6.92959100E-11-4.28169100E-15 2
1.63513273E+04 5.97355100E+00 4.13332700E+00-3.78789300E-04-2.77785400E-06 3
5.37011200E-09-2.39400600E-12 1.60276973E+04 1.61153500E-01 4
Zhou: R.C. Shiell, X.K. Hu, Q.J. Hu, J.W. Hepburn, J. Phys. Chem. A 104 (2000) 4339–4342.
!H2S 121286H 2S 1 G 0300.00 5000.00 1000.00 1
! 0.02883147E+02 0.03827835E-01-0.01423398E-04 0.02497999E-08-0.01660273E-12 2
!-0.03480743E+05 0.07258162E+02 0.03071029E+02 0.05578261E-01-0.01030967E-03 3
! 0.01201953E-06-0.04838370E-10-0.03559826E+05 0.05935226E+02 4
H2S g 4/01H 2.S 1. 0. 0.G 200.000 6000.000 1000. 1 ! -4.92 49.18
2.97879430E+00 3.59760372E-03-1.22803151E-06 1.96833209E-10-1.16716162E-14 2
-3.51607638E+03 6.77921228E+00 4.12024455E+00-1.87907426E-03 8.21426650E-06 3
-7.06425730E-09 2.14234860E-12-3.68215173E+03 1.53174068E+00-2.47759639E+03 4
! GBR 1509
HSOO H 1O 2S 1 0G 300.00 5000.00 1000.00 1 ! 32.29 67.63
5.87948232E+00 4.58580173E-03-2.93621833E-06 1.10178148E-09-1.86219122E-13 2
1.41706015E+04-1.04622817E+00 3.04640372E+00 1.52114268E-02-1.84762707E-05 3
1.13862234E-08-2.72421836E-12 1.48073744E+04 1.28748017E+01 4
! Zhou: C. Zhou, K. Sendt, B.S. Haynes, J. Phys. Chem. A 113 (2009) 2975–2981.
!S2 121386S 2 G 0300.00 5000.00 1000.00 1
! 0.03904443E+02 0.06925733E-02-0.01233097E-05 0.08783809E-11 0.01374662E-13 2
! 0.01425693E+06 0.04956834E+02 0.03157673E+02 0.03099480E-01-0.01560746E-04 3
!-0.01357891E-07 0.01137444E-10 0.01439187E+06 0.08596062E+02 4
S2 tpis89S 2 0 0 0G 200.000 6000.000 1 ! 30.73 54.52
3.83249656E+00 8.88970881E-04-2.59080844E-07 3.63847115E-11-1.72606371E-15 2
1.42836134E+04 5.33000845E+00 2.87736627E+00 5.00301430E-03-6.04370732E-06 3
3.04738962E-09-3.87017618E-13 1.44342379E+04 9.79873919E+00 1.54669367E+04 4
! Zhou - Burcat
!HS2 burc94H 1S 2 0 0G 298.150 5000.000 2000.00 0 1
! 0.46552282E+01 0.29202531E-02-0.11010941E-05 0.18878697E-09-0.12318000E-13 2
! 0.16492900E+04 0.27987542E+01 0.40214995E+01 0.31961918E-02 0.21507270E-05 3
!-0.48650943E-08 0.21391804E-11 0.18942796E+04 0.64213003E+01 0.32457475E+04 4
HS2 H 1S 2 0G 300.00 2000.00 1000.00 1 ! 25.84 60.94
3.59075969E+00 4.98506901E-03-3.43045513E-06 1.19341826E-09-1.67403033E-13 2

1.17649789E+04 8.92475572E+00 2.81672268E+00 1.03969679E-02-1.55535096E-05 3
1.24197562E-08-3.90834999E-12 1.18156870E+04 1.21143632E+01 4
! Zhou - K. Sendt, B.S. Haynes, J. Phys. Chem. A 109 (2005) 8180–8186;
! K. Sendt, M. Jazbec, B.S. Haynes, Proc. Combust. Inst. 29 (2003) 2439–2446.
!H2S2 burc94H 2S 2 0 0G 298.150 5000.000 2000.00 0 1
! 0.65731735E+01 0.25619139E-02-0.69109315E-06 0.94286242E-10-0.52907210E-14 2
!-0.24677791E+03-0.72991840E+01 0.21128554E+01 0.21398828E-01-0.33893856E-04 3
! 0.28468801E-07-0.95576325E-11 0.67951055E+03 0.14205983E+02 0.20128667E+04 4
H2S2 H 2S 2 0G 300.00 2000.00 1000.00 1 ! 3.70 61.61
4.69311463E+00 6.01993785E-03-3.01832133E-06 7.52297526E-10-7.91533129E-14 2
1.72179592E+02 2.47728860E+00 2.07852476E+00 1.94742814E-02-2.93966240E-05 3
2.37295586E-08-7.52058161E-12 5.96292301E+02 1.44741864E+01 4
! Zhou - K. Sendt, B.S. Haynes, J. Phys. Chem. A 109 (2005) 8180–8186;
! K. Sendt, M. Jazbec, B.S. Haynes, Proc. Combust. Inst. 29 (2003) 2439–2446.
H2S2O2 H 2O 2S 2 G 300.00 5000.00 1000.00 1 ! -69.74 77.82
1.16213004E+01 3.43806006E-03-5.74448284E-07-3.13293096E-10 1.00662179E-13 2
-3.91048380E+04-2.90177401E+01 8.28112013E-01 4.74477762E-02-6.95648159E-05 3
4.87812487E-08-1.32222441E-11-3.69287907E+04 2.29903159E+01 4
! Zhou - K. Sendt, B.S. Haynes, J. Phys. Chem. A 109 (2005) 8180–8186;
! K. Sendt, M. Jazbec, B.S. Haynes, Proc. Combust. Inst. 29 (2003) 2439–2446.
H2S3O H 2O 1S 3 G 300.00 5000.00 1000.00 1 ! -17.86 80.56
1.18514105E+01 3.33850673E-03-6.86562800E-07-2.02600304E-10 7.47780445E-14 2
-1.28853402E+04-2.85026663E+01 3.67805059E+00 4.07191390E-02-6.67990246E-05 3
5.28547092E-08-1.60811288E-11-1.13979874E+04 9.98571106E+00 4
! Zhou - K. Sendt, B.S. Haynes, J. Phys. Chem. A 109 (2005) 8180–8186;
! K. Sendt, M. Jazbec, B.S. Haynes, Proc. Combust. Inst. 29 (2003) 2439–2446.
HSSSOH H 2O 1S 3 G 300.00 5000.00 1000.00 1 ! -28.04 82.12
1.10809208E+01 3.73387762E-03-2.44411342E-07-6.13453741E-10 1.64649581E-13 2
-1.78355780E+04-2.35331548E+01 2.93988478E+00 4.05695638E-02-6.59918573E-05 3
5.33283075E-08-1.67311298E-11-1.63029028E+04 1.49845285E+01 4
! Zhou - K. Sendt, B.S. Haynes, J. Phys. Chem. A 109 (2005) 8180–8186;
! K. Sendt, M. Jazbec, B.S. Haynes, Proc. Combust. Inst. 29 (2003) 2439–2446.
HSSO2 H 1O 2S 2 0G 300.00 2000.00 1000.00 1 ! -40.89 73.61
7.76282262E+00 7.02637234E-03-4.08428794E-06 1.12459784E-09-1.18489230E-13 2
-2.33271862E+04-9.48284274E+00 3.49856646E+00 2.50749289E-02-3.40614452E-05 3
2.40531480E-08-6.85626593E-12-2.24794312E+04 1.09552126E+01 4

! Zhou: PhD; L.A. Curtiss, K. Raghavachari, P.C. Redfern, V.
! Rassolov, J.A. Pople, J. Chem. Phys. 109 (1998) 7764–7776. ??
S4 tpis89S 4. 0. 0. 0.G 200.000 6000.000 1 ! 32.41 70.15
9.12781762E+00 9.13784446E-04-3.62719239E-07 6.24637076E-11-3.90794764E-15 2
1.33309374E+04-1.74976107E+01 1.62124479E+00 3.69694158E-02-6.92243749E-05 3
6.03240791E-08-1.99529262E-11 1.46879795E+04 1.76312033E+01 1.63127271E+04 4
! Zhou - Burcat
S5 tpis89S 5. 0. 0. 0.G 200.000 6000.000 1 ! 31.78 84.61
1.33325960E+01 2.09782536E-04-3.36431685E-07 8.53311588E-11-6.48294924E-15 2
1.13787913E+04-3.48611560E+01 3.27621083E+00 4.32967838E-02-8.47662885E-05 3
8.12574426E-08-2.97793536E-11 1.36965078E+04 1.41196663E+01 1.59953327E+04 4
! Zhou - Burcat
S6 tpis89S 6. 0. 0. 0.G 200.000 2500.000 1 ! 24.21 85.50
1.34043558E+01 3.42127317E-03-1.12816145E-06 1.46420087E-10-6.61286087E-15 2
8.10860569E+03-3.42545590E+01 2.69715935E+00 6.86818730E-02-1.43788282E-04 3
1.35427080E-07-4.71805554E-11 9.35349932E+03 1.24775267E+01 1.21853457E+04 4
! Zhou - Burcat
S7 tpis89S 7. 0. 0. 0.G 200.000 6000.000 1 ! 26.73 96.74
1.78534018E+01 1.21114205E-03-4.83082305E-07 8.34576672E-11-5.23294619E-15 2
7.80776842E+03-5.40618730E+01 2.91732736E+00 8.29649517E-02-1.73743030E-04 3
1.63959287E-07-5.74388498E-11 1.01380200E+04 1.37221660E+01 1.34572415E+04 4
! Zhou - Burcat
S8 tpis89S 8. 0. 0. 0.G 200.000 6000.000 1 ! 24.20 103.35
2.04307658E+01 5.18092908E-03-2.91895357E-06 5.97574588E-10-4.13758389E-14 2
5.11843364E+03-6.74373075E+01 4.13158109E+00 9.43298552E-02-2.05775943E-04 3
2.05747851E-07-7.51844045E-11 8.20318834E+03 7.83537207E+00 1.21807686E+04 4
! Zhou - Burcat
HS2O H 1O 1S 2 0G 300.00 2000.00 1000.00 1 ! -7.89 68.60
6.11859237E+00 5.59523243E-03-3.70626629E-06 1.22524738E-09-1.62789560E-13 2
-6.05886590E+03-1.97720682E+00 2.70484711E+00 2.32126968E-02-3.77894894E-05 3
3.04178811E-08-9.47692405E-12-5.52811032E+03 1.36259179E+01 4
! Zhou: PhD; L.A. Curtiss, K. Raghavachari, P.C. Redfern, V.
! Rassolov, J.A. Pople, J. Chem. Phys. 109 (1998) 7764–7776. ??
SSO2 O 2S 2 0G 300.00 2000.00 1000.00 1 ! -40.72 68.23
6.34280650E+00 6.05027505E-03-4.24571996E-06 1.40852829E-09-1.81318004E-13 2
-2.27684952E+04-3.78737520E+00 2.80168627E+00 1.99919280E-02-2.56401242E-05 3

1.65559742E-08-4.33620009E-12-2.20225598E+04 1.34189370E+01 4

! Zhou: PhD; L.A. Curtiss, K. Raghavachari, P.C. Redfern, V.

! Rassolov, J.A. Pople, J. Chem. Phys. 109 (1998) 7764–7776. ??

VDW1 H 2O 3S 1 G 300.00 5000.00 1000.00 1 ! -131.26 82.88

1.01262222E+01 3.57132793E-03-7.13009073E-09-5.82222901E-10 1.37375969E-13 2

-6.93881691E+04-1.74036743E+01 8.13179120E+00 8.32444914E-03-2.04192137E-06 3

-2.95153810E-09 1.78217150E-12-6.88287103E+04-6.98378761E+00 4

! H2O...SO2??:

! Zhou - K. Sendt, B.S. Haynes, J. Phys. Chem. A 109 (2005) 8180–8186;

! K. Sendt, M. Jazbec, B.S. Haynes, Proc. Combust. Inst. 29 (2003) 2439–2446.

OSSO O 2S 2 0G 300.00 2000.00 1000.00 1 ! -28.15 71.33

8.06932897E+00 2.78600929E-03-1.65788135E-06 4.55717434E-10-4.76687943E-14 2

-1.68597542E+04-1.12637659E+01 4.27684328E+00 1.71764292E-02-2.30032367E-05 3

1.50850596E-08-3.93335889E-12-1.60275576E+04 7.31095245E+00 4

! Zhou: PhD; L.A. Curtiss, K. Raghavachari, P.C. Redfern, V.

! Rassolov, J.A. Pople, J. Chem. Phys. 109 (1998) 7764–7776. ??

HSSO2 H 1O 2S 2 0G 300.00 2000.00 1000.00 1 ! -40.89 73.61

7.76282262E+00 7.02637234E-03-4.08428794E-06 1.12459784E-09-1.18489230E-13 2

-2.33271862E+04-9.48284274E+00 3.49856646E+00 2.50749289E-02-3.40614452E-05 3

2.40531480E-08-6.85626593E-12-2.24794312E+04 1.09552126E+01 4

! Zhou: PhD; L.A. Curtiss, K. Raghavachari, P.C. Redfern, V.

! Rassolov, J.A. Pople, J. Chem. Phys. 109 (1998) 7764–7776. ??

CH3NO BUR0302 T12/92C 1H 3N 1O 1G 200.00 6000.00 1000. 1 !BURCAT

0.50677397E+01 0.93871079E-02-0.33958317E-05 0.55076729E-09-0.33095301E-13 2
!H298 = 18.88 kcal/mol

0.71852464E+04-0.10709779E+01 0.52463494E+01-0.68175691E-02 0.46713959E-04 3
!S298 = 62.33 cal/mol/K

-0.53482743E-07 0.19916692E-10 0.79241319E+04 0.18687355E+01 0.95017371E+04 4 !

!

!Termodinamica nuevas especies S/C del sacadas del Burcat

!

COS g5/01C 1O 1S 1 0G 200.000 6000.000 1000. 1

5.37456093E+00 2.10411234E-03-7.76417533E-07 1.29745227E-10-7.92407725E-15 2

-1.89178351E+04-3.78473799E+00 1.77198991E+00 1.71486966E-02-2.73082140E-05 3

2.25553393E-08-7.34373482E-12-1.81328604E+04 1.36810097E+01-1.70424956E+04 4

CS2 g6/95C 1S 2 0 0G 200.000 6000.000 1000. 1

5.94905043E+00 1.69288150E-03-6.74333823E-07 1.16460519E-10-6.37363519E-15 2

1.20171256E+04-6.17036834E+00 2.17230835E+00 1.81263444E-02-3.08080090E-05 3
2.65150564E-08-8.92801520E-12 1.28063739E+04 1.19826948E+01 1.40357038E+04 4
CS g11/01C 1S 1 0 0G 200.000 6000.000 1000. 1
3.76959667E+00 7.30980640E-04-2.42920716E-07 2.88070971E-11-5.21956199E-17 2
3.22498707E+04 3.42022942E+00 3.73124786E+00-3.09803648E-03 1.24828276E-05 3
-1.41633372E-08 5.33370965E-12 3.24420956E+04 4.54855088E+00 3.35016830E+04 4
!
CS2OH dummy C 1H 1S 2O 1G 200.000 6000.000 1000. 1
5.94905043E+00 1.69288150E-03-6.74333823E-07 1.16460519E-10-6.37363519E-15 2
1.20171256E+04-6.17036834E+00 2.17230835E+00 1.81263444E-02-3.08080090E-05 3
2.65150564E-08-8.92801520E-12 1.28063739E+04 1.19826948E+01 1.40357038E+04 4
!
!COS2 pG/13 C 1O 1S 2 0G 200.000 6000.000 1000. 1
! 2.82500000E+00 2.02120000E-02-2.87800000E-05 1.86200000E-08-4.55300000E-12 2
! 1.54100000E+03 1.23600000E+01 2.82500000E+00 2.02120000E-02-2.87800000E-05 3
! 1.86200000E-08-4.55300000E-12 1.54100000E+03 1.23600000E+01 2.82500000E+00 4
!
!
CH3S IU3/03H 3C 1S 1 0G 200.000 6000.000 1000. 1
4.62809340E+00 7.50242892E-03-2.70631691E-06 4.37671177E-10-2.61526827E-14 2
1.30328459E+04 4.15868210E-02 2.56437070E+00 1.15796385E-02-4.50119584E-06 3
-5.02342418E-10 6.95252997E-13 1.37469790E+04 1.12504946E+01 1.49857923E+04 4
CH3SH T12/08C 1H 4S 1 0G 200.000 6000.000 1000. 1
4.50369870E+00 9.49866516E-03-3.34303841E-06 5.31967412E-10-3.15164389E-14 2
-4.46153406E+03 1.51156041E+00 3.78634471E+00 3.77026048E-03 1.96468694E-05 3
-2.65727342E-08 1.05290360E-11-3.87921543E+03 7.09507940E+00-2.45670376E+03 4
CH2S T11/08C 1H 2S 1 0G 200.000 6000.000 1000. 1
4.19801901E+00 5.14114256E-03-1.90400104E-06 3.33562196E-10-2.14380834E-14 2
1.21202116E+04 1.89538934E+00 3.98890625E+00-4.48093468E-03 3.23152583E-05 3
-3.98564197E-08 1.57804745E-11 1.26210562E+04 5.29851918E+00 1.38253747E+04 4
CH3CHO C 2H 4O 1 0G 200.000 6000.000 1000. 1
0.54041108E+01 0.11723059E-01-0.42263137E-05 0.68372451E-09-0.40984863E-13 2
-0.22593122E+05-0.34807917E+01 0.47294595E+01-0.31932858E-02 0.47534921E-04 3
-0.57458611E-07 0.21931112E-10-0.21572878E+05 0.41030159E+01-0.19987949E+05 4
CH3SO2 (ZHU2006) C 1H 3S 1O 2G 200.00 6000.00 1000. 1
0.28260000E+01 0.25630000E-01-0.21440000E-04 9.25300000E-09-0.15790000E-13 2

-0.28809000E+05 1.32900000E+01 0.28260000E+01 0.25630000E-01-0.21440000E-04 3
9.25300000E-09-0.15790000E-13-0.28809000E+05 1.32900000E+01 0.28260000E+01 4
CH3OSO C 1H 3S 1O 2G 200.000 6000.000 1000. 1
0.22960000E+01 0.25080000E-01-0.19940000E-04 8.14500000E-09-0.13260000E-13 2
-0.29221000E+05 1.92800000E+01 0.22960000E+01 0.25080000E-01-0.19940000E-04 3
8.14500000E-09-0.13260000E-13-0.29221000E+05 1.92800000E+01 0.22960000E+01 4
S2O tpis89S 2O 1 0 0G 200.000 6000.000 1000. 1
6.02401811E+00 1.00035579E-03-3.91923038E-07 6.69240060E-11-4.16275707E-15 2
-8.76531218E+03-2.93690271E+00 3.01869800E+00 1.08575811E-02-1.25419070E-05 3
6.57657832E-09-1.21573834E-12-8.02370855E+03 1.21738889E+01-6.73948254E+03 4
S3 S 3 G 200.000 6000.000 1000. 1
6.53302278E+00 4.89117086E-04-1.94120477E-07 3.34257105E-11-2.09106833E-15 2
1.53186530E+04-4.42378063E+00 2.67426151E+00 1.85725510E-02-3.39241252E-05 3
2.89518256E-08-9.41515882E-12 1.60320458E+04 1.37269667E+01 1.74079204E+04 4
CH3SCH3 C 2H 6S 1 0G 200.000 6000.000 1000. 1
6.46633952E+00 1.55897399E-02-5.49135107E-06 8.74455165E-10-5.18380108E-14 2
-7.34925770E+03-8.01940674E+00 5.28055093E+00 2.44703498E-03 4.47525603E-05 3
-5.76668384E-08 2.25740377E-11-6.22993885E+03 2.04977549E+00-4.25469691E+03 4
CH3CH2S C 2H 5S 1 0G 200.000 6000.000 1000. 1
6.06146203E+00 1.35096776E-02-4.79809612E-06 7.68421362E-10-4.57369490E-14 2
8.87147183E+03-5.21760983E+00 4.12080784E+00 6.77995700E-03 2.82399071E-05 3
-3.90230535E-08 1.53781094E-11 1.00274180E+04 7.80653672E+00 1.17370255E+04 4
CH2CH2SH C 2H 5S 1 0G 200.000 6000.000 1000. 1
6.32502214E+00 1.54070231E-02-5.45709466E-06 8.72281676E-10-5.18467041E-14 2
-8.26561807E+03-5.41769249E+00 5.40529602E+00 2.42610602E-03 4.12377755E-05 3
-5.18768956E-08 1.99031036E-11-7.22408589E+03 3.16335395E+00-5.23345332E+03 4
H2SO4 T 8/03H 2S 1O 4 0G 200.000 6000.000 1000. 1
1.13355392E+01 5.60829109E-03-1.94574192E-06 3.07136054E-10-1.81109544E-14 2
-9.21087435E+04-2.96094003E+01 4.53388173E+00 3.10347679E-02-4.10421795E-05 3
2.95752341E-08-8.81459071E-12-9.05459072E+04 3.93961412E+00-8.81230524E+04 4
CH3SO C 1H 3S 1O 1G 200.00 6000.00 1000. 1
2.49700000E+00 1.79300000E-02-1.24500000E-05 4.60900000E-09-7.05600000E-13 2
-1.09760000E+04 1.51000000E+01 2.49700000E+00 1.79300000E-02-1.24500000E-05 3
4.60900000E-09-7.05600000E-13-1.09760000E+04 1.51000000E+01 2.49700000E+00 4
HCS C 1H 1S 1 0G 200.000 6000.000 1000. 1
4.24664932E+00 2.35823084E-03-8.25468697E-07 1.30882236E-10-7.73500263E-15 2

```
 3.24994581E+04 3.27483332E+00 3.79164958E+00-4.94798913E-04 1.27553978E-05    3
-1.73549729E-08 7.20528315E-12 3.27828773E+04 6.50582055E+00 3.39731635E+04    4
!
!
!
!
END
!
!
REACTIONS
C2H3+O2=C2H2+HO2                1.34E6     1.61    -383.5 !
C2H4+O2=CH2HCO+OH                2.0E08     1.500   39000.000 !
C2H4+O2=C2H3+HO2                 4.2E13     0.00    57630.000 !
C2H2+O=HCCO+H                  1.4E07     2.000   1900.000 !
H+C2H2(+M)=C2H3(+M)            3.64E10    1.09    2640 ! Marinov 1996
xxxxxxxxxxxx
 LOW/2.254E40  -7.269 6577./
 TROE/0.5 675. 675./
  H2/2/ CO/2/ CO2/3/ H2O/5/
CH3+CH3(+M)=C2H6(+M)             2.1E16  -0.97   620. ! GRI2.11
 LOW /1.26E50 -9.67 6220/
 TROE/ 0.5325 151 1038 4970 /
  N2/1.43/ H2O/8.59/ H2/2/ CO/2/ CO2/3/
!#!  H2O/8.59/ H2/2/ CO/2/ CO2/3/
CH3+H(+M)=CH4(+M)              1.3E16     -0.63   383.  ! GRI-MECH2.11
 LOW/1.75E33  -4.76 2440.0/
 TROE/0.783  74.0 2941.0 6964.0/
 H2/2.86/ H2O/8.57/ CH4/2.86/  CO/2.14/ CO2/2.86/ C2H6/4.29/ N2/1.43/
CH4+O2=CH3+HO2                0.790E+14  0.000  56000.000 ! SKINNER ET AL 1972
!CH4+O2=CH3+HO2                4.000E+13  0.000  57000.000 !  CEC 1994
CH4+H=CH3+H2                  1.3E4    3.0   8040.  !cec 92
CH4+OH=CH3+H2O                 0.160E+07  2.100   2460.000 ! TULLY
CH4+O=CH3+OH                   1.02E9     1.5     8604. !TSANG
CH4+HO2=CH3+H2O2               0.180E+12  0.000  18700.000 ! NBS
CH3+HO2=CH3O+OH                8.0E12   0.0  0.0 ! Jam&PG rbn (Troe unpub.)
CH3+O=CH2O+H                   8.0E13   0.0   0.0    !GUTMAN
```

```
CH3+O2=CH3O+O                2.87E13      0.0   30481  !frenk JPC 1995
CH3+O2=CH2O+OH               1.85E12      0.0   20315 !Frenk jpc 1995
CH2OH+H=CH3+OH               0.100E+15  0.000      0.000 ! NBS 87
CH3O+H=CH3+OH                0.100E+15  0.000      0.000 ! EST JAM
CH3+OH=CH2+H2O               0.750E+07  2.000   5000.000 ! JAM
CH3+HCO=CH4+CO                1.2E14    0.0      0.0   ! NBS 86
CH3+H=CH2+H2                 0.900E+14  0.000  15100.000 ! PG
CH3+OH(+M)=CH3OH(+M)          6.3E13    0.0      0.0   !GRI2.11
  LOW/1.89E38  -6.3   3100/
  TROE/0.2105 83.5 5398 8370/
  N2/1.43/ H2O/8.58/ CO2/3/ CO/2/ H2/2/
!#!  H2O/8.58/ CO2/3/ CO/2/ H2/2/
!CH3OH+OH=CH2OH+H2O           5.30E4    2.53     960.    ! NBS
!cojo la del mecanismo etanol
!CH3OH+OH=CH3O+H2O            1.32E4    2.53     960.    !
!cojo la del mecanismo etanol
CH3OH+O=CH2OH+OH             3.88E5     2.5     3080.    ! NBS
!CH3OH+H=CH2OH+H2             1.7E7     2.1     4868     ! NBS
!cojo la del mecanismo etanol
!CH3OH+H=CH3O+H2              4.24E6     2.1     4868     ! NBS
!cojo la del mecanismo etanol
!CH3OH+HO2=CH2OH+H2O2          9.64E10     0.0   12578.    ! NBS
!cojo la del mecanismo etanol
CH2O+H(+M)=CH3O(+M)           5.4E11  0.454  2600. ! GRI2.11
  LOW/1.54E30  -4.8  5560 /
  TROE/ 0.758 94 1555 4200/
   N2/1.43/  H2O/8.58/ CO/2/ H2/2/ CO2/3/
!#!  H2O/8.58/ CO/2/ H2/2/ CO2/3/
H+CH2O(+M)=CH2OH(+M)          5.4E11   0.454   3600. ! GRI2.11
    LOW/.91E32 -4.82 6530/
    TROE/0.7187 103 1291 4160/
   N2/1.43/ H2O/8.58/ CO/2/ CO2/3/ H2/2/
!#!  H2O/8.58/ CO/2/ CO2/3/ H2/2/
CH3O+H=CH2O+H2               0.200E+14  0.000      0.000 ! PG
!CH2OH+H=CH2O+H2              0.200E+14  0.000      0.000
!cojo la del mecanismo etanol
```

```
CH3O+OH=CH2O+H2O              0.100E+14  0.000      0.000 ! PG
CH2OH+OH=CH2O+H2O             0.100E+14  0.000      0.000
CH3O+O=CH2O+OH                0.100E+14  0.000      0.000 ! PG
!CH2OH+O=CH2O+OH              0.100E+14  0.000      0.000
!cojo la del mecanismo etanol
CH3O+O2=CH2O+HO2              0.630E+11  0.000   2600.000 ! PG
CH2OH+O2=CH2O+HO2             1.57E15    -1.0       0.0   ! EURCOM 1992
 DUP
CH2OH+O2=CH2O+HO2             7.23E13    0.0      3577.  !
 DUP
CH2+H=CH+H2                   0.100E+19 -1.560      0.000 ! THORNE,ET AL
CH2+OH=CH+H2O                 0.113E+08  2.000   3000.000 ! JAM
CH2+OH=CH2O+H                 0.250E+14  0.000      0.000 ! PG
CH+O2=HCO+O                   0.330E+14  0.000      0.000 ! PG
CH+O=CO+H                     0.570E+14  0.000      0.000 ! PG
CH+OH=HCO+H                   0.300E+14  0.000      0.000 ! PG
CH+CO2=HCO+CO                 0.340E+13  0.000    690.000 ! PG
CH+H2O=CH2O+H                 5.72E12    0.0     -751.0    !LIN
CH+CH2O=CH2CO+H               0.946E+14  0.000   -515.000 ! THORNE
CH+C2H2=C3H2+H                0.100E+15  0.000      0.000 ! THORNE
CH+CH2=C2H2+H                 0.400E+14  0.000      0.000 ! PG
CH+CH3=C2H3+H                 0.300E+14  0.000      0.000 ! PG
CH+CH4=C2H4+H                 0.600E+14  0.000      0.000 ! PG
CH2+CO2=CH2O+CO               0.110E+12  0.000   1000.000 ! PG
CH2+O=CO+H+H                  0.500E+14  0.000      0.000 ! JAM 2/87
CH2+O=CO+H2                   0.300E+14  0.000      0.000 ! JAM 2/87
CH2+O2=CO+H2O     2.20E22   -3.3  2867. ! DOMBROWSKY(HGGW) BER.BUN.1992
CH2+O2=CO2+H+H    3.29E21   -3.3  2867.  !
CH2+O2=CH2O+O     3.29E21   -3.3  2867. !
CH2+O2=CO2+H2     2.63E21   -3.3  2867. !
CH2+O2=CO+OH+H    1.64E21   -3.3  2867. !
CH2+CH2=C2H2+H+H              0.400E+14  0.000      0.000 ! BRAUN,ET AL
CH2+HCCO=C2H3+CO              0.300E+14  0.000      0.000 ! JAM,1/11/82
CH2+C2H2=H2CCCH+H             0.120E+14  0.000   6600.000 ! BOHLAND ET AL,21S
CH2+CH4=CH3+CH3               4.3E12     0.0     10030. ! PG 86
CH2O+OH=HCO+H2O               0.343E+10  1.180   -447.000 ! NBS
```

```
CH2O+H=HCO+H2                1.3E8     1.62    2166. ! CEC 94
CH2O+M=HCO+H+M               0.331E+17  0.000  81000.000 ! DEAN,C 1980
    H2/2/ CO/2/ CO2/3/  H2O/5/
CH2O+O=HCO+OH                0.180E+14  0.000   3080.000 ! NBS
CH2O+CH3=HCO+CH4              7.8E-8      6.1     1967. ! CEC 1994
CH2O+HO2=HCO+H2O2             3.0E12    0.0     13000.  !CEC 1994
CH2O+O2=HCO+HO2               6.0E13     0.0      40660 ! CEC 94
HCO+OH=H2O+CO                 0.100E+15  0.000      0.000 ! TEMPS
HCO+M=H+CO+M                  3.48E17   -1.0    17010.0  ! Timoen et al 1987
   CO/1.87/   H2/1.87/  CH4/2.81/ CO2/3./ H2O/5./
HCO+H=CO+H2                  0.119E+14  0.250    0.000 ! HARD.. 21ST, JAM
HCO+O=CO+OH                   0.300E+14  0.000      0.000 ! PG
HCO+O=CO2+H                  0.300E+14  0.000      0.000 ! PG
HCO+O2=HO2+CO                 7.58E12    0.0    406. !TIMONEN(GUTMAN)JPC 1988
CO+O+M=CO2+M                  0.617E+15  0.000   3000.000 ! NBS
    H2/2/ CO/2/ CO2/3/  H2O/16/
CO+OH=CO2+H                  1.51E7     1.3     -758   ! BAULCH&DRYSDALE
CO+O2=CO2+O                   2.53E12    0.0     47688. !TSANG,BAULCH
!HO2+CO=CO2+OH                0.580E+14  0.000  22934.000 ! ATRI ET AL ,C 197
HO2+CO=CO2+OH                 1.570E5    2.18    17900.000 ! YOU/WANG,2007
C2H4+H=C2H3+H2                5.42E14    0.0     14902    ! EURCOM 1992
C2H4+O=CH3+HCO                8.1E6      1.88     180. ! CEC 94
C2H4+O=CH2CO+H2               6.8E5      1.88     180  !
C2H4+OH=C2H3+H2O              0.202E+14  0.000   5955.000 ! TULLY 1987
C2H4+CH3=C2H3+CH4             5.0E11     0.0     15000 !JAM&Pg rbn (Zhang 1990)
CH2+CH3=C2H4+H                0.400E+14  0.000      0.000 ! JAM
C2H4+H(+M)=C2H5(+M)           1.081E12   0.454    1822.  ! MARINOV
  LOW/1.112E34  -5.0   4448.0/
 TROE/0.5 95.0  95.0    200./
   H2/2/ CO/2/ CO2/3/ H2O/5/
C2H3+H=C2H2+H2                0.400E+14  0.000      0.000 ! HOYERMANN
C2H3+O=CH2CO+H                0.300E+14  0.000      0.000 ! HOYERMANN 21ST
C2H3+O2=CH2O+HCO              4.58E16    -1.39   1015 !  Mebel,et al.
C2H3+OH=C2H2+H2O               2.0E13    0.0     0.0   ! JAM
C2H3+C2H=C2H2+C2H2            0.300E+14  0.000      0.000 ! MMSK
C2H3+CH3=C2H2+CH4              2.1E13   0.0     0.0 ! NBS, Fahr 91(rbn PG)
```

```
C2H3+CH2O=C2H4+HCO              5.4E3   2.81   5860 ! NBS 86
C2H3+HCO=C2H4+CO               9.0E13    0.0    0.0  ! NBS 86
C2H3+C2H3=H2CCCH+CH3            1.8E13  0.0   0.0 ! CJP 091699 adj
C2H3+C2H3=C2H4+C2H2             6.3E13  0.0   0.0 ! CJP 091699 adj
C2H3+CH=CH2+C2H2               0.500E+14  0.000      0.000 ! JAM
OH+C2H2=C2H+H2O                 3.37E7    2.0   14000. ! MILLER
OH+C2H2=HCCOH+H                 5.04E5    2.3   13500. ! MILLER
OH+C2H2=CH2CO+H                 2.18E-4   4.5   -1000. ! MILLER
OH+C2H2=CH3+CO                  4.83E-4   4.0   -2000. ! MILLER
!OH+C2H2(+M)=C2H2OH(+M)          1.52E8  1.7    1000. ! MILLER&MELIUS!
!
!   LOW/1.81E23  -2.0   0.0 /                ! Atkinson(cited in CEC 92)/PG
!  H2/2/  CO/2/   CO2/3/   H2O/5/
!          HO2+C2H2=CH2HCO+O               1.0E12   0.0   10000 ! JAM           xxxxxx
!          HO2+C2H2=CH2O+HCO               1.0E12   0.00   10000 ! JAM           xxxxxx
! last 2 k's crudely based on calculations of Mebel,Morokuma,Lin,et al(C2H3+O2)
HCCOH+H=HCCO +H2                3.0E7   2.0     1000. ! JAM
HCCOH+OH=HCCO+H2O               1.0E7   2.0     1000. !JAM
HCCOH+O=HCCO+OH                 2.0E7  3.0     1900. !JAM(O+C2H2)
C2H2+O=C2H+OH                  0.316E+16 -0.600  15000.000 !MMSK
C2H2OH+O=OCHCHO+H               5.0E13   0.0     0.0  ! JAM 1996
C2H2OH+O2=OCHCHO+OH             1.0E12   0.0    5000. ! JAM 1996
OCHCHO+M=HCO+HCO+M              1.0E17    0.0  25000. ! JAM
xxxxxxxxxx
OCHCHO+H=CH2O+HCO               3.0E13    0.0   0.0  !JAM
CH2CO+O=CO2+CH2                0.175E+13  0.000   1350.000 ! SEE WAGNER,TEMPS ET
CH2CO+H=CH3+CO                 5.93E6   2.0    1300. ! CEC 92 / JAM
CH2CO+H=HCCO+H2                 3.0E7     2.0  10000.000 ! JAM 1996
CH2CO+O=HCCO+OH                 2.0E7  2.0   10000.000 !
CH2CO+OH=HCCO+H2O               1.0E7   2.0   3000.000 !
CH2CO+OH=CH2OH+CO               7.2E12   0.0   0.0 ! Temps,HggW,et al 1992
CH2CO+OH=CH3+CO2                3.0E12  0.0   0.0 ! Grussdorf 94 (PG rbn)
CH2+CO(+M)=CH2CO(+M)            8.1E11    0.5  4510. ! GRI2.11
  LOW/ 1.88E33 -5.11 7095./
  TROE/ 0.5907 275 1226 5185/
     H2/2/ CO/2/ CO2/3/  H2O/8.58/  N2/1.43/
```

```
C2H+O2=CO+CO+H          2.52E13    0.0    0.0   ! GLASS&CURL(STEPHENS)JPC1987
C2H+CH4=CH3+C2H2             7.23E12   0.0    976 ! Leone JPC 1996
CH+CO(+M)=HCCO(+M)           5.0E13   0.0    0.0  ! GRI2.11
 LOW/ 1.88E28  -3.74 1936 /
 TROE/ 0.5757 237  1652 5069 /
  N2/1.43/ H2O/8.58/ CO/2/ CO2/3/ H2/2/
!#!  H2O/8.58/ CO/2/ CO2/3/ H2/2/
HCCO+C2H2=H2CCCH+CO          1.0E11   0.0     3000. ! JAM
H+HCCO=CH2(S)+CO             0.100E+15  0.000      0.000 ! PEETERS 1985
O+HCCO=H+CO+CO               0.100E+15  0.000      0.000 ! PEETERS 1985
HCCO+O2=CO2+CO+H              1.4E7    1.7        1000. ! HGGW.Peeters,JAM
HCCO+O2=CO +CO +OH           2.88E7     1.7       1000. !
CH+HCCO=C2H2+CO              0.500E+14  0.000      0.000 ! JAM EST
HCCO+HCCO=C2H2+CO+CO          0.100E+14  0.000      0.000 ! MMSK
HCCO+OH=C2O+H2O               6.0E13     0.0    0.0    ! JAM
C2O+H=CH+CO                  1.0E13    0.0     0.0    ! JAM
C2O+O=CO+CO                  5.0E13    0.0      0.0   ! JAM
C2O+OH=CO+CO+H               2.0E13    0.0     0.0    ! JAM
C2O+O2=CO+CO+O               2.0E13  0.0   0.0  ! JAM
C2H+O=CH+CO                  0.500E+14  0.000      0.000 ! BROWNE
C2H+OH=HCCO+H                0.200E+14  0.000      0.000 ! JAM,12/22
C2H+OH=C2+H2O           4.0E7    2.0     8000.   !  JAM
C2+H2=C2H+H              4.0E5    2.4     1000.   !  JAM
C2+O2=CO+CO              5.0E13    0.0     0.0   ! JAM
C2+OH=C2O+H              5.0E13    0.0     0.0   ! JAM
!C2H2+O2=HCCO+OH              0.200E+09  1.500  30100.000 ! MMSK
C2H2+O2=HCO+HCO              0.200E+09  1.500  30100.000 ! MMSK/Benson 1996
C2H2+M=C2H+H+M               9.08E30    -3.7  127138. !TSANG&HAMP(TAN&GARD)
    H2/2/ CO/2/ CO2/3/  H2O/5/
C2H4+M=C2H2+H2+M             3.50E+16  0.000  71500. ! CEC 94
     N2/1.5/  H2O/10/
!#!     H2O/10/
C2H3+H(+M)=C2H4(+M)              6.1E12  0.27  280.000 !   GRI2.11
     LOW /0.98E30 -3.86 3320./
     TROE /0.7820 207.50 2663.00 6095.00/
  H2/2.85/ CO/2.1/ CO2/2.85/  H2O/7.14/ CH4/2.85/ C2H6/4.29/  N2/1.43/
```

```
!
!
!
!REACCIONES MECANISMO REBURNING
!
!
!
 ! *****************************************
 ! *   H2/O2 Subset                        *
 ! *****************************************
 !
O+OH=O2+H                  2.0E14 -0.40      0
O+H2=OH+H                  5.0E04  2.67   6290
OH+H2=H2O+H                  2.1E08  1.52   3450
2OH=O+H2O                  4.3E03  2.70  -2486
H+H+M=H2+M                   1.0E18 -1.00      0
   H2O/0/
H+H+H2O=H2+H2O               6.0E19 -1.25      0
H+O+M=OH+M                  6.2E16 -0.60      0
   H2O/5/
H+OH+M=H2O+M                 1.6E22 -2.00      0
   H2O/5/
O+O+M=O2+M                 1.9E13  0.00  -1788
   H2O/5/
!
!Pruebas reacción H+O2+M
!
!H+O2(+M)=HO2(+M)            1.48E+12  0.6    0.0
!    LOW /3.50E+16 -0.41 -1116.0/
!    TROE /0.5 100000 10/
! AR/0.0/ H2O/10.6/ H2/1.5/ CO2/2.4/
!H+O2(+AR)=HO2(+AR)          1.480E+12  0.6    0.0
!    LOW /7.00E+17 -0.8  0.0/
!    TROE /0.45 10 100000/
!H+O2(+M)=HO2(+M)             4.66E12  0.44      0 ! (Konnov/C&F 2008)
!     LOW /5.70E19 -1.4 0/
```

```
!    TROE/ 0.5 1.0E-30 1.0E30 /
!     H2O/0/  N2/0/  H2/1.5/   O2/0/  AR/0/
!H+O2(+AR)=HO2(+AR)            4.66E12  0.44      0 ! (Konnov/C&F 2008)
!     LOW /7.43E18 -1.2 0/
!    TROE/ 0.5 1.0E-30 1.0E30 /
!H+O2(+O2)=HO2(+O2)            4.66E12  0.44      0 ! (Konnov/C&F 2008)
!     LOW /5.69E18 -1.094 0/
!    TROE/ 0.5 1.0E-30 1.0E30 /
!H+O2(+H2O)=HO2(+H2O)          9.06E12  0.2       0 ! (Konnov/C&F 2008)
!     LOW /3.67E19 -1.0 0/
!    TROE/ 0.8 1.0E-30 1.0E30 /
!H+O2+M=HO2+M                  4.5E18  0.00      0 ! (Glarborg 1995 CST, basada en Atkinson et al.1992)
!     H2O/10/  N2/0/
!H+O2+M=HO2+M                  4.5E18  0.00      0 ! (Glarborg 1995 CST, basada en Atkinson et al.1992)
    !H2O/10/  N2/0/
!H+O2+M=HO2+M                  5.69E18 -1.09      0 ! (Michael 2002 J.Phis.Chem, 2002)
   ! H2O/16/  N2/0/
!!!!!!!
!!!!!!
!H+O2=HO2                     1E11    0.00      0 ! (Para sacar K para una Temp dada)
!!!!!!!!
!H+O2+M=HO2+M                  1E11 -1.00      0! (la que había)
   !H2O/16/  N2/0/
H+O2+M=HO2+M                  8E17   -0.80      0 ! (Dagaut 2009 E&F)
    H2O/20/  N2/0/  CO2/4/                              !
H+O2+N2 = HO2+N2              6.7E19 -1.42      0 ! *
H+HO2=H2+O2                   4.3E13  0.00   1411
H+HO2=OH+OH                   1.7E14  0.00    874
H+HO2=O+H2O                   3.0E13  0.0    1721
O+HO2=O2+OH                   3.3E13  0.0       0
OH+HO2=H2O+O2                 1.9E16 -1.0       0
HO2+HO2=H2O2+O2               4.2E14  0.0   11982
 DUP
HO2+HO2=H2O2+O2               1.3E11  0.0   -1629
 DUP
```

```
H2O2+M=OH+OH+M              1.3E17  0.0   45500
  H2O/5/
H2O2+H=HO2+H2              1.7E12  0.0    3755
H2O2+H=OH+H2O              1.0E13  0.0    3576
H2O2+O=OH+HO2              6.6E11  0.0    3974
H2O2+OH=H2O+HO2            7.8E12  0.0    1330
 DUP
H2O2+OH=H2O+HO2            5.8E14  0.0    9560 ! +
 DUP
!*****NUEVAS O3*****
O+O2+M=O3+M 1.88E+21 -2.8 0.0 !private communication
O+O3=O2+O2 4.80E+12 0.0 4090.0 !Atkinson et al. (2004)
H+O3=OH+O2 8.43E+13 0.0 950.0 !Atkinson et al. (2004)
OH+O3=HO2+O2 1.14E+12 0.0 2000.0 !Atkinson et al. (2004)
HO2+O3=OH+O2+O2 8.43E+09 0.0 1200.0 !Zahniser et al. (1980)
 ! ********************************************
 ! *   CH4/CH3/CH2/CH/C Subset              *
 ! ********************************************
 !
CH2(S)+H2=CH3+H            7.2E13  0.0      0 !
CH2(S)+H2O=CH3+OH          3.0E15 -0.6      0 !
CH2(S)+N2=CH2+N2           1.3E13  0.0    430 !
CH2(S)+AR=CH2+AR           1.5E13  0.0    884 !
CH2(S)+H=CH2+H             2.0E14  0.0      0 !
CH2(S)+H2O=CH2+H2O         3.0E13  0.0      0 !
CH2(S)+H=CH+H2             3.0E13  0.0      0 !
CH2(S)+O=CO+H+H            3.0E13  0.0      0 !
CH2(S)+OH=CH2O+H           3.0E13  0.0      0 !
CH2(S)+O2=CO+OH+H          7.0E13  0.0      0 !
CH2(S)+CO2=CH2O+CO         3.0E12  0.0      0 !
CH2(S)+CH4=CH3+CH3         4.3E13  0.0      0 !
CH2(S)+CH3=C2H4+H          2.0E13  0.0      0 !
CH2(S)+CH2CO=C2H4+CO       1.6E14  0.0      0 !
CH2(S)+C2H6=CH3+C2H5       1.2E+14 0.0      0 !
CH+H=C+H2                  1.5E14  0.0      0 !
CH+OH=C+H2O                4.0E7   2.0   3000 !
```

```
C+OH=CO+H                  5.0E13  0.00      0 !
C+O2=CO+O                  2.0E13  0.00      0 !
C+CH3=C2H2+H               5.0E13  0.00      0 !
C+CH2=C2H+H                5.0E13  0.00      0 !
 !
 ! ****************************************
 ! *   CH3OH/CH2OH/CH2O subset            *
 ! ****************************************
CH2OH+O2=CH2O+HO2           1.6E15 -1.0       0 !
 DUP
CH2OH+O2=CH2O+HO2           7.2E13  0.0    3577 !
 DUP
 !
 ! ****************************************
 ! *   C2H6/C2H5/C2H4/C2H3/C2H2/C2H/C2 subset *
 ! ****************************************
 !
C2H6+H=C2H5+H2              5.4E02  3.50   5210 !
C2H6+O=C2H5+OH              3.0E07  2.00   5115 !
C2H6+OH=C2H5+H2O            7.2E6   2.0     864 !
C2H6+HO2 = C2H5+H2O2        1.3E13  0.00  20460 !
C2H6+O2=C2H5+HO2            5.0E13  0.0   55000 !
C2H6+CH3=C2H5+CH4           5.5E-1  4.00   8300 !
C2H5+H(+M) = C2H6(+M)     5.2E17 -0.99   1580 !
  LOW  /  2.0E41 -7.08 6685/
  TROE/  0.8422 125 2219 6882 /
  N2/1.0/ H2O/6/  AR/0.7/
C2H5+H=CH3+CH3              4.9E12  0.35      0 !
C2H5+O = CH3+CH2O         4.2E13  0.00      0 !
C2H5+O = CH3HCO+H         5.3E13  0.00      0 !
C2H5+O = C2H4+OH          3.0E13  0.00      0 !
C2H5+OH = C2H4+H2O        2.4E13  0.00      0 !
C2H5+O2 = C2H4+HO2        1.0E10  0.00  -2190 !
C2H5+CH2O = C2H6+HCO      5.5E03  2.81   5860 !
C2H5+HCO = C2H6+CO        1.2E14  0.00      0 !
C2H5+CH3 = C2H4+CH4       1.1E12  0.00      0 !
```

```
C2H5+C2H5 = C2H6+C2H4      1.5E12  0.00      0 !
C2H4+O = CH2HCO+H           4.7E06  1.88    180 !
C2H4+HO2=CH3HCO+OH          2.2E12  0.0   17200 !
C2H3+O2 = CH2HCO+O          3.03E11 -0.29 10.73 !
H2+C2H=C2H2+H               4.1E05  2.39    864 !
C2H2+O=CH2+CO               6.1E6   2.00   1900 !
OH+C2H2(+M)=C2H2OH(+M)      1.5E8   1.7    1000 !
  LOW/1.81E23  -2.0   0.0 /                  !
 H2/2/  CO/2/   CO2/3/   H2O/5/
!HO2+C2H2=CH2HCO+O          1.0E12  0.0   10000 !
!HO2+C2H2=CH2O+HCO          1.0E12  0.0   10000 !
 !
 ! *****************************************************
 ! *   CH3HCO/CH2HCO/CH3CO/CH2CO/HCCOH/HCCO/C2O subset *
 ! *****************************************************
 !
CH3HCO = CH3+HCO            7.1E15  0.00  81280 !
CH3HCO+H = CH3CO+H2         4.1E09  1.16   2400 !
CH3HCO+O = CH3CO+OH         5.8E12  0.00   1800 !
CH3HCO+OH=CH3CO+H2O         2.3E10  0.73  -1110 !
CH3HCO+HO2 = CH3CO+H2O2     3.0E12  0.00  12000 !
CH3HCO+O2 = CH3CO+HO2       3.0E13  0.00  39000 !
CH3HCO+CH3=CH3CO+CH4        2.0E-6  5.6    2464 !
CH2HCO=CH3+CO               1.0E13  0.0   42000 !
!CH2HCO+M=CH3+CO+M          2.0E16  0.0   42000 !
!    H2/2/ CO/2/ CO2/3/  H2O/5/
CH2HCO+H=CH3+HCO            1.0E14  0.0       0 !
CH2HCO+H=CH3CO+H            3.0E13  0.0       0 !
CH2HCO+O=CH2O + HCO         5.0E13  0.0       0 !
CH2HCO+OH=CH2CO+H2O         2.0E13  0.0       0 !
CH2HCO+OH=CH2OH+HCO         1.0E13  0.0       0 !
CH2HCO+O2 = CH2O+CO+OH      2.2E11  0.0    1500 !
CH2HCO+CH3=C2H5CHO          5.0E13  0.0       0 !
CH2HCO+CH2=C2H4+HCO         5.0E13  0.0       0 !
CH2HCO+CH =C2H3+HCO         1.0E14  0.0       0 !
C2H5+HCO = C2H5CHO          1.8E13  0.0       0 !
```

```
C2H5CHO+H = C2H5CO+H2          8.0E13  0.0       0 !
C2H5CHO+O = C2H5CO+OH          7.8E12  0.0    1730 !
C2H5CHO+OH = C2H5CO+H2O        1.2E13  0.0       0 !
C2H5+CO = C2H5CO               1.5E11  0.0    4800 !
C2H2OH+H=CH2HCO+H              5.0E13  0.0       0 !
CH3CO(+M)=CH3+CO(+M)           2.8E13  0.0   17100 !
  LOW/2.1E15  0.0  14000./
  TROE/ 0.5 1.0E-30 1.0E30 /
     H2/2/ CO/2/ CO2/3/  H2O/5/
CH3CO+H = CH3+HCO              2.1E13  0.00      0 !
CH3CO+H = CH2CO+H2             1.2E13  0.00      0 !
CH3CO+O = CH3+CO2              1.5E14  0.00      0 !
CH3CO+O = CH2CO+OH             4.0E13  0.00      0 !
CH3CO+OH = CH2CO+H2O           1.2E13  0.00      0 !
  !
  ! *****************************************************
  ! *   H/N/O subset                                    *
  ! *   taken from [nh2no2] except where noted          *
  ! *****************************************************
  !
H+NO+M=HNO+M                   4.0E20 -1.75      0 ! a (GLA 1998, se ha quitado la eficacia
del tercer cuerpo para el N2 ya que se tiene en cuenta en la siguiente reacción)
     H2O/10/  O2/1.5/ H2/2/ CO2/3/ N2/0/
H+NO+N2=HNO+N2                 7.0E19 -1.50      0 !
NO+O+M=NO2+M                   7.5E19 -1.41      0 !
  N2/1.7/   O2/1.5/  H2O/10/
!!!!OH+NO+M=HONO+M             5.1E23 -2.51    -68 !
!!!!  H2O/5/
!HO2+NO=NO2+OH                 2.1E12  0.00   -479 !
HO2+NO=NO2+OH                        2.32E10          0.58     1433 ! (actualizada)
!NO2+OH=NO+HO2                       1.35E13          0.0     7613 !
!NO2+OH=NO+HO2                1.02E13          0.0       5962 !
NO2+H=NO+OH                    8.85E13  0.0       0 ! (actualizada)
NO2+O=NO+O2                   3.9E12  0.0    -238 !
!NO2+O=NO+O2                         1.050E14  -0.520   0 ! (actualizar?) Juanma JUnio
NO2+SO=SO2+NO                        8.43E12   0.0   0 ! (Prueba juanma junio)
```

```
NO2+SO2=SO3+NO              6.31E12          0.0  2.7E4 ! (Prueba juanma junio)
NO2+O(+M)=NO3(+M)           1.3E13  0.0      0 !
   LOW/1.0E28  -4.08 2470./
  N2/1.5/ O2/1.5/  H2O/18.6/
NO2+NO2=NO+NO+O2            1.6E12  0.0   26123 !
NO2+NO2=NO3+NO              9.6E09  0.73  20900 !
NO3+H=NO2+OH                6.0E13  0.0      0 !
NO3+O=NO2+O2                1.0E13  0.0      0 !
NO3+OH=NO2+HO2              1.4E13  0.0      0 !
NO3+HO2=NO2+O2+OH           1.5E12  0.0      0 !
NO3+NO2=NO+NO2+O2           5.0E10  0.0    2940 !
HNO+H=H2+NO                 4.5E11  0.72    655 !
HNO+O=NO+OH                 1.0E13  0.0      0 !
HNO+OH=NO+H2O               3.6E13  0.0      0 !
!!!!!!!HNO+O2=HO2+NO            1.0E13  0.0   25000 !
HNO+NO2=HONO+NO             6.0E11  0.0    2000 !
HNO+HNO=N2O+H2O             9.0E08  0.0    3100 !
HNO+NH2=NH3+NO              3.63E6  1.63  -1252 !
H2NO+M=HNO+H+M              2.5E15  0.0   50000 !
  H2O/5/  N2/2/
H2NO+H=HNO+H2               3.0E7   2.0    2000 !
H2NO+H=NH2+OH               5.0E13  0.0      0 !
H2NO+O=HNO+OH               3.0E7   2.0    2000 !
H2NO+O = NH2+O2             2.0E14   0       0 !
H2NO+OH=HNO+H2O             2.0E7   2.0    1000 !
H2NO+NO=HNO+HNO             2.0E04  2.0   13000 !
H2NO+NO2=HNO+HONO           6.0E11  0.0    2000 !
HONO+H=H2+NO2               1.2E13  0.0    7352 !
HONO+O=OH+NO2               1.2E13  0.0    5961 !
HONO+OH=H2O+NO2             4.0E12  0.0      0 !
NH3+M = NH2+H+M             2.2E16   0    93470 !
NH3+H=NH2+H2                6.4E05  2.39  10171 !
NH3+O=NH2+OH                9.4E06  1.94   6460 !
NH3+OH=NH2+H2O              2.0E06  2.04    566 !
NH3+HO2=NH2+H2O2            3.0E11  0.0   22000 !
NH2+H=NH+H2                 4.0E13  0.00   3650 !
```

```
NH2+O=HNO+H                6.6E14 -0.50      0 !
NH2+O=NH+OH                6.8E12  0.        0 !
NH2+OH=NH+H2O               4.0E06  2.     1000 !
NH2+HO2=H2NO+OH              5.0E13  0.0       0 !
NH2+HO2=NH3+O2              1.0E13  0.0       0 !
NH2+NO=NNH+OH               8.9E12 -0.35      0 !
NH2+NO=N2+H2O               1.3E16 -1.25      0 !
 DUP
NH2+NO=N2+H2O              -8.9E12 -0.35      0 !
 DUP
NH2+NO2=N2O+H2O             3.2E18 -2.2       0 !
NH2+NO2=H2NO+NO             3.5E12  0.        0 !
NH2+H2NO=NH3+HNO             3.0E12  0.0    1000 !
HONO+NH2=NO2+NH3             71.1    3.02  -4941 !
NH2+NH2=N2H2+H2             8.5E11  0.        0 !
NH2+NH=N2H2+H               5.0E13  0.        0 !
NH2+N=N2+H+H                7.2E13  0.        0 !
NH+H=N+H2                  3.0E13  0.        0
NH+O=NO+H                   9.2E13  0.        0
NH+OH=HNO+H                 2.0E13  0.        0
NH+OH=N+H2O                 5.0E11  0.50   2000
NH+O2=HNO+O                 4.6E05  2.     6500 !
NH+O2=NO+OH                 1.3E06  1.5     100 !
NH+NO=N2O+H                 2.9E14 -0.4       0 !
 DUP
NH+NO=N2O+H                -2.2E13 -0.23      0
 DUP
NH+NO=N2+OH                 2.2E13 -0.23      0
NH+NO2=N2O+OH                1.0E13  0.        0
NH+NH=N2+H+H                2.5E13  0.        0
NH+N=N2+H                  3.0E13  0.        0
N+OH=NO+H                   3.8E13  0.        0
N+O2=NO+O                  6.4E09  1.     6280
N+NO=N2+O                  3.3E12  0.30      0
N2H2+M=NNH+H+M               5.0E16  0.    50000
   H2O/15/ O2/2/ N2/2/ H2/2/
```

```
N2H2+H=NNH+H2                5.0E13  0.     1000
N2H2+O=NH2+NO                1.0E13  0.        0
N2H2+O=NNH+OH                2.0E13  0.     1000
N2H2+OH=NNH+H2O              1.0E13  0.     1000
N2H2+NO=N2O+NH2              3.0E12  0.        0
N2H2+NH2=NH3+NNH             1.0E13  0.     1000
N2H2+NH=NNH+NH2              1.0E13  0.     1000
NNH=N2+H                   1.0E7   0.        0 !
NNH+H=N2+H2                  1.0E14  0.        0
NNH+O=N2+OH                  8.0E13  0.        0
NNH+O=N2O+H                  1.0E14  0.        0
NNH+O=NH+NO                  5.0E13  0.        0
NNH+OH=N2+H2O                5.0E13  0.        0
NNH+O2=N2+HO2                2.0E14  0.        0 !
NNH+O2=N2+O2+H               5.0E13  0.        0 !
NNH+NO=N2+HNO                5.0E13  0.        0
NNH+NH2=N2+NH3               5.0E13  0.        0
NNH+NH=N2+NH2                5.0E13  0.        0
N2O+M=N2+O+M                 4.0E14  0.    56100
 N2/1.7/   O2/1.4/ H2O/12/ CO/1.5/  CO2/3/
N2O+H=N2+OH                  3.3E10  0.     4729
 DUP
N2O+H=N2+OH                  4.4E14  0.    19254
 DUP
N2O+O=NO+NO                  6.6E13  0.    26630 !
N2O+O=N2+O2                 1.0E14  0.    28000 !
N2O+OH=N2+HO2                1.3E-2  4.72  36561 !
N2O+OH=HNO+NO                1.2E-4  4.33  25081 !
!HNO+NO = N2O+OH              2.0E12  0.0   26000 !
N2O+NO=NO2+N2                5.3E05  2.23  46281 !
 !
 ! *****************************************************
 ! *  cyanide subset                          *
 ! *****************************************************
 !
CN+H2=HCN+H                  3.0E05  2.45   2237 !
```

HCN+O=NCO+H 1.4E04 2.64 4980
HCN+O=NH+CO 3.5E03 2.64 4980
HCN+O=CN+OH 2.7E09 1.58 29200
HCN+OH = CN+H2O 3.9E06 1.83 10300 !
HCN+OH=HOCN+H 5.9E04 2.40 12500
HCN+OH=HNCO+H 2.0E-3 4. 1000
HCN+OH=NH2+CO 7.8E-4 4. 4000
HCN+CN=C2N2+H 1.5E07 1.71 1530 !
CN+O=CO+N 7.7E13 0. 0 !
CN+OH=NCO+H 4.0E13 0. 0 !
CN+O2=NCO+O 7.5E12 0. -389 !
CN+CO2=NCO+CO 3.7E06 2.16 26884 !
CN+NO2=NCO+NO 5.3E15 -0.752 344 !
CN+NO2=CO+N2O 4.9E14 -0.752 344 !
CN+NO2=N2+CO2 3.7E14 -0.752 344 !
CN+HNO=HCN+NO 1.8E13 0.00 0
CN+HONO=HCN+NO2 1.2E13 0.00 0
CN+N2O=NCN+NO 3.9E03 2.6 3696 !
CN+HNCO=HCN+NCO 1.5E13 0. 0 !
CN+NCO=NCN+CO 1.8E13 0. 0 !
HNCO=NH+CO 1.1E16 0. 86000 !
HNCO+H=NH2+CO 2.2E07 1.7 3800 !
HNCO+O=HNO+CO 1.5E08 1.57 44012 !
HNCO+O=NH+CO2 9.8E7 1.41 8524 !
HNCO+O=NCO+OH 2.2E6 2.11 11425 !
HNCO+OH=NCO+H2O 6.4E05 2. 2563 !
HNCO+HO2=NCO+H2O2 3.0E11 0. 22000 !
HNCO+O2=HNO+CO2 1.0E12 0. 35000 !
HNCO+NH2=NH3+NCO 5.0E12 0. 6200 !
HNCO+NH=NH2+NCO 3.0E13 0. 23700 !
HOCN+H=NCO+H2 2.0E07 2. 2000 !
HOCN+O=NCO+OH 1.5E04 2.64 4000 !
HOCN+OH=NCO+H2O 6.4E05 2. 2563 !
HCNO+H=HCN+OH 1.0E14 0 12000 !
HCNO+O=HCO+NO 2.0E14 0. 0 !
HCNO+OH=CH2O+NO 4.0E13 0. 0 !

```
NCO+M=N+CO+M                3.1E16 -0.50  48000 !
NCO+H=NH+CO                 5.0E13  0.       0 !
NCO+O=NO+CO                 4.7E13  0.       0 !
NCO+OH=NO+HCO               5.0E12  0.    15000 !
NCO+O2=NO+CO2               2.0E12  0.    20000 !
NCO+H2=HNCO+H               7.6E02  3.     4000 !
NCO+HCO=HNCO+CO             3.6E13  0.       0 !
NCO+NO=N2O+CO               6.2E17 -1.73    763 !
NCO+NO=N2+CO2               7.8E17 -1.73    763 !
NCO+NO2=CO+NO+NO            2.5E11  0.     -707 !
NCO+NO2=CO2+N2O             3.0E12  0.     -707 !
NCO+HNO=HNCO+NO             1.8E13  0.       0 !
NCO+HONO=HNCO+NO2           3.6E12  0.       0 !
NCO+N=N2+CO                 2.0E13  0.       0 !
NCO+NCO=N2+CO+CO            1.8E13  0.       0 !
C2N2+O=NCO+CN               4.6E12  0.     8880 !
C2N2+OH=HOCN+CN             1.9E11  0.     2900 !
NCN+O=CN+NO                 1.0E14  0.       0 !
NCN+OH=HCN+NO               5.0E13  0.       0 !
NCN+H=HCN+N                 1.0E14  0.       0 !
NCN+O2=NO+NCO               1.0E13  0.       0 !
H+CH3CN=HCN+CH3             4.0E7   2.     2000 !
H+CH3CN=CH2CN+H2            3.0E7   2.     1000 !
O+CH3CN=NCO+CH3             1.5E4   2.64   4980 !
OH+CH3CN=CH2CN+H2O          2.0E7   2.     2000 !
CH2CN+O=CH2O+CN             1.0E14    0.   0.   !
CN+CH2OH=CH2CN+OH           5.0E13  0.       0 !
H2CN+M=HCN+H+M              3.0E14  0.    22000 !
 !
 ! *****************************************************
 ! *  subset for CxHyOz+nitrogen species reactions     *
 ! *****************************************************
 !
CO+NO2 = CO2+NO             9.0E13  0.    33779 !
CO+N2O=N2+CO2               3.2E11  0.    20237 !
CO2+N=NO+CO                 1.9E11  0.     3400 !
```

```
CH2O+NCO=HNCO+HCO            6.0E12  0.       0 !
CH2O+NO2 = HCO+HONO          8.0E02  2.77  13730 !
!!!!!HCO+NO=HNO+CO            7.2E12  0.       0 !
HCO+NO2 = CO+HONO           1.2E23 -3.29   2355 !
HCO+NO2 = H+CO2+NO           8.4E15 -0.75   1930 !
HCO+HNO=CH2O+NO             6.0E11  0.     2000 !
CH4+CN=CH3+HCN              6.2E04  2.64   -437 !
NCO+CH4 = CH3+HNCO           9.8E12  0.00   8120 !
CH3+NO=HCN+H2O              1.5E-1  3.523  3950 !
CH3+NO=H2CN+OH              1.5E-1  3.523  3950 !
CH3+N=H2CN+H                7.1E13  0.       0 !
CH3+CN=CH2CN+H              1.0E14  0.       0 !
CH3+HOCN=CH3CN+OH            5.0E12  0.     2000 !
CH2+NO=HCN+OH               2.2E12  0.     -378 !
CH2+NO=HCNO+H               1.3E12  0.     -378 !
CH2+NO2=CH2O+NO              5.9E13  0.       0 !
CH2+N=HCN+H                 5.0E13  0.       0 !
CH2+N2=HCN+NH                1.0E13  0.    74000 !
H2CN+N=N2+CH2               2.0E13  0.       0 !
CH2(S)+NO=HCN+OH             2.0E13  0.       0 !
CH2(S)+NO=CH2+NO             1.0E14  0.       0 !
CH2(S)+HCN=CH3+CN            5.0E13  0.       0 !
CH+NO2=HCO+NO                1.0E14  0.       0 !
CH+NO = HCN+O                4.8E13  0.00     0 !
CH+NO = HCO+N                3.4E13  0.00     0 !
CH+NO = NCO+H                1.9E13  0.00     0 !
CH+N=CN+H                   1.3E13  0.       0 !
CH+N2=HCN+N                  3.7E07  1.42  20723 !
CH+N2O=HCN+NO                1.9E13  0.     -511 !
C+NO=CN+O                   2.0E13  0.       0 !
C+NO=CO+N                   2.8E13  0.       0 !
C+N2=CN+N                   6.3E13  0.    46019 !
C+N2O=CN+NO                  5.1E12  0.       0 !
C2H6+CN=C2H5+HCN             1.2E05  2.77  -1788 !
C2H6+NCO = C2H5+HNCO         1.5E-9  6.89  -2910 !
C2H4+CN = C2H3+HCN           5.9E14 -0.24     0 !
```

```
C2H3+NO=C2H2+HNO              1.0E12  0.     1000 !
C2H3+N=HCN+CH2                2.0E13  0.        0 !
C2H2+NCO = HCCO+HCN           1.4E12  0.00   1815 !
!!!!!C2H+NO=CN+HCO            2.1E13  0.        0 !
CH2CO+CN=HCCO+HCN             2.0E13  0.        0 !
HCCO+NO=HCNO+CO               7.2E12  0.        0 !
HCCO+NO=HCN+CO2               1.6E13  0.        0 !
HCCO+NO2=HCNO+CO2             1.6E13  0.        0 !
HCCO+N=HCN+CO                 5.0E13  0.        0 !
!
!
! REACCIONES MECANISMO ETANOL
!
!
! *********************************************************
! *   C2H6OH subset                                       *
! *********************************************************
!
C2H5OH(+M) = CH2OH+CH3(+M)      5.9E23  -1.68   91163! MAR99 *
  LOW /2.9E85 -18.9 109914/
  TROE/ 0.5 200 890 4600 /
  H2O/5.0/ H2/2/ CO/2/ CO2/3/
C2H5OH(+M) = C2H5+OH(+M)        1.2E23  -1.54   96005! MAR99 *
  LOW /3.2E85 -18.8 114930/
  TROE/ 0.5 300 900 5000 /
  H2O/5.0/ H2/2/ CO/2/ CO2/3/
C2H5OH(+M) = C2H4+H2O(+M)       2.8E13   0.09   66136! MAR99 *
  LOW /2.6E83 -18.8 86452/
  TROE/ 0.7 350 800 3800 /
  H2O/5.0/
C2H5OH(+M) = CH3HCO+H2(+M)      7.2E11   0.09   91007! MAR99 *
  LOW /4.5E87 -19.4 115586/
  TROE/ 0.9 900 1100 3500 /
  H2O/5.0/
C2H5OH+OH = C2H4OH+H2O          1.7E11   0.27     600! MAR99  * overall
!C2H5OH+OH = CH3CHOH+H2O         2.6E06   2.00   -1373! DRY
```

```
!C2H5OH+OH = CH3CHOH+H2O        4.6E11   0.15       0! MAR99
C2H5OH+OH = CH3CH2O+H2O         7.5E11   0.30    1634! MAR99
C2H5OH+H = C2H4OH+H2           1.2E07   1.80    5098! MAR99  * fit
!C2H5OH+H = CH3CHOH+H2          2.6E07   1.65    2827! MAR99
C2H5OH+H = CH3CH2O+H2           1.5E07   1.60    3038! MAR99
C2H5OH+O = C2H4OH+OH           9.4E07   1.70    5459! MAR99  * overall
!C2H5OH+O = CH3CHOH+OH          1.9E07   1.85    1824! MAR99
C2H5OH+O = CH3CH2O+OH           1.6E07   2.00    4448! MAR99
C2H5OH+CH3 = C2H4OH+CH4         2.2E02   3.18    9622! MAR99  * fit
!C2H5OH+CH3 = CH3CHOH+CH4        7.3E02   2.99    7948! MAR99
C2H5OH+CH3 = CH3CH2O+CH4        1.4E02   2.99    7649! MAR99
C2H5OH+HO2 = C2H4OH+H2O2        1.2E04   2.55   15750! MAR99
C2H4OH+O2 = CH2O+CH2O+OH        6.0E10   0.00   24500! MAR99
!C2H5OH+HO2 = CH3CHOH+H2O2       8.2E03   2.55   10750! MAR99
C2H5OH+HO2 = CH3CH2O+H2O2       2.5E12   0.00   24000! MAR99
!
CH3CH2O+M = CH3HCO+H+M          1.2E35  -5.89   25274! MAR99
CH3CH2O+M = CH3+CH2O+M          1.3E38  -6.96   23800! MAR99
CH3CH2O+CO = C2H5+CO2           4.7E02   3.16    5380! MAR99  * anal to ch3o+co
CH3CH2O+O2 = CH3HCO+HO2         4.0E10   0.00    1100! HAR90
CH3CH2O+H = CH3+CH2OH           3.0E13   0.00       0! MAR99 *
CH3CH2O+H = C2H4+H2O            3.0E13   0.00       0! MAR99 *
CH3CH2O+OH = CH3HCO+H2O         1.0E13   0.00       0! MAR99 *
!
!CH3CHOH+O2 = CH3HCO+HO2         4.8E14   0.00    5017! MAR99 * anal to ch2oh+o2
! DUP
!CH3CHOH+O2 = CH3HCO+HO2         8.4E15  -1.20       0! MAR99 *
! DUP
!CH3CHOH+CH3 = C3H6+H2O          2.0E13   0.00       0! MAR99 *
!CH3CHOH+O = CH3HCO+OH           1.0E14   0.00       0! MAR99 *
!CH3CHOH+H = CH3+CH2OH           3.0E13   0.00       0! MAR99 *
!CH3CHOH+H = C2H4+H2O            3.0E13   0.00       0! MAR99 *
!CH3CHOH+HO2 = CH3HCO+OH+OH      4.0E13   0.00       0! MAR99 *
!CH3CHOH+OH = CH3HCO+H2O         5.0E12   0.00       0! MAR99 *
!CH3CHOH+M = CH3HCO+H+M          1.0E14   0.00   25000! MAR99 *
!!CH3HCO+OH = CH3CO+H2O          9.2E06   1.50    -962! TAY96 *
```

```
!!CH3HCO+OH = CH2HCO+H2O          1.7E05   2.40     815! TAY96 *
!
!*****************************************************
! ***   CH2O/HCO Subset
!*****************************************************
!
HCO+HCO=CO+CH2O                3.0E13  0.00      0 ! cec94 (300)
!
!*****************************************************
! *** CH3OH/CH2OH/CH2O Subset ***
!*****************************************************
!
!CH3OH(+M)=CH3+OH(+M)           1.9E16  0.0   91730 !TSA87+Held98
!  LOW/2.95E44  -7.35 95640/
!  TROE/0.414 279 5459/
!  N2/1.43/ H2O/8.58/
CH3OH(+M)=CH2OH+H(+M)          2.7E16 -0.08  98940 !TSA87+Held98
  LOW/2.34E40  -6.33 103100/
  TROE/0.773 693 5333/
CH3OH+H=CH2OH+H2               1.7E7   2.1    4868
CH3OH+H=CH3O+H2                4.2E6   2.1    4868
!CH3OH+H=CH2OH+H2              1.67E7   2.0    4520 ! LI/WILL96
!CH3OH+H=CH3O+H2               3.8E7   2.0    5860 ! LI/WILL96
!CH3OH+O=CH2OH+OH              3.9E5   2.5    3080
!CH3OH+OH=CH2OH+H2O            5.30E4  2.53    960
!CH3OH+OH=CH2OH+H2O            7.1E06  1.80   -600 ! BOT/COH91
!CH3OH+OH=CH3O+H2O             1.32E4  2.53    960
!CH3OH+OH=CH3O+H2O             1.0E06  2.10    500 ! BOT/COH91
CH3OH+OH=CH2OH+H2O             1.4E06  2.00   -3510 ! LI/WILL96
CH3OH+OH=CH3O+H2O              6.3E06  2.00    6300 ! LI/WILL96
!CH3OH+HO2=CH2OH+H2O2          9.6E10  0.0   12578 ! nbs87
!CH3OH+HO2=CH2OH+H2O2          3.0E12  0.0   12578 !
! A factor fit to ch3oh oxidation data
CH3OH+HO2=CH2OH+H2O2           1.0E12  0.0   10040 ! 81tsu
CH3OH+O2=CH2OH+HO2             2.1E13  0.00  44900 ! nbs87
CH3OH+CH3=CH2OH+CH4            3.2E01  3.17   7170 ! nbs87
```

```
CH3OH+CH3=CH3O+CH4            1.5E01  3.10   6940 ! nbs87
CH3O+HO2=CH2O+H2O2            3.0E11  0.00      0 ! nbs86
CH3O+CO=CH3+CO2               1.6E13  0.00  11800 ! nbs86
CH3O+CH3=CH2O+CH4             2.4E13  0.00      0 ! nbs86
CH3O+CH2O=CH3OH+HCO           1.0E11  0.00   3000 ! nbs86
CH3O+HCO=CH3OH+CO             9.0E13  0.00      0 ! nbs86
CH3O+CH3OH=CH3OH+CH2OH        3.0E11  0.00   4100 ! nbs86
CH3O+CH3O=CH3OH+CH2O          6.0E13  0.00      0 ! nbs86
!CH2OH+H=CH2O+H2              2.0E13  0.00      0
! PG98: removed
CH2OH+H=CH2O+H2               4.8E13  0.00      0 ! DOB/WAG94
!CH2OH+O=CH2O+OH              1.0E13  0.00      0
! PG98: removed
CH2OH+O=CH2O+OH               6.5E13  0.00   -700 ! SEE/GUT94
CH2OH+O2=CH2O+HO2             1.6E15 -1.0       0
 DUP
CH2OH+O2=CH2O+HO2             7.2E13  0.0    3577
 DUP
CH2OH+HO2=CH2O+H2O2           3.6E13  0.0       0 ! Grotheer ea 85
CH2OH+HCO=CH3OH+CO            1.2E14  0.0       0 ! nbs87
CH2OH+HCO=CH2O+CH2O           1.8E14  0.0       0 ! nbs87
CH2OH+CH2O=CH3OH+HCO          5.5E03  2.8    5860 ! nbs87
CH2OH+CH2OH=CH3OH+CH2O        5.0E12  0.0       0 ! nbs87
CH2OH+CH3O=CH3OH+CH2O         2.4E12  0.0       0 ! nbs87
!
!*****************************************************
! *** H/N/O Subset ***
!*****************************************************
!
HONO2+OH=NO3+H2O              1.0E10  0.0   -1240 ! LAM/BEN84
H2NO+O2=HNO+HO2               3.0E12  0.0   25000 ! a (JAM 6/98)
HONO+HONO=>NO+NO2+H2O         3.5E-1  3.64  12100 ! MEB/LIN98
H2NO+HO2=HNO+H2O2             2.9E04  2.69   1600 ! a (BOZ/DEA98)
HNOH+H=NH2+OH                 4.0E13  0.0       0 ! a (BOZ/DEA98)
HNOH+H=HNO+H2                 4.8E8   1.5     378 ! a (BOZ/DEA98)
HNOH+O=HNO+OH                 7.0E13  0.0       0 ! a (BOZ/DEA98)
```

```
DUP
HNOH+O=HNO+OH              3.3E08  1.5    -358 ! a (BOZ/DEA98)
DUP
HNOH+OH=HNO+H2O             2.4E6   2.0   -1192 ! a (BOZ/DEA98)
HNOH+NH2=NH3+HNO            1.8E6   1.94  -1152 ! a (BOZ/DEA98)
HNOH+HO2=HNO+H2O2           2.9E4   2.69  -1600 ! a (BOZ/DEA98)
HNOH+M=HNO+H+M              2.0E24 -2.84  58934 ! a (BOZ/DEA98)
 H2O/10/
HNOH+O2=HNO+HO2             3.0E12  0.0   25000 ! a (JAM 10/98)
HNOH+NO2=HONO+HNO            6.0E11  0.0    2000 ! a (JAM 98)
!
!*******************************************************
! ***  Subset for CxHyOz+nitrogen species reactions ***
!*******************************************************
!
CH3OH+NO2=CH2OH+HONO         3.7E11  0.0   21400 ! ANA/HAN88
CH2OH+NO=CH2O+HNO            1.3E12  0.0       0 ! NES/STI89/p (300)
CH2OH+NO2=CH2O+HONO           5.0E12  0.0       0 ! NES/STI89/p (300)
CH2OH+HNO=CH3OH+NO           3.0E12  0.0       0 ! PG98 est.
CH3O+NO=CH2O+HNO             1.3E14 -0.7       0 ! ATK92
CH3O+NO2=CH2O+HONO           6.0E12  0.0    2285 ! MCC/KAU85
CH3O+HNO=CH3OH+NO            3.2E13  0.0       0 ! HE/LIN88
CH3+NO(+M)=CH3NO(+M)         9.0E12  0.0     119 ! DAV/PIL91
LOW/3.2E23  -1.87 0/
 H2O/10/ N2/1.5/
CH3+NO2=CH3O+NO              4.0E13 -0.20      0 ! PG98
CH3+HONO=CH4+NO2             1.0E12  0.0       0 ! PG98 est.
! analogy NH2+HONO
CH3NO=HCN+H2O                3.0E13  0.0   50000 ! LIF93 est.
!
!NUEVAS REACCIONES AÑADIDAS
!
CH3+O2(+M)=CH3O2 (+M)          7.8E8   1.2       0
LOW/5.8E25  -3.3  0/
CH3O2+O=CH3O+O2              2.59E13   0       0
CH3O2+H=CH3O+OH               9.64E13   0       0
```

CH3O2+NO=CH3O+NO2 3.10E12 0 -358

CH3O2+CH3=CH3O+CH3O 3.24E13 0 0

!

!

!

C2H+NO=CN+HCO 6.03E13 0. 570

!

!

!

!

!

!

!!!!**********Mecanismo NO-NO2 (articulo P. Glarborg et al., Combustion and Flame 132, 629-638, 2003

!

OH+NO+M=HONO+M 5.1E23 -2.51 -68 ! Cambio en las eficacias de tercer cuerpo antes: H2O/5/ Ahora en relación cn NO+O+M=NO2+M

N2/1.7/ O2/1.5/ H2O/10/

!!!!!!H2O/5/

!

!

NO2+HO2=HONO+O2 6.3E08 1.25 5000 !Hori et al., 1998

HNO+O2=NO+HO2 2.0E13 0.0 16000 !Dean et al., 2000

HCO+NO=CO+HNO 7.0E13 -0.40 0 ! Veyret et al., 1981

!

!!!HO2+NO+M=HONO2+M 2.23E12 -3.5 2200 !

!!!NO2+H+M=HONO+M 1.40E18 -1.5 900

!!!NO3+M=O2+NO+M 2.05E8 1 12122

!!! NO2/0/

!

!

!SON REACCIONES DEL ARTI DE GLARBORG 2003, ACTUALIZANDO VALORES, DEJO LOS ANTERIORES EXCEPTO LAS QUE NO ESTABAN ANTERIORMENTE

!!!CH2O+M=HCO+H+M 6.1E+15 0.000 76900 ! Kumaran, 1998 (Glarborg 2003)

!!! H2O/5/

!!!!H2/2/ CO/2/ CO2/3/ H2O/5/

```
        CH2O+M=CO+H2+M                    2.8E15  0         63800   !KUMARAN, 1998
(GLARBORG 2003)
                H2O/5/
        !!!H2/2/ CO/2/ CO2/3/  H2O/5/
        !!!CH2O+H=HCO+H2              5.7E07    1.90    2740 ! JUST 1981 (GLARBORG 2003)
        !!!!CH2O+HO2=HCO+H2O2           4.1E04    2.5     10200  ! EITENEER 1998
(GLARBORG 2003)
        !!!!CH2O+O2=HCO+HO2             5.0E04    3.0     39000 ! GLARBORG 2003
        !!!HCO+M=H+CO+M                4.8E17   -1.20    17700.0  ! fRIEDRICHS, 2002
(GLARBORG 2003)
        !!!!       H2O/5./
        !!!!CO/1.87/   H2/1.87/  CH4/2.81/ CO2/3./ H2O/5./
        HCO+HO2=CO2+OH+H                  3.0E13  0         0         ! TSANG 1986
(GLARBORG 2003)
        !!!!!HCO+O2=HO2+CO              7.58E12    0.0    406. !DESAIN 2001 (GLARBORG
2003)
        !
        !!!!**************************************************************************
**********
        !!
        !!  sulphur subset: Alzueta 2001
        !!  a: ref: Glarborg, Kubel, Dam-Johansen, Chiang, *
        !!         Bozzelli, IJCK 28:773 (1996)
        !!
        !!**************************************************************************
********
        !!
        ! ******** H2S subset: taken from Song ea 2013. 24/Sept:JM   *********
        !
        ! ******* H2S reactions *******
        !
        H2S+M = S+H2+M      1.6E24  -2.613   89100 ! Shiina+98 (9911)
           N2/1.5/ SO2/10/ H2O/10/
        H2S+S = SH+SH         7.4E6    2.3     9007 ! Gao ea 2011
        DUP
        H2S+S = SH+SH         4.7E7    1.33    -436 !
        DUP
        H2S+H = SH+H2         3.5E07   1.94     904 ! Peng eaJPCA1999
```

```
!H2S+H = SH+H2       1.2E07  2.10   700 ! a (Yoshimura+92)
H2S+O = SH+OH        7.5E07   1.75     2900 ! Goumri ea 95
H2S+OH = SH+H2O              8.7E13  -0.7        0 ! Ellingson ea, JACS2007 /Zhou ea 2013
DUP
H2S+OH = SH+H2O              4.1E7   1.77        0 ! Ellingson ea, JACS2007
DUP
SH+H2O2=H2S+HO2              5E12    0.0    0 ! ESTIMATED PRESENT WORK
!SH+H2O2=H2S+HO2             5.6E4    2.823    8668 ! Zhou TST (2009)
!H2S+HO2=SH+H2O2             3.16E12    0.0    16890 ! Marwan 2011 PRUEBA
H2S+HO2=HSO+H2O              1.0E0    3.29     6224 ! Zhou (Molina Sendt TST) 2009
SH+HO2=H2S+O2        3.8E4    2.78    -1529 ! Zhou TST (2009)
!H2S+O2=HO2+SH       9.53E5   2.13   39124 ! (Prueba JM O2 singlet)
!SH+HO2=H2S+O2               3.5E16   -1.84    -2758 ! Prueba chinos
H2S+O2=HSO+OH                1.0E11   0.0     49100 ! Zhou est (2009)
H2S+O3=SO2+H2O               5.3E8    1.66    11665 ! MOU/MORJPCA2013
H2S+O3=HOSO+OH               1.1E3    2.77    11369 ! MOU/MORJPCA2013
!H2S+SO=SH+HSO               5.4E3    3.21    26824 ! Zhou TST (2009) (Glarborg dice: rv
too fast; la suprime) y utiliza la siguiente
H2S+SO(S)=HSO+SH             1.0E13   0.000   11000 ! (NUEVA) Zhou est 2009
H2S+SO=SH+HOS        1.0E13   0.0     36500 ! Zhou est (2009)
H2S+SO2=S2O+H2O              1.7E6    1.86    37740 ! Sendt ea 2005
!H2S+M=H+SH+M                1.8E14   0.0     64000 ! (NUEVA) Frenklach 1981
H2S+S(+M)=H2S2(+M)           6.4E7    1.28     -478 ! Zhou 2009
   LOW /2.4E21 -1.612 1670/
   TROE /0.5 726 726/
H2S+SO2=H2S2O2         3.5E18  -2.12    33530 ! (NUEVA) Sendt ea 2005
H2S+HSO=SH+HSOH        1E13     0.0     17300 ! (NUEVA) Zhou est 2009
H2S+HOS=SH+HSOH        1E13     0.0     12500 ! (NUEVA) Zhou est 2009
H2S+S2O=H2S3O                2.4E19  -2.3     30450 ! (NUEVA) Sendt ea 2005
H2S+S2O=S3+H2O               8E7      1.51    34010 ! (NUEVA) Sendt ea 2005
H2S+S2O=HSSSOH               2.9      3.64    22681 ! (NUEVA) Sendt ea 2005
!
! ***HS2/H2S2 reactions****
!
!
HS2+H=H2S+S          1.5E8    1.55     2259 ! Zhou ea 2009
```

```
DUP
HS2+H=H2S+S          4.2E18  -1.56     472 ! Zhou ea 2009
DUP
HS2+H=H2+S2          1.0E08   1.750   -877 ! (Updated) Zhou ea 2009 (113)
DUP
HS2+H=H2+S2          2.9E16  -0.894    -56 ! (Updated) Zhou ea 2009 (113)
DUP
HS2+H+M = H2S2+M             1.0E16   0.0        0 ! est Maria
HS2+H=SH+SH          9.7E7    1.62   -1030 ! Sendt ea 2002
DUP
HS2+H=SH+SH          1.6E18  -0.983    261 !
DUP
HS2+O = S2+OH        7.5E07   1.75    2900 ! est h2s+O  **no rev
!HS2+O = S2+OH       1.0E14   0.0        0 ! (Update?) Zhou est 2009
HS2+OH = S2+H2O              2.7E12   0.0        0 ! est h2s+oh **no rev
!HS2+OH = S2+H2O             1.0E14   0.0        0 ! (Update?) Zhou est 2009
HS2+O2=S2+HO2        8.4E01   2.95    7071 ! Song ea 2016
HS2+SH=S2+H2S        6.3E3    3.05   -1105 ! Sendt ea 2002
HS2+S = S2+SH        2.0E13   0.0     7400 ! est h2s+s **no rev
!HS2+S = S2+SH       4.2E6    2.2     -600 ! (Update?) Sendt 2002
H2S2+H=HS2+H2        5.0E07   1.93   -1408 ! (Updated) Sendt 2002
H2S2+O = HS2+OH              7.5E07   1.75    2900 ! est h2s+o **no rev
!H2S2+O = HS2+OH             1.0E14   0.0        0 ! (Update?) Zhou est 2009
H2S2+OH = HS2+H2O            1.0E13   0.0        0 ! (Updated) Zhou est 2009 (antes 2.7E12)
H2S2+S = HS2+SH      2.0E13   0.0     7400 ! est h2s+s **no rev
!H2S2+S=HS2+SH               2.9E6    2.3     1204 ! (Update?) Sendt 2002
H2S2+SH=HS2+H2S              6.4e03   2.98   -1480 ! Sendt ea PCI2002
HS2+O2=HSO+SO        6.6E3    1.9     7071 ! Song ea 2016 (Juanma nueva Julio '17)
H2S2+H=H2S+SH        3.7E8    1.72     477 ! (NUEVA) Sendt ea 2002
H2S2+O=HSO+SH                1.0E14   0.0        0 ! (NUEVA) Zhou est 2009
H2S2+HO2=HS2+H2O2            1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
H2S2+O2=HS2+HO2              1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
H2S2+SO=HS2+HSO              1.0E13   0.0    15000 ! (NUEVA) Zhou est 2009
H2S2+SO=HS2+HOS              1.0E13   0.0    19000 ! (NUEVA) Zhou est 2009
H2S2+HSO=HS2+HSOH            1.0E13   0.0     2000 ! (NUEVA) Zhou est 2009
H2S2+HOS=HS2+HSOH            1.0E13   0.0     2000 ! (NUEVA) Zhou est 2009
```

```
HS2+O=SH+SO                 1.0E14   0.0        0 ! (NUEVA) Zhou est 2009
HS2+HO2=S2+H2O2             1.0E13   0.0    26000 ! (NUEVA) Zhou est 2009
HS2+SO=S3+OH                1.0E13   0.0    14900 ! (NUEVA) Zhou est 2009
HS2+SO3=HS2O+SO2 1.0E13   0.0    10000 ! (NUEVA) Zhou est 2009
HS2+HSO=HS2O+SH             1.0E13   0.0     7000 ! (NUEVA) Zhou est 2009
HS2+HSO=S2+HSOH             1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HS2+HOS=S2+HSOH             1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HS2+HS2=H2S2+S2             9.6E0    3.37    -1672 ! (NUEVA) Sendt 2002
!
!
! ****** SH reactions *********
!
SH+O = H+SO           4.25E11  0.724   -1027 ! Sendt/Hay2007
SH+O=S+OH             1.8E12   0.0        0 ! zhou ea ijck2016
DUP
SH+O=S+OH             4.3E11   0.724      0 !
DUP
SH+OH=S+H2O           1.0E14   0.0        0 ! Song ea 2016
!SH+OH=S+H2O          1.7E5    2.47    -1637 ! Zhou TST 2009
SH+OH=HOS+H           1.0E13   0.0     7400 ! Zhou ea PCI 2013
SH+HO2=SO+H2O               3.2E2    2.58    -2071 ! Zhou ea 2013
SH+HO2=HSO+OH       2.5E8    1.48    -2169 ! Zhou TST 2009
S+H2O2=SH+HO2       4.1E6    2.2     12619 ! Zhou ea 2013
SH+O2=HSO+O           2.3E6    1.816   20008 ! Zhou ea 2009
SH+O2=S+HO2           4.7E6    2.02    36913 ! Zhou ea 2009
SH+O2=SO+OH           7.5E4    2.05    16384 ! Zhou ea 2009
SH+O2=SO2+H           1.5E5    2.12    11020 ! Song ea 2016
SH+O2(+M)=HSOO(+M)          8.7E14  -0.26      298 ! Goumri ea JPCA99! check
A=2E14???)
        LOW /3.1E19 -0.201 20/
SH+O3=HSO+O2          5.7E12   0.0      556 ! Atk2004
SH+H2O2=HSOH+OH             9.5E3    2.8      9829 ! Zhou ea2009
SH+SH(+M)=H2S2(+M)          9E11     0.155   -1432 ! Zhou ea JPCA2009
        LOW /2.3E31 -4.94 1998/           ! Gao ea 2011
        TROE/ 1.0 254 2373 /
!SH+S+M=HS2+M                6E11     0.0        0 !
```

```
!SH+SH = S2+H2         1.0E12   0.0        0 ! **no rev
!SH+S = S2+H           3.0E13   0.0        0 ! **no rev
SH+S=S2+H            3.3E12   0.543     -29 ! (NUEVA) Zhou QRRK 2009
SH+SO=HSO+S           1.0E13   0.0     25000 ! (NUEVA) Zhou est 2009
SH+SO=HOS+S                    1.0E13   0.0     30000 ! (NUEVA) Zhou est 2009
SH+HSO=S+HSOH                  1.0E11   0.0     11000 ! (NUEVA) Zhou est 2009
SH+HSO=S2O+H2                  1.0E14   0.0     14250 ! (NUEVA) Zhou est 2009
SH+SO=S2O+H                    1.0E12   0.0      5000 ! (NUEVA) Zhou est 2009
SH+SO2=HSO+SO                  1.0E14   0.0     32000 ! (NUEVA) Zhou est 2009
SH+SO2=HOS+SO                  1.0E14   0.0     36000 ! (NUEVA) Zhou est 2009
SH+SO2=OH+S2O                  1.0E14   0.0     32000 ! (NUEVA) Zhou est 2009
SH+SO2=HSSO2                   1.0E13   0.0     33000 ! (NUEVA) Zhou est 2009
!
!
! ***** S/S2/S3... reactions ********
!
S+H+M=SH+M           6.2E16  -0.6        0 ! Sendt ea PCI2002  **no rev
S+H2 = SH+H          1.4E14   0       19300 ! Shiina+98 (9906) **no rev
S+OH = H+SO          1.5E13   0.2     -1361 ! Sendt ea PCI2007
S+HO2=SO+OH          5.7E13   0.0        0 ! Ballester/VAr IJCK2008
S+O2 = SO+O          5.4E05   2.1     -1450 ! Lu ea JCM2004
S+HO2=HOS+O                    1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
S+O3=SO+O2           7.2E12   0.0        0 ! (NUEVA) Atkinson 2004
S+H2O2=HOS+OH                  1.0E12   0.0        0 ! (NUEVA) Zhou est 2009
S+S(+M)=S2(+M)        1.4E10   0.0      -825 ! (Updated) Du 2008 (tenía la inversa sin ref)
   LOW  /7.2E14 0.0 -408 /
S2+H+M=HS2+M          1.2E25  -2.840    1665 ! (Updated) Sendt 2002 (tenía 1E16)
  H2S /1.1/ AR /0.88/
S2+O=SO+S            1.4E11   0.7      -231 ! (Updated) Zhou TST 2009
S2+O+M=S2O+M                   1.9E21  -2.8        0 ! (NUEVA) Zhou est O+O+M 2009
S2+O2=S2O+O           1.7E4    2.54    34376 ! (NUEVA) Zhou TST 2009
S2+O2=SO+SO           2.3      2.45    30440 ! (NUEVA) Zhou TST 2009
S2+S+M=S3+M           1.9E15   0.0     -1788 ! (NUEVA) Zhou est 2009
S2+S2+M=S4+M          1.9E15   0.0     -1788 ! (NUEVA) Zhou est 2009
S3+H2O=HSSSOH          1.0E14   0.0     25000 ! (NUEVA) Zhou est 2009
S3+S2+M=S5+M          1.9E15   0.0     -1788 ! (NUEVA) Zhou est 2009
```

```
S3+S3+M=S6+M          1.9E15   0.000   -1788 ! (NUEVA) Zhou est 2009
S3+S2O=S4+SO          1.0E14   0.000   16000 ! (NUEVA) Zhou est 2009
S3+S4+M=S7+M          1.9E15   0.000   -1788 ! (NUEVA) Zhou est 2009
S4+S4+M=S8+M          1.9E15   0.000   -1788 ! (NUEVA) Zhou est 2009
!
!
!***** S2O reactions *******
!
S2O+H2=SH+HOS       1.0E13   0.0     46000 ! (NUEVA) Zhou est 2009
S2O+H+M=HS2O+M         6.4E22  -2.59      287 ! (NUEVA) Zhou est HSO+M 2009
S2O+H=OH+S2           1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
S2O+O=SO+SO           9.3E11   0.0        0 ! (NUEVA) Singleton 1988
S2O+OH=S2+HO2          1.0E13   0.0     40000 ! (NUEVA) Zhou est 2009
S2O+S=SO+S2           1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
S2O+SH=HSO+S2          1.0E12   0.0      5000 ! (NUEVA) Zhou est 2009
S2O+SH=HS2+SO          1.0E13   0.0      8000 ! (NUEVA) Zhou est 2009
S2O+SH=S3+OH          1.0E13   0.0     21450 ! (NUEVA) Zhou est 2009
S2O+SO2=S2+SO3         1.0E13   0.0     20000 ! (NUEVA) Zhou est 2009
S2O+HSO2=HS2O+SO2      1.0E13   0.0     32000 ! (NUEVA) Zhou est 2009
S2O+S2=S3+SO          1.0E14   0.000   18000 ! (NUEVA) Zhou est 2009 (Glarborg la tenía suprimida)
S2O+S2O=S3+SO2         1.0E12   0.000    2600 ! (NUEVA) Zhou est 2009
!
!
!***** SOx reactions ******
!
!SO+O(+M) = SO2(+M)           3.2E13   0.0        0 ! COB85,Plach/Troe84
!    LOW/1.2E21 -1.54  0/
!    TROE/0.55 1E-30 1E30/
!    N2/1.5/ SO2/10/ H2O/10/
SO+O+M=SO2+M          4.1E22  -2.170       0 ! (NUEVA) Lu 2003
 N2/1.5/ SO2/10/ H2O/10/
SO+M = S+O+M          4.0E14   0      107000 ! Plach/Troe 1984
SO+O2=SO2+O           7.6E03   2.37     2970 ! Tsuchiya+97/Woiki+95 (9906) !
!SO+HO2=SO2+OH               3.7E3    2.42     7660 ! Est Rasmussen2007
SO+HO2=SO2+OH               1.0E12   0.0        0 ! (NUEVA) (Glarborg suprime la anterior y dice que usa esta, barrierless pw)
```

```
SO+H+M=HSO+M          1.9E20  -1.31      662 ! (NUEVA) Rasmussen 2007 (Tengo la inversa + antigua)
    N2/1.5/ SO2/10/ H2O/10/
!HSO+M=SO+H+M         8.43E15  0.0     58600 ! Tsuchiya1994
!    N2/1.5/ SO2/10/ H2O/10/
SO+O3=SO2+O2                  2.7E12   0.0      2325 ! (NUEVA) Atkinson 2004
SO+S+M=S2O+M                  4.1E22  -2.170       0 ! (NUEVA) Song ea 2016 (est as SO+O+M)
    N2/1.5/ SO2/10/ H2O/10/
SO+SH=S2+OH                   1.0E12   0.0      4320 ! (NUEVA) Zhou est 2009
SO(S)+M=SO+M          1.0E13   0.0         0 ! Est Rasmussen2007
SO(S)+O2=SO2+O        1.0E13   0.0         0 ! Est Rasmussen2007
!SO+OH=SO2+H                  1.1E17  -1.35         0 ! Alzueta 2001 (disponible la inversa de 2002)
SO2+H=SO+OH           6.7E21  -2.22    30736 ! (Updated) Blitz 2002
H+SO2(+M)=OH+SO(+M)    9.19E25  2.77    20850 ! * Blitz 2006  (La teníamos suprimida, update?)
   LOW/1.35E22 -2.30 30965/            !
   TROE/0.283 272 3995/
   N2/1.0/ SO2/10/ H2O/10/ !CO2/2.5/
H+SO+M=HOS+M          3.6E20  -1.924     -29 ! (NUEVA) Sendt 2007
 N2 /0/
H+SO+N2=HOS+N2         2.0E21  -2.093     -72 ! (NUEVA) Sendt 2007
SO2*+M = SO2+M        1.3E14   0.0      3600 ! Strickler/Ito 1985
SO2*+SO2 = SO3+SO  2.6E12   0.0      2430 ! Heicklen+1980
SO2+O(+M) = SO3(+M)           3.7E11   0.0      1689 ! (Updated) Yilmaz 2006
   LOW/2.9E27 -3.58 5206/ !
   TROE/0.43 371 7442/
   SO2/10/ H2O/10/ N2/1/ !CO2/10/
SO2+O(+N2) = SO3(+N2)         3.7E11   0.00     1689 ! Naidoo2005/Yilmaz06
   LOW/2.9E27 -3.58 5206/ !
   TROE/0.43 371 7442/
SO2+OH(+M)=HOSO2(+M)     5.7E12  -0.27        0 ! Blitz2003
   LOW/1.7E27 -4.09 0/
   TROE/1.0 1E-30 412/
   N2/1.0/ SO2/5/ H2O/5/ !CO2/2.5/
SO2+H2O=VDW1                  1.0E14   0.0         0 ! (NUEVA) Zhou est 2009
```

```
SO2+O3=SO3+O2                1.8E12   0.0     14000 ! (NUEVA) Zhou est 2009
SO2+S=SO+SO          6.0E-16  8.21    -9600 ! Murakami2003
SO3+H = HOSO+O               2.5E05   2.92    50300 ! a
SO3+H = SO2+OH       8.4E09   1.22     3319 ! Hindiyarti2007
SO3+O = SO2+O2       2.8E04   2.57    29212 ! Hindiyarti2007
SO3+OH = SO2+HO2             4.8E04   2.46    27225 ! Hindiyarti2007
SO3+SO=SO2+SO2       7.6E3    2.37     2980 ! Glarborg2004 (Chung75+est depT)
SO3+S=SO+SO2                 1.0E13   0.0         0 ! (NUEVA) Zhou est 2009
!
!
!***** HSO/HOS reactions ******
!
HSO+O2=SO+HO2                6.4E5    2.63    19013 ! Zhou ea PCI2013
DUP
HSO+O2=SO+HO2                2.9E1    3.2         14529 !
DUP
HSO+O2=HSO2+O                8.4E-7   5.1         11312 ! Zhou ea PCI2013
HSO+O2=SO2+OH                3.7E01   2.764     6575 ! zHOOU EA PCI2013
HSO+O3=SH+O2+O2              1.5E12   0.0       2230 ! ATK 2004/LEE94
HSO+O3=HSO2+O2               1.3E12   0.0       2230 !
HSO+O3=SO+OH+O2              5.0E0    3.6       7191 ! Song ea IJCK2016
HSO+H = HSOH         2.5E20  -3.14       920 ! a
HSO+H = SH+OH        4.9E19  -1.86      1560 ! a
HSO+H = S+H2O        1.6E09   1.37      -340 ! a
HSO+H = H2SO         1.8E17  -2.47       50 ! a
H2S+O=HSO+H          1.4E9    1.1      5099 ! Goumri ea95
!HSO+H = H2S+O        1.1E06   1.03    10400 !
HSO+H = SO+H2        1.0E13   0.00        0 ! * est (a 1E12)
HSO+O+M = HSO2+M             1.1E19  -1.73      -50 ! a
HSO+O = SO2+H        4.5E14  -0.40        0 ! a
HSO+O+M = HOSO+M             6.9E19  -1.61     1590 ! a
HSO+O = O+HOS        4.8E08   1.02     5340 ! a
HSO+O = OH+SO        1.4E13   0.15      300 ! a
HSO+OH = HOSHO               5.2E28  -5.44     3170 ! a
HSO+OH = HOSO+H              5.3E07   1.57     3750 ! a
HSO+OH = SO+H2O              1.7E09   1.03      470 ! a
```

```
HSOO(+M)=HSO+O(+M)        2.0E19   -1.070  28374 ! Goumri ea 99
   LOW  /9.3E34 -5.87 30957/
HSO+H=HOS+H               1.0E14   0.0     4000 ! (NUEVA) Zhou est 2009
HSO+OH=H2+SO2             1.0E11   0.0        0 ! (NUEVA) Zhou est 2009
HSO+HO2=SO+H2O2           1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO+HSO=SO+HSOH           1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO+S2=HS2+SO             1.0E12   0.0     3000 ! (NUEVA) Zhou est 2009
HOS+M=HSO+M           5.8E11   0.0     32722 ! (NUEVA) Sendt 2007
   N2 /0/
HOS+N2=HSO+N2         2.9E11   0.0     24601 ! (NUEVA) Sendt 2007
HOS+H=H2+SO               1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HOS+O=OH+SO               1.0E14   0.0        0 ! (NUEVA) Zhou est 2009
HOS+O=H+SO2               1.0E14   0.0        0 ! (NUEVA) Zhou est 2009
HOS+OH=SO+H2O             1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HOS+OH=H2+SO2             1.0E11   0.0        0 ! (NUEVA) Zhou est 2009
HOS+O2=HO2+SO             6.4E5    2.63    19013 ! (NUEVA) Zhou est 2009
HOS+O2=SO2+OH             3.7E1    2.76     6575 ! (NUEVA) Zhou est 2009
HOS+HO2=SO+H2O2           1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HOS+HOS=SO+HSOH           1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HOS+S2=HS2+SO             1.0E12   0.0     1000 ! (NUEVA) Zhou est 2009
HOS+S2=S3+OH              1.0E13   0.0    13000 ! (NUEVA) Zhou est 2009
!
!
!***** HSOH reactions ******
!
HSOH = SH+OH          2.8E39  -8.75     75200 ! a
HSOH = S+H2O          5.8E29  -5.60    54500 ! a
HSOH = H2S+O          9.8E16  -3.40     86500 ! a
HSOH+HO2=HSO+H2O2         1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSOH+HO2=HOS+H2O2         1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSOH+O2=HSO+HO2           1.0E13   0.0    26000 ! (NUEVA) Zhou est 2009
HSOH+O2=HOS+HO2           1.0E13   0.0    30000 ! (NUEVA) Zhou est 2009
HSOH+O=HSO+OH             1.0E14   0.0        0 ! (NUEVA) Zhou est 2009
HSOH+O=HOS+OH             1.0E14   0.0        0 ! (NUEVA) Zhou est 2009
HSOH+H=HSO+H2             1.0E14   0.0        0 ! (NUEVA) Zhou est 2009
HSOH+H=HOS+H2             1.0E14   0.0        0 ! (NUEVA) Zhou est 2009
```

```
HSOH+OH=HSO+H2O          1.0E14   0.0        0 ! (NUEVA) Zhou est 2009
HSOH+OH=HOS+H2O          1.0E14   0.0        0 ! (NUEVA) Zhou est 2009
!
!
!***** HOSO reactions ******
!
!H+SO2(+M)=HOSO(+M)     2.37E8   1.63     7339 ! Blitz06  (Glarborg la utiliza en 2016)
!   LOW/1.85E37 -6.14 11075/
!   TROE/0.283 272 3995/
!    N2/1.0/ SO2/10/ H2O/10/ !CO2/2.5/
HOSO(+M)=H+SO2(+M)      1.7E10   0.80    46933 ! Alzueta2001(Goumri1999)
   LOW/1.5E31 -4.53 49178/
   TROE/0.30 1E-30 1E30/
   N2/1.0/ SO2/10/ H2O/10/
HOSO(+M) = HSO2(+M)         1.0E09   1.03     50000 ! GOU/MAR99
   LOW/1.7E35 -5.64 55400/
   TROE/0.40 1.E-30 1.E30/
   N2/1.0/ SO2/10/ H2O/10/ !CO2/2.5/
HOSO(+M)=OH+SO(+M)      9.9E21  -2.540   75891 ! (Updated) Blitz 2002 (Tenía puesta la
inversa de Goumri 1999)
   LOW /1.2E46 -9.020 52953/
   TROE/0.95 2989 1.1/
!SO+OH(+M)=HOSO(+M)       1.6E12  0.50      -400 ! (PRUEBA con la inversa de
GOumri'99)
!          SO2/10/ H2O/10/ N2/1.5/
!          LOW/9.5E27 -3.48 974/
!HOSO=OH+SO                  3.6E18  0.0       86746 !
HOSO+M = O+HOS+M            2.5E30  -4.8    119000 ! Glarborg 1996
HOSO+H=SO(S)+H2O            2.4E14   0.0        0 ! Marshall-Hu05
HOSO+H=SO2+H2       1.8E7    1.72    -1286 ! Marshall-Hu05
HOSO+O=SO2+OH               1.0E13   0.0        0 ! (Updated) Zhou est 2009 (Tenía puesta
la inversa con valores de ref desconocida)
HOSO+OH=SO2+H2O         6.0E12   0.0        0 ! (Updated) Rasmussen est 2007 (Yo tenía
est 1E12)
HOSO+HO2=SO2+H2O2       1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
!HOSO+O2=HO2+SO2            9.6E1    2.35   -10130 ! (Updated) Rasmussen 2007 (La tenía
suprimida, y utilizaba valor Glarborg 96)
HOSO+O2=SO2+HO2     1.0E12   0.00  500  !Alzueta01 (Glarborg1996)
```

```
HOSO+SH=SO2+H2S            1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HOSO+S=SO2+SH              1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HOSO+SO=SO2+HSO            1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HOSO+SO=SO2+HOS            1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HOSO+HSO=SO2+HSOH       1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HOSO+HOS=SO2+HSOH       1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HOSO+HS2=SO2+H2S2          1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HOSO+S2=SO2+HS2            1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
!
!
!***** HSO2 reactions ******
!
H+SO2(+M)=HSO2(+M)      5.31E8   1.59      2472 ! Blitz 2006
   LOW/1.41E31 -5.19 4513/           !
   TROE/0.390 167 2191/
   N2/1.0/ SO2/10/ H2O/10/ !CO2/2.5/
!HSO2(+M)=H+SO2(+M)         2.03E11            0.9     18360 ! Goumri '99 inversa
!    LOW/5.74E1 -3.29 19095/
!    N2/1.0/ SO2/10/ H2O/10/
HSO2+H = SO2+H2      5.0E12   0.46     -262 ! Marshall/Hu2005
HSO2+O2 = HO2+SO2          1.1E3    3.20     -235 ! Est Rasmussen2007
HSO2+O=SO2+OH              1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO2+OH=SO2+H2O            1.0E13   0.0        0 ! la tenía estimada así ya
HSO2+HO2=SO2+H2O2          1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO2+O3=SO2+OH+O2          1.0E13   0.0        0 ! (NUEVA) Song est 2016
HSO2+SH=SO2+H2S            1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO2+S=SO2+SH              1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO2+SO=SO2+HSO            1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO2+SO=SO2+HOS            1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO2+HSO=SO2+HSOH          1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO2+HS2=SO2+H2S2          1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO2+S2=SO2+HS2            1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSOO=HSO2              1E17   0.0        21300 ! est present work
!HSOO=HSO2              1E13   0.0        0 ! est present work
!
!
```

```
!***** HS2O reactions ******
!
HS2O+H=S2O+H2              1.0E12   0.0      2600 ! (NUEVA) Zhou est 2009
HS2O+H=HS2+OH              1.0E13   0.0         0 ! (NUEVA) Zhou est 2009
HS2O+O=S2O+OH              1.0E13   0.0       0 ! (NUEVA) Zhou est 2009
HS2O+O=SH+SO2              1.0E13   0.0       0 ! (NUEVA) Zhou est 2009
HS2O+OH=S2O+H2O            1.0E13   0.0       0 ! (NUEVA) Zhou est 2009
HS2O+OH=HS2+HO2            1.0E13   0.0   27000 ! (NUEVA) Zhou est 2009
HS2O+HO2=S2O+H2O2          1.0E13   0.0       0 ! (NUEVA) Zhou est 2009
HS2O+S=HS2+SO              1.0E13   0.0       0 ! (NUEVA) Zhou est 2009
HS2O+S=S2O+SH              1.0E13   0.0       0 ! (NUEVA) Zhou est 2009
HS2O+SH=S2O+H2S            1.0E13   0.0       0 ! (NUEVA) Zhou est 2009
HS2O+HS2=S2O+H2S2          1.0E13   0.0       0 ! (NUEVA) Zhou est 2009
!
!
!***** SSO2 reactions ******
!
SO2+S(+M)=SSO2(+M)      3.7E12   0.0      1689 ! (NUEVA) Song es 2016 (est 10 x SO2+O+M)
  LOW  /2.9E28 -3.58 5206/
  TROE /0.43 371 7442/
  N2/1/ SO2/10/ H2O/10/
!SSO2+M=S+SO2+M   1.0E15   0.0     30000 ! (NUEVA) Zhou est 2009 (glarborg la tenía suprimida)
SSO2+H=SH+SO2              1.0E13   0.0       0 ! (NUEVA) Song est 2016
SSO2+O=SO+SO2              1.0E13   0.0         0 ! (NUEVA) Song est 2016
SSO2+OH=HOS+SO2            1.0E13   0.0       0 ! (NUEVA) Song est 2016
SSO2+S=S2+SO2              1.0E13   0.0       0 ! (NUEVA) Song est 2016
!
!
!***** OSSO reactions ******
!
SO+SO+M=OSSO+M             3.2E32  -5.75     3044 ! (NUEVA) Zhou TST 2009
OSSO+H=OH+S2O              1.0E13   0.0         0 ! (NUEVA) Zhou est 2009
OSSO+H=SO+HSO              1.0E13   0.0         0 ! (NUEVA) Zhou est 2009
OSSO+H=SO+HOS              1.0E13   0.0         0 ! (NUEVA) Zhou est 2009
OSSO+H=HO2+S2              1.0E13   0.0    12570 ! (NUEVA) Zhou est 2009
```

```
OSSO+O=SO+SO2              1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
OSSO+O=O2+S2O              1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
OSSO+OH=HO2+S2O            1.0E13   0.0    11350 ! (NUEVA) Zhou est 2009
OSSO+OH=HOSO+SO            1.0E12   0.0        0 ! (NUEVA) Zhou est 2009
OSSO+SO=SO2+S2O            1.0E10   0.0        0 ! (NUEVA) Zhou est 2009
OSSO+S=S2O+SO              1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
OSSO+S=S2+SO2              1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
OSSO+SH=HSO+S2O            1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
OSSO+S2=S2O+S2O            1.0E12   0.0        0 ! (NUEVA) Zhou est 2009
!
!
!***** HOSO2/HOSHO ******
!
HOSO2+S=SH+SO3             1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HOSO2 = HOSO+O      5.4E18  -2.34   106300 ! Glarborg 1996
HOSO2 = SO3+H       1.4E18  -2.91    54900 ! Glarborg 1996
HOSO2+H = SO2+H2O          1.0E12   0.0        0 ! Glarborg 1996
HOSO2+O = SO3+OH           5.0E12   0.0        0 ! Glarborg 1996
HOSO2+OH = SO3+H2O         1.0E12   0.0        0 ! Glarborg 1996
HOSO2+O2 = HO2+SO3         7.8E11   0.0      656 ! Atkinson 2004
HOSHO = HOSO+H             6.4E30  -5.89    73800 ! Glarborg 1996
HOSHO = SO+H2O      1.2E24  -3.59    59500 ! Glarborg 1996
HOSHO+H = HOSO+H2          1.0E12   0.0        0 ! Glarborg 1996
HOSHO+O = HOSO+OH          5.0E12   0.0        0 ! Glarborg 1996
HOSHO+OH = HOSO+H2O        1.0E12   0.0        0 ! Glarborg 1996
!
!
!***** OTHERS ******
!
H2SO = H2S+O          4.9E28  -6.66     71700 ! Glarborg 1996
HSSO2+M=SH+SO2+M           1.0E17   0.0     3000 ! (NUEVA) Zhou est 2009
HSSO2=S2O+OH               1.0E13   0.0    33700 ! (NUEVA) Zhou est 2009
H2S2O2+H2O=H2S+VDW1        3.9E5    1.66    3740 ! (NUEVA) Sendt 2005
H2S2O2+H2O=2H2O+S2O        3.6E5    1.56   14290 ! (NUEVA) Sendt 2005
H2S2O2+SH=H2S2+HOSO        1.0E13   0.0     8000 ! (NUEVA) Sendt 2005
!
```

```
!
SO2+CO=SO+CO2    1.9E13    0    65900   ! Bacskay2005
CO+SO=CO2+S      5.10E13   0    53400   ! Bacskay2005
!
!
!
!*************Subset de Murakami et al. Bull.Chem.Soc.Jpn., 74 (2001)
!
O+CS2=CS+SO                  3.6E13 0        1696 !
O+CS=CO+S             3.2E13 0        0 !
O+CS2=CO+S2                  1.7E12 0        1194 !
O+CS2=COS+S                  7.1E12 0        2102 !
S+CS2=CS+S2           1.0E14 0        4060 !
CS2+O2=CS+SO2                1.0E12 0        31050 !
!
!
!Optimizadas
CS+O2=COS+O                  6.1E12 0        16500 ! Murakami2001- Opt. Ea
!!!!CS+O2=COS+O               1.3E07 1.970    28124 ! Glarborg 2014 CS2
CS+O2=CO+SO                  6.1E12 0        16500 ! Analogia a CS+O2=COS+O
!
!
!
CS2 + OH = COS + SH 5.79E8     0     -1174  ! Leu1982
COS + OH = CO2 + SH      2.41E10     0.0    0    ! COX1980
CS2 + OH => CS2OH    1.04E10          0        1743 ! MURRELLS 1990
CS2OH + O2 => COS + HSO2  1.57E10          0        0 !BASADA EN MURRELLS
1990, CS2OH + O2
!
CS2 + H2O = H2S + COS        2.07E13          0        41497 ! nuestra, basada en Ling2011
COS + H2O = H2S + CO2        1.54E13          0        35299 ! nuestra, basada en Ling2011
!
CS2 + SO = COS + S2  6.90E-05    0     -6339   ! Wood1971
!
!
!!!!CS + S + M = CS2 + M       0.617E15         0        3000 ! analogía a
CO+O+M=CO2+M NBS
```

```
!
!!!!CO + S + M = COS + M       0.617E15        0       3000 ! analogía a
CO+O+M=CO2+M NBS
CO+SH=COS+H                    2.50E10         0       15200
COS+O=CO+SO                    4.7E13  0       5200
 DUP
COS+O=CO+SO                    -2.0E130        7385
 DUP
COS+O=CO2+S                    2.0E13 0        7385
COS+S=CO+S2                    4.0E04 2.57     2345
COS+M=CO+S+M          2.50E+14    0.0    61400.0
!
CS+S(+M)=CS2(+M)                1.9E26  -4.300      0 !
 LOW  / 6.2E23 -2.42 0 /                        !
! Troe, J.; Marshall, P.; Glarborg, P., in preparation (2013).
CS+SH=CS2+H                    1.2E13   0.000      0 !
! Woiki, D.; Roth, P. Int J Chem Kinet 1995, 27, 59-71.
! P Glarborg B Halaburt P Marshall J Troe M Thellefsen K Christensen, pw
!
!
!**************MECANISMO CxHy-SO2 *********************************
!
!
C2 + H2S = C2H + SH  5.36E12          0         0 ! Huang2004
C2 + SO2 = C2O + SO  1.40E12          0         0 ! Huang2004
C2H + M = C2 + H + M1.74E35           -5.16     57367 ! Kruse1997
  N2/1.0/ SO2/5/ H2O/5/
CO + CH3S = COS + CH3   6.62E07     1.57   6675   ! Tang2008
CH3S + H2O2 = CH3SH + HO2  1.81E11  0      0      ! Turnipseed1996
CH3S+O2 = CH2S+HO2      4.74E24     -4.70  8300   ! Zhu2006
CH3S + O2 = CH3 + SO2   9.47E25     -3.80  12300  ! Zhu2006
!CH3SH + H = CH3 + H2S   6.90E12     0      1671   ! Amano1983
!CH3SH + OH = CH3S + H2O 1.31E07     1.77   -1689  ! Masgrau2003
CH3 + SH = CH3SH        1.00E13     0      0      ! Shum1985
CH3 + SO2 = CH3OSO      1.55E12     0.0    1291   ! Frank1999
CH3 + SO2 = CH3SO2      9.69E10     2.90   -340   ! Frank1999
```

CH3SO2 = CH3OSO 1.20E11 0.75 46300 ! zhu2006
CH3OSO = CH3O + SO 4.00E08 0.0 57300 ! zhu2006
CH3OSO = CH2O + HSO 2.44E06 1.82 53000 ! zhu2006
CH3O2 + SO2 = CH3O + SO3 3.01E07 0.0 0 ! ATKINSON1989
CH2S + CH3 = CH3CH2S 3.98E11 0.0 2007 ! SHUM1985
CH3SCH3 + H = CH3SH + CH3 1.80E08 1.70 2152 ! ZHANG2005
CH3CH2S = CH2CH2SH 2.00E13 0.0 32000 ! SHUM1985
CH2CH2SH = C2H4 + SH 1.58E13 0.0 11000 ! SHUM1985
CH3SCH3 + O = CH3 + CH3SO 7.83E12 0 -813 ! Baulch2004
CH3S + O2 = O + CH3SO 5.24E13 -1.50 1.69E04 ! zHU2006
CH3SCH3 + OH = CH3OH + CH3S 0.04 0 0 ! BARONE1995
CH3SCH3 = CH3 + CH3S 6.10E15 0 75800 ! MOUSAVIPOUR2002
CH4 + S = CH3 + SH 2.04E14 0.0 19900 ! TSUCHIYA1996
CH3 + H2S = CH4 +SH 3.80E11 0.0 2603 ! ARTHUR1978
C2H + C2H = C2H2 + C2 1.81E12 0 0 ! Tsang1986
!!!!!H2S+CO=COS+H2 1.0E11 0 0 ! nuestra est.
SO + C2H2 = COS + CH2 1.0E11 0 0 ! nuestra est.
SO + C2H4 = COS + CH4 1.0E11 0 0 ! nuestra est.
SO + CH2 = COS + H2 1.0E11 0 0 ! nuestra est.
SO + CH = COS + H 1.0E11 0 0 ! nuestra est.
SO + HCO = COS + OH 1.0E11 0 0 ! nuestra est.
SO + CH2O = COS + H2O 1.0E11 0 0 ! nuestra est.
SO + C2H2 = CS + CH2O 1.0E11 0 0 ! nuestra est.
SO + C2H4 = CS + CH3OH 1.0E11 0 0 ! nuestra est.
SO + CH2 = CS + H2O 1.0E11 0 0 ! nuestra est.
SO + CH = CS + OH 1.0E11 0 0 ! nuestra est.
SO2 + CH = CS + HO2 1.0E11 0 0 ! nuestra est.
SO2 + CH = COS + OH 1.0E11 0 0 ! nuestra est.
SO2 + CH2 = COS + H2O 1.0E11 0 0 ! nuestra est.
SO2 + CH2 = CS + H2O2 1.0E11 0 0 ! nuestra est.
SO2 + C2H = CS + HCOO 1.0E11 0 0 ! nuestra est.
S2 + C2H2 = CS2 + CH2 1.0E11 0 0 ! nuestra est.
S2 + CH2 = CS2 + H2 1.0E11 0 0 ! nuestra est.
S2 + CH = CS2 + H 1.0E11 0 0 ! nuestra est.
SH + C2H = CS + CH2 1.0E11 0 0 ! nuestra est.
SH + C2H2 = CS + CH3 1.0E11 0 0 ! nuestra est.

SH + C2H3 = CS + CH4 1.0E11 0 0 ! nuestra est.

H2S + C2H2 = CS + CH4 1.0E11 0 0 ! nuestra est.

CS + H2S = CS2 + H2 1.0E11 0 0 ! nuestra est.

!!!!!!!!!COS + SO = CO2 + S2 1.0E11 0 0 ! nuestra est.
DIAGRAMA DE CLARK2001

!

!***Bibliography***

!

! * Abian ea 2015: Abian M, Millera A, Bilbao R, Alzueta MU, FUEL 159, 550-558, 2015

! * Atkinson 2004: Atkinson R, J Atmos Chem Phys, 4, 2004

! * Blitz 2002: Hughes KJ Blitz MA, Proc Combust Inst, 29, 2002

! * Blitz 2006: MA Blitz, J Phys Chem A, 110, 2006

! * Du 2008: Du SY, J Chem Phys, 128, 2008

! * Ellingson ea, JACS2007: Ellingson BA, J Am Chem Soc, 129, 2007

! * Frenklach ea 1981: Frenklach M, Combustion Flame, 41, 1981

! * Gao ea 2011: Y Gao CR Zhou K Sendt BS Haynes P Marshall Proc Combust Inst, 33, 2011

! * Glarborg 1996: P Glarborg, Int J Chem Kinet, 28, 1996

! * Goumri ea 95: Goumri A, J Chem Phys, 102, 1995

! * Goumri ea 99: A Goumri, J.-D.R. Rocha, D. Laakso, C.E. Smith, P. Marshall, J. Phys. Chem. A 1999, 103, 11328-11335.

! * MOU/MORJPCA2013: Mousavipour SH, Hematti O, J Phys Chem A, 117, 2013

! * Lu 2003: Lu C-W Wu Y-J Lee Y-P Zhu RS Lin MC J Phys Chem A, 107, 2003

! * Peng eaJPCA1999: Jingping Peng, J. Phys. Chem. A, 103, 1999

! * Plach/Troe 1994: Plach HJ, Troe J, Int J Chem Kinet, 16, 1984

! * Rasmussen 2007: Rasmussen CL, Proc Combust Inst, 31, 2007

! * Sendt ea 2002: Sendt K Jazbec M Haynes BS PROC COMBUST INST, 29, 2002

! * Sendt ea 2005: Sendt K Haynes BS J PHYS CHEM A 109, 2005

! * Sendt ea 2007: Sendt K Haynes BS Proc Combust Inst, 31, 2007

! * Singleton 1988: Singleton DL Cvetanovic RJ JPCRD 17:1377 1988

! * Song ea 2016: Song Yu, Int J Chem Kinetics, 49, 2016

! * Shiina+98 (9911): Shiina H, J Phys Chem A, 102, 1998

! * Yilmaz 2006: A Yilmaz, J. Phys. Chem. A, 110, 2006

! * Zhou 2009: CR Zhou K Sendt BS Haynes J. Phys. Chem. A 2009, 113, 2975–2981

! * Zhou 2009: CR Zhou K Sendt BS Haynes J. Phys. Chem. A 2009, 112, 3239-3247

!

END

C.3 Reacciones agregadas

La siguiente lista de reacciones contiene todas aquellas que han sido agregadas al mecanismo al mecanismo final del presente trabajo y que, en el mecanismo inicial no se tenían en cuenta. Se han ordenado por bibliografía, por tanto, cada una de las tablas pertenece a un autor diferente y que se señala al inicio de esta. Los parámetros cinéticos para cada una de las reacciones también se encuentran expuestos en las siguientes tablas.

Tabla C.3.1 Parámetros cinéticos de las reacciones involucradas en el submecanismo de CH_4 de Giménez-López [12]. Unidades: mol, cm, s, cal, K.

Reacción	A	β	Ea
H+H+H2=H2+H2	0.920E+17	-0.6	0.0
H+H+CO2=H2+CO2	0.549E+21	-2.0	0.0
CH3O2+OH = CH3OH+O2	6.0E13	0.0	0
CH3O2+HO2 = CH3OOH+O2	2.5E11	0.0	-1570
CH3O2+H2O2 = CH3OOH+HO2	2.4E12	0.0	9940
CH3O2+CH2O = CH3OOH+HCO	2.0E12	0.0	11665
CH3O2+CH4 = CH3OOH+CH3	1.8E11	0.0	18500
CH3O2+CH3O = CH2O+CH3OOH	3.0E11	0.0	0
CH3O2+CH2OH = CH2O+CH3OOH	1.2E13	0.0	0
CH3O2+CH3OH = CH3OOH+CH2OH	1.8E12	0.0	13700
CH3O2+CH3O2 = CH3O+CH3O+O2	1.0E11	0.0	300
CH3O2+CH3O2 = CH3OH+CH2O+O2	4.0E09	0.0	-2210
CH3OOH = CH3O+OH	6.3E14	0.0	42300

CH3OOH+H = CH3O2+H2	8.8E10	0.0	1860
CH3OOH+H = CH3O+H2O	8.2E10	0.0	1860
CH3OOH+O = CH3O2+OH	1.0E12	0.0	3000
CH3OOH+OH = CH3O2+H2O	1.8E12	0.0	-378
C2H3+CH2=C3H4+H	3.0E13	0.0	0.0
C2H3+C2H=H2CCCCH+H	3.0E13	0.0	0.0
C2H3+C2H3=CH2CHCCH2+H	9.0E12	0.0	0.0
CH2HCO+CH3=C2H5+HCO	5.0E13	0.0	0.0
CH2HCO+O2=OH+OCHCHO	2.22E11	0.0	1500.
CH2HCO+M=CH3+CO+M Eficiencias de 3er cuerpo: H2/2/ CO/2/ CO2/3/ H2O/5/	2.0E16	0.0	42000
C2H+C2H2=C4H2+H	2.47E12	0.5	-391.
CH2(S)+M=CH2+M Eficiencias de 3er cuerpo: H/0.0/ H2O/0.0/ C2H2/0.0/ C6H6/0.0/ N2/0.0/ AR/0.0/	0.100E+14	0.000	0.000
CH2(S)+C2H2=CH2+C2H2	4.0E13	0.0	0.0
NH+CO2=CO+HNO	8.2E13	0.0	34500
HNCO+M=CO+NH+M Eficiencias de 3er cuerpo: N2/1.0/ CO2/2.0/ AR/0.7/	1.1E16	0.0	86000
HNCO+OH=NH2+CO2	1.8E06	1.5	3597
SH+SH = S2+H2	1.0E12	0.0	0.0

CH3SH(+M)=CH2SH+H(+M) Límite de baja presión: Parámetros de TROE: 0.773 693 5333	2.7E16 2.34E40	-0.08 -6.33	98940 103100
CH3SH = CH4+S	1.0E13	0	73000
CH3SH + O = CH3 + HSO	1.78E10	0	0
CH3SH + O = CH3SO + H	1.07E10	0	0
CH3SH + O = CH3O + SH	1.78E10	0	0
CH3SH + OH = CH3 + H2SO	1.0E13	0	0
CH3SH + OH = CH4 + HSO	1.0E13	0	0
CH3SH + O2 = CH2SH + HO2	2.1E13	0.00	44900
CH2SH + O2 = CH2S + HO2 DUP	1.6E15	-1.0	0
CH2SH + O2 = CH2S + HO2 DUP	7.2E13	0.0	3577
CH2SH+H=CH2S+H2	4.8E13	0.00	0
CH2SH+O=CH2S+OH	6.5E13	0.00	-700

Tabla C.3.2 Parámetros cinéticos de las reacciones involucradas en el submecanismo Gri 3.0[14] de CH_4. Unidades: mol,cm,s,cal, K.

Reacción	A	β	Ea
O+CH2=H+HCO	8.000E+13	.000	.00

O+CH2(S)=H2+CO	1.500E+13	.000	.00
O+CH2(S)=H+HCO	1.500E+13	.000	.00
O+CH3OH=OH+CH3O	1.300E+05	2.500	5000.00
H+2O2=HO2+O2	2.080E+19	-1.240	.00
H+O2+H2O=HO2+H2O	11.26E+18	-.760	.00
H+CH2(+M)=CH3(+M) Límite de baja presión: Parámetros de TROE: .5620 91.00 5836.00 8552.00 Eficiencias de 3er cuerpo: H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/	6.000E+14 1.040E+26	.000 -2.760	.00 1600.00
H+CH2OH=CH2(S)+H2O	3.280E+13	-.090	610.00
H+CH3O(+M)=CH3OH(+M) Límite de baja presión: Parámetros de TROE: .700 100.00 90000.0 10000.00 Eficiencias de 3er cuerpo: H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/	2.430E+12 4.660E+41	.515 -7.440	50.00 14080.0
H+CH3O=H+CH2OH	4.150E+07	1.630	1924.00
H+CH3O=CH2(S)+H2O	2.620E+14	-.230	1070.00
HO2+CH2=OH+CH2O	2.000E+13	.000	.00

CH2+CH2=H2+C2H2	1.600E+15	.000	11944.00
CH2(S)+O2=CO+H2O	1.200E+13	.000	.00
CH2(S)+H2O(+M)=CH3OH(+M) Límite de baja presión: Parámetros de TROE: .6027 208.00 3922.00 10180.0 Eficiencias de 3er cuerpo: H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/	4.820E+17 1.880E+38	-1.160 -6.360	1145.00 5040.00
CH2(S)+CO=CH2+CO	9.000E+12	.000	.00
CH2(S)+CO2=CH2+CO2	7.000E+12	.000	.00
HCO+H2O=H+CO+H2O	1.500E+18	-1.000	17000.00
C2H+O2=HCO+CO	1.000E+13	.000	-755.00
NH+H2O=HNO+H2	2.000E+13	.000	13850.00
NNH+M=N2+H+M Eficiencias de 3er cuerpo: H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/	1.300E+14	-.110	4980.00
NNH+CH3=CH4+N2	2.500E+13	.000	.00
HCN+M=H+CN+M Eficiencias de 3er cuerpo: H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/	1.040E+29	-3.300	126600.00

CH+N2(+M)=HCNN(+M) Límite de baja presión: Parámetros de TROE: .6670 235.00 2117.00 4536.00 Eficiencias de 3er cuerpo: !H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ 1.0/	3.100E+12 1.300E+25	.150 -3.160	.00 740.00
CH2(S)+N2=NH+HCN	1.000E+11	.000	65000.00
CH2+NO=H+HNCO	3.100E+17	-1.380	1270.00
CH2(S)+NO=H+HNCO	3.100E+17	-1.380	1270.00
CH2(S)+NO=H+HCNO	3.800E+13	-.360	580.00
HCNN+O=CO+H+N2	2.200E+13	.000	.00
HCNN+O=HCN+NO	2.000E+12	.000	.00
HCNN+O2=O+HCO+N2	1.200E+13	.000	.00
HCNN+OH=H+HCO+N2	1.200E+13	.000	.00
HCNN+H=CH2+N2	1.000E+14	.000	.00
HCNO+H=H+HNCO	2.100E+15	-.690	2850.00
HCNO+H=NH2+CO	1.700E+14	-.750	2890.00
HOCN+H=H+HNCO	2.000E+07	2.000	2000.00
CH3+N=HCN+H2	3.700E+12	.150	-90.00
O+CH3=H+H2+CO	3.370E+13	.000	.00

O+C2H4=H+CH2CHO	6.700E+06	1.830	220.00
O+C2H5=H+CH3CHO	1.096E+14	.000	.00
OH+CH3=H2+CH2O	8.000E+09	.500	-1755.00
CH+H2(+M)=CH3(+M) Límite de baja presión: Parámetros de TROE: . 578 122.0 2535.0 9365.0 Eficiencias de 3er cuerpo: H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/	1.970E+12 4.820E+25	.430 -2.80	-370.00 590.0
CH2(S)+H2O=H2+CH2O	6.820E+10	.250	-935.00
C2H3+O2=O+CH2CHO	3.030E+11	.290	11.00
O+CH3CHO=OH+CH2CHO	2.920E+12	.000	1808.00
O+CH3CHO=OH+CH3+CO	2.920E+12	.000	1808.00
O2+CH3CHO=HO2+CH3+CO	3.010E+13	.000	39150.00
H+CH3CHO=CH2CHO+H2	2.050E+09	1.160	2405.00
H+CH3CHO=CH3+H2+CO	2.050E+09	1.160	2405.00
OH+CH3CHO=CH3+H2O+CO	2.343E+10	0.730	-1113.00
HO2+CH3CHO=CH3+H2O2+CO	3.010E+12	.000	11923.00
CH3+CH3CHO=CH3+CH4+CO	2.720E+06	1.770	5920.00
H+CH2CO(+M)=CH2CHO(+M) Límite de baja presión:	4.865E+11 1.012E+42	0.422 -7.63	-1755.00 3854.0

Parámetros de TROE: 0.465 201.0 1773.0 5333.0 Eficiencias de 3er cuerpo: H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/			
O+CH2CHO=H+CH2+CO2	1.500E+14	.000	.00
O2+CH2CHO=OH+CO+CH2O	1.810E+10	.000	.00
O2+CH2CHO=OH+2HCO	2.350E+10	.000	.00
H+CH2CHO=CH3+HCO	2.200E+13	.000	.00
H+CH2CHO=CH2CO+H2	1.100E+13	.000	.00
OH+CH2CHO=H2O+CH2CO	1.200E+13	.000	.00
OH+CH2CHO=HCO+CH2OH	3.010E+13	.000	.00
CH3+C2H5(+M)=C3H8(+M) Límite de baja presión: Parámetros de TROE: .1527 291.0 2742.0 7748.0 Eficiencias de 3er cuerpo: H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/	.9430E+13 2.710E+74	.000 -16.82	.00 13065.0
O+C3H8=OH+C3H7	1.930E+05	2.680	3716.00
H+C3H8=C3H7+H2	1.320E+06	2.540	6756.00
OH+C3H8=C3H7+H2O	3.160E+07	1.800	934.00

C3H7+H2O2=HO2+C3H8	3.780E+02	2.720	1500.00
CH3+C3H8=C3H7+CH4	0.903E+00	3.650	7154.00
CH3+C2H4(+M)=C3H7(+M) Límite de baja presión: Parámetros de TROE: .1894 277.0 8748.0 7891.0 Eficiencias de 3er cuerpo: H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/	2.550E+06 3.00E+63	1.600 -14.6	5700.00 18170
O+C3H7=C2H5+CH2O	9.640E+13	.000	.00
H+C3H7(+M)=C3H8(+M) Límite de baja presión: Parámetros de TROE: .315 369.0 3285.0 6667.0 Eficiencias de 3er cuerpo: H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/	3.613E+13 4.420E+61	.000 -13.545	.00 11357.0
H+C3H7=CH3+C2H5	4.060E+06	2.190	890.00
OH+C3H7=C2H5+CH2OH	2.410E+13	.000	.00
HO2+C3H7=O2+C3H8	2.550E+10	0.255	-943.00
HO2+C3H7=OH+C2H5+CH2O	2.410E+13	.000	.00
CH3+C3H7=2C2H5	1.927E+13	-0.320	.00

Tabla C.3.3 Parámetros cinéticos de las reacciones involucradas en el submecanismo de CH_4+H_2S de S. Gersen [9]. Unidades: mol, cm, s, cal, K.

Reacción	A	β	Ea
CH3O2+SH=CH3O+HSO	2.5E7	1.477	-2169
CH3OOH+SH=CH3O2+H2S	5.6E3	2.823	8668
CH3SH+H=CH3S+H2	1.3E8	1.729	986
CH3SH+H=CH2SH+H2	4.1E3	2.925	4750
CH3SH+H=CH3+H2S	7.1E10	0.766	3220
CH3SH+H=CH4+SH	7.0E6	1.983	16530
CH3SH+O=CH3S+OH	4.2E7	1.818	80
CH3SH+O=CH2SH+OH	3.3E3	2.864	1224
CH3SH+OH=CH3S+H2O	1.3E7	1.770	-1689
CH3SH+OH=CH2SH+H2O	1.9E5	2.220	718
CH3SH+HO2=CH3S+H2O2	9.1E12	0.0	14300
CH3SH+HO2=CH2SH+H2O2	2.0E11	0.0	14500
CH3S+HO2=CH3SH+O2	1.7E-15	7.49	-12060
CH3SH+CH3=CH3S+CH4	8.1E5	1.9	1700
CH3SH+CH3=CH2SH+CH4	1.5E12	0.0	6500
CH3SH+SH=CH3S+H2S	1.2E14	0.0	5920
CH3S=CH2S+H	2.5E38	-7.8	62053
CH3S+O2=CH3+SO2	9.5E25	-3.8	12300

CH2S+H=CH2SH	9.5E08	1.700	-700
CH2SH+O2=CH2S+HO2 DUP	3.8E10	-0.280	4113
CH2SH+O2=CH2S+HO2 DUP	6.1E19	-2.820	5124
CH2S+H=CHS+H2	2.8E07	2.020	7760
CH2S+O=CHS+OH	2.1E13	0.000	3000
CH2S+OH=CHS+H2O	5.2E12	0.000	500
CH2S+CH3=CHS+CH4	2.3E04	2.370	12280
CHS+H2S=CH2S+SH	7.3E12	0.000	6425
CHS+SH=CH2S2	7.3E12	0.230	-578
CHS+S=CS2+H	2.0E13	0.000	0
CHS+H2S2=CH2S+HS2	1.1E13	0.000	3900
CHS+S2=CS2+SH	3.0E11	0.000	4000
CHS+C2H6=CH2S+C2H5	2.0E14	0.000	24360

Tabla C.3.4 Parámetros cinéticos de las reacciones involucradas en el submecanismo de CH_4+H_2S de Mulvihill et al.[13]. Unidades: mol, cm, s, cal, K.

Reacción	A	β	Ea
H2O+H2O=H+OH+H2O	1.01E+26	-2.4	120180

O+O2+M=O3+M	1.88E+21	-2.8	0
O+O3=O2+O2	4.80E+12	0	4090
H+O3=OH+O2	8.43E+13	0	950
OH+O3=HO2+O2	1.14E+12	0	2000
HO2+O3=OH+O2+O2	8.43E+09	0	1200
HSO+SH=SO+H2S	1.00E+13	0	0
HOSO(+M)=OH+SO(+M) Límite de baja presión: Parámetros de TROE: 0.95 2989 1.1	9.90E+21 1.2E46	-2.5 -9.020	75891 52953
CS2+OH(+M)=>CS2OH(+M) Límite de baja presión:	4.80E+12 2.9E17	0 0	0 0
CS2OH(+M)=>CS2+OH(+M) Límite de baja presión:	1.60E+13 9.6E17	0 0	10250 10250
CS2+O2=COS+SO	1.60E+13	0	61600
CS2+O2=COS+SO(S)	3.60E+11	0	35574
CS2+S(+M)=CS3(+M) Límite de baja presión:	1.30E+12 2.5E21	0 -1.600	0 0
CS2+SO=CS+S2O	1.00E+12	0	10000
CS2+SO2=COS+S2O	7.80E+12	0	48600
CS+OH=COS+H	1.00E+14	0	0

CS+OH=CO+SH	2.00E+13	0	0
CS+O3=COS+O2	4.50E+12	0	6000
CS+COS=CS2+CO	2.00E+12	0	37700
CS+SO=COS+S	3.60E+05	2.2	3465
CS+SO2=COS+SO	2.70E+12	0	24300
COS+O2=CO+SO2	1.00E+12	0	32000
COS+SO=S2O+CO	2.00E+12	0	37700
COS2+O=COS+SO	6.00E+13	0	0
COS2+S=COS+S2	6.00E+13	0	0
COS2+O2=COS+SO2	1.00E+12	0	0
CS3+O=CS2+SO	6.00E+13	0	0
CS3+S=CS2+S2	6.00E+13	0	0
CS2OH+O2=>COS+HOSO	1.40E+10	0	0
CS2OH+O2=>HCO+SO2+S	3.00E+09	0	0
CH3+H2S2=CH4+HS2	2.20E+13	0	3900
C2H5+H2S=C2H6+SH	9.90E+11	0	5470
C2H5+H2S2=C2H6+HS2	1.40E+12	0	2770
C2H3+H2S2=C2H4+HS2	2.80E+13	0	1360
C2H3+H2S=C2H4+SH	1.80E+13	0	3900
CH3SH+O3=CH2S+H2O+O2	3.90E+11	0	14900

CH3SH+C2H5=CH3S+C2H6	6.70E+11	0	5250
CH3SH+C2H5=CH2SH+C2H6	7.50E+11	0	7500
CH3SH+C2H3=C2H4+CH2SH	6.40E+12	0	10400
CH3SH+C2H3=C2H4+CH3S	1.20E+13	0	3580
CH2SH+H2S=CH3SH+SH	2.30E+12	0	7620
CH3S+H2S2=CH3SH+HS2	7.40E+13	0	3730
CH2SH+H2S2=CH3SH+HS2	1.50E+12	0	3270
CH3SH+CH2SH=CH3SH+CH3S	1.60E+12	0	6800
CH3SH+CHS=CH2S+CH2SH	2.50E+13	0	21900
CH3SH+CHS=CH2S+CH3S	4.90E+12	0	6110
CH3S+H=CH3+SH	2.00E+13	0	0
CH3S+OH=CH2S+H2O	1.80E+13	0	0
CH3S+HO2=CH2S+H2O2	3.00E+11	0	0
CH3S+CH3=CH2S+CH4	2.40E+13	0	0
CH3S+SH=CH3SSH	9.00E+11	0.2	-1432
CH3S+CS=CH3+CS2	5.90E+04	1.7	1080
C2H6S+H=CH3SH+CH3	5.74E+13	0	6568
C2H6S+CH3=CH4+C2H5S	1.41E+13	0	15190
C2H6S+C2H5=C2H6+C2H5S	2.34E+12	0	16002
C2H6S+CHS=CH2S+C2H5S	4.93E+13	0	21877

C2H6S+CH2SH=CH3SH+C2H5S	2.03E+12	0	18677
C2H6S(1)+H=H2S+C2H5	6.31E+13	0	6591.8
C2H6S(1)+CH3=CH4+C2H5S(1)	1.42E+13	0	13446
C2H6S(1)+CH3=CH4+C2H5S(2)	3.00E+13	0	17674
C2H6S(1)+CH3=CH4+C2H5S(3)	9.78E+12	0	6114.2
C2H6S(1)+C2H5=C2H6+C2H5S(1)	2.09E+12	0	14187
C2H6S(1)+C2H5=C2H6+C2H5S(2)	4.35E+12	0	18892
C2H6S(1)+C2H5=C2H6+C2H5S(3)	6.68E+11	0	5254.4
C2H6S(1)+C2H3=C2H4+C2H5S(1)	1.28E+13	0	8645.8
C2H6S(1)+C2H3=C2H4+C2H5S(2)	2.72E+13	0	12873
C2H6S(1)+C2H3=C2H4+C2H5S(3)	1.21E+13	0	3582.5
C2H6S(1)+SH=H2S+C2H5S(3)	1.20E+14	0	5923.1
C2H6S(1)+HS2=H2S2+C2H5S(3)	1.85E+13	0	17268
C2H6S(1)+CH3S=CH3SH+C2H5S(3)	5.21E+13	0	6902.3
C2H6S(1)+CHS=CH2S+C2H5S(1)	5.15E+13	0	20134
C2H6S(1)+CHS=CH2S+C2H5S(2)	9.62E+13	0	24361
C2H6S(1)+CHS=CH2S+C2H5S(3)	4.89E+12	0	6114.2
C2H6S(1)+CH2SH=CH3SH+C2H5S(1)	2.05E+12	0	16456
C2H6S(1)+CH2SH=CH3SH+C2H5S(2)	7.99E+12	0	22235
C2H6S(1)+CH2SH=CH3SH+C2H5S(3)	1.56E+12	0	6806.8

C2H6S(1)+C2H5S=C2H6S+C2H5S(1)	2.05E+12	0	16456
C2H6S(1)+C2H5S=C2H6S+C2H5S(2)	7.99E+12	0	22235
C2H6S(1)+C2H5S=C2H6S+C2H5S(3)	1.56E+12	0	6806.8
C2H6S(1)+C2H5S(2)=C2H6S(1)+C2H	2.09E+12	0	14187
C2H5S+H2S=C2H6S+SH	2.27E+12	0	7618.8
C2H5S+H2S2=C2H6S+HS2	1.51E+12	0	3272
C2H5S+CH3SH=C2H6S+CH3S	1.56E+12	0	6806.8
C2H5S+CH3SSH=C2H6S+CH3S2(1)	7.55E+11	0	3224.3
C2H5S(1)+H2S=C2H6S(1)+SH	4.33E+12	0	6233.6
C2H5S(1)+H2S2=C2H6S(1)+HS2	2.63E+12	0	1719.6
C2H5S(1)+CH3SH=C2H6S(1)+CH3S	3.02E+12	0	5517.1
C2H5S(1)+C2H6S(1)=C2H6S(1)+C2H	3.02E+12	0	5517.1
C2H5S(2)=C2H5S(3)	7.94E+01	3	11703
C2H5S(2)=C2H4+SH	3.02E+13	0	8263.7
C2H5S(2)+H2S=C2H6S(1)+SH	9.86E+11	0	5469.3
C2H5S(2)+H2S2=C2H6S(1)+HS2	1.38E+12	0	2770.5
C2H5S(2)+CH3SH=C2H6S(1)+CH3S	6.68E+11	0	5254.4
C2H5S(2)+C2H6S(1)=C2H6S(1)+C2H	6.68E+11	0	5254.4
C2H5S(3)=CH2S+CH3	3.98E+15	0	41557
CH3SSH+H=CH3S2(1)+H2	2.22E+04	3.1	-644.9

CH3SSH+CH3=CH3S2+CH4	7.06E+12	0	15190
CH3SSH+CH3=CH3S2(1)+CH4	1.12E+13	0	3845.2
CH3SSH+C2H5=C2H6+CH3S2	1.17E+12	0	16002
CH3SSH+C2H5=CH3S2(1)+C2H6	6.91E+11	0	2722.7
CH3SSH+C2H3=C2H4+CH3S2	6.39E+12	0	10389
CH3SSH+C2H3=C2H4+CH3S2(1)	1.38E+13	0	1313.6
CH3SSH+SH=H2S+CH3S2(1)	1.31E+14	0	3009.3
CH3SSH+HS2=H2S2+CH3S2(1)	9.51E+12	0	7475.5
CH3SSH+CH3S=CH3SH+CH3S2(1)	3.69E+13	0	3725.8
CH3SSH+CH2SH=CH3SH+CH3S2(1)	7.55E+11	0	3224.3
CH3SSH+CHS=CH2S+CH3S2	2.47E+13	0	21877
CH3SSH+CHS=CH2S+CH3S2(1)	5.60E+12	0	3845.2
CH3SSH+C2H5S(1)=C2H6S(1)+CH3S2(1)	1.32E+12	0	1671.8
CH3SSH+C2H5S(2)=C2H6S(1)+CH3S2(1)	6.91E+11	0	2722.7
CH3SSH+CH3S2=CH3SSH+CH3S2(1)	7.55E+11	0	3224.3
CH3S2+H2S=CH3SSH+SH	2.27E+12	0	7618.8
CH3S2+H2S2=CH3SSH+HS2	1.51E+12	0	3272
CH3S2+CH3SH=CH3SSH+CH3S	1.56E+12	0	6806.8
CH3S2+C2H6S=CH3SSH+C2H5S	2.03E+12	0	18677
CH3S2+C2H6S(1)=CH3SSH+C2H5S(1)	2.05E+12	0	16456

CH3S2+C2H6S(1)=CH3SSH+C2H5S(2)	7.99E+12	0	22235
CH3S2+C2H6S(1)=CH3SSH+C2H5S(3)	1.56E+12	0	6806.8
CH3S2+CH2S2=CH3SSH+CHS2	2.08E+12	0	6090.3
S2+CH3=CH3S2(1)	1.53E+03	3	23.9
CH3S2(1)+C2H6S(1)=CH3SSH+C2H5S(3)	1.77E+13	0	17268
CH3S2(1)+CH2S2=CH3SSH+CHS2	5.06E+13	0	17029
CH2S2+H=CHS2+H2	1.74E+04	2.9	1402
CH2S2+C2H5=C2H6+CHS2	8.87E+11	0	4537.9
CH2S2+C2H3=C2H4+CHS2	1.61E+13	0	2866
CH2S2+SH=H2S+CHS2	5.28E+13	0	4179.6
CH2S2+HS2=H2S2+CHS2	5.25E+13	0	17029
CH2S2+CHS=CH2S+CHS2	6.49E+12	0	5397.7
CH2S2+CH2SH=CH3SH+CHS2	2.08E+12	0	6090.3
CH2S2+C2H5S=C2H6S+CHS2	2.08E+12	0	6090.3
CH2S2+C2H5S(1)=C2H6S(1)+CHS2	4.01E+12	0	4800.6
CH2S2+C2H5S(2)=C2H6S(1)+CHS2	8.87E+11	0	4537.9
CHS2=CS2+H	1.14E+14	0	32768
CHS2+C2H6S(1)=CH2S2+C2H5S(3)	6.97E+13	0	13470
C2H6S2+CH3=CH4+C2H5S2	1.42E+13	0	13446
C2H6S2+CH3=CH4+C2H5S2(1)	3.00E+13	0	17674

C2H6S2+CH3=CH4+C2H5S2(2)	1.12E+13	0	3845.2
C2H6S2+C2H5=C2H6+C2H5S2	2.09E+12	0	14187
C2H6S2+C2H5=C2H6+C2H5S2(1)	4.35E+12	0	18892
C2H6S2+C2H3=C2H4+C2H5S2	1.28E+13	0	8645.8
C2H6S2+C2H3=C2H4+C2H5S2(1)	2.72E+13	0	12873
C2H6S2+C2H3=C2H4+C2H5S2(2)	1.38E+13	0	1313.6
C2H6S2+C2H5=C2H6+C2H5S2(2)	6.91E+11	0	2722.7
C2H6S2+SH=H2S+C2H5S2(2)	1.31E+14	0	3009.3
C2H6S2+HS2=H2S2+C2H5S2(2)	9.51E+12	0	7475.5
C2H6S2+CH3S=CH3SH+C2H5S2(2)	3.69E+13	0	3725.8
C2H6S2+CH2SH=CH3SH+C2H5S2(2)	7.55E+11	0	3224.3
C2H6S2+CH2SH=CH3SH+C2H5S2	2.05E+12	0	16456
C2H6S2+CH2SH=CH3SH+C2H5S2(1)	7.99E+12	0	22235
C2H6S2+CHS=CH2S+C2H5S2	5.15E+13	0	20134
C2H6S2+CHS=CH2S+C2H5S2(1)	9.62E+13	0	24361
C2H6S2+CHS=CH2S+C2H5S2(2)	5.60E+12	0	3845.2
C2H6S2+C2H5S=C2H6S+C2H5S2	2.05E+12	0	16456
C2H6S2+C2H5S=C2H6S+C2H5S2(1)	7.99E+12	0	22235
C2H6S2+C2H5S=C2H6S+C2H5S2(2)	7.55E+11	0	3224.3
C2H6S2+C2H5S(1)=C2H6S(1)+C2H5S	1.32E+12	0	1671.8

C2H6S2+C2H5S(2)=C2H6S(1)+C2H5S	6.91E+11	0	2722.7
C2H6S2+CH3S2=CH3SSH+C2H5S2	2.05E+12	0	16456
C2H6S2+CH3S2=CH3SSH+C2H5S2(1)	7.99E+12	0	22235
C2H6S2+CH3S2=CH3SSH+C2H5S2(2)	7.55E+11	0	3224.3
C2H6S2+CH3S2(1)=CH3SSH+C2H5S2(2)	1.39E+14	0	15859
C2H6S2+CHS2=CH2S2+C2H5S2(2)	8.31E+13	0	10556
C2H5S2+H2S=C2H6S2+SH	4.33E+12	0	6233.6
C2H5S2+H2S2=C2H6S2+HS2	2.63E+12	0	1719.6
C2H5S2+CH3SH=C2H6S2+CH3S	3.02E+12	0	5517.1
C2H5S2+C2H6S(1)=C2H6S2+C2H5S(1)	3.84E+12	0	15739
C2H5S2+C2H6S(1)=C2H6S2+C2H5S(2)	1.43E+13	0	21997
C2H5S2+CH3SSH=C2H6S2+CH3S2(1)	1.32E+12	0	1671.8
C2H5S2+CH2S2=C2H6S2+CHS2	4.01E+12	0	4800.6
C2H5S2+C2H6S(1)=C2H6S2+C2H5S(3)	3.02E+12	0	5517.1
C2H5S2+C2H6S2=C2H6S2+C2H5S2(2)	1.32E+12	0	1671.8
C2H5S2(1)+H2S=C2H6S2+SH	9.86E+11	0	5469.3
C2H5S2(1)+H2S2=C2H6S2+HS2	1.38E+12	0	2770.5
C2H5S2(1)+CH3SH=C2H6S2+CH3S	6.68E+11	0	5254.4
C2H5S2(1)+C2H6S(1)=C2H6S2+C2H5S(1)	2.09E+12	0	14187
C2H5S2(1)+C2H6S(1)=C2H6S2+C2H5S(2)	4.40E+12	0	18892

C2H5S2(1)+C2H6S(1)=C2H6S2+C2H5S(3)	6.68E+11	0	5254.4
C2H5S2(1)+CH3SSH=C2H6S2+CH3S2(1)	6.91E+11	0	2722.7
C2H5S2(1)+CH2S2=C2H6S2+CHS2	8.87E+11	0	4537.9
C2H5S2(1)+C2H6S2=C2H6S2+C2H5S2	2.09E+12	0	14187
C2H5S2(1)+C2H6S2=C2H6S2+C2H5S2(2)	6.91E+11	0	2722.7
C2H5S2(2)+C2H6S(1)=C2H6S2+C2H5S(3)	1.77E+13	0	17268
HS2+O2=HSSO+O	1.00E+13	0	26000
HS2+SO3=HSSO+SO2	1.00E+13	0	10000
HS2+HSO=HSSO+SH	1.00E+13	0	7000
S2O+H+M=HSSO+M	6.40E+22	-2.6	287
S2O+HSO2=HSSO+SO2	1.00E+13	0	32000
HSSO+H=S2O+H2	1.00E+13	0	0
HSSO+H=HS2+OH	1.00E+13	0	0
HSSO+O=S2O+OH	1.00E+13	0	0
HSSO+O=SH+SO2	1.00E+13	0	0
HSSO+OH=S2O+H2O	1.00E+13	0	0
HSSO+OH=HS2+HO2	1.00E+13	0	27000
HSSO+HO2=S2O+H2O2	1.00E+13	0	0
HSSO+S=HS2+SO	1.00E+13	0	0
HSSO+S=S2O+SH	1.00E+13	0	0

HSSO+SH=S2O+H2S	1.00E+13	0	0
HSSO+HS2=S2O+H2S2	1.00E+13	0	0
HSSO+S2=S2O+HS2	1.00E+13	0	0

Tabla C.3.5 Parámetros cinéticos de las reacciones involucradas en el submecanismo de CH_4 de Mulvihill et al.[13]. Unidades: mol, cm, s, cal, K.

Reacción	A	β	Ea
CO+OH=HOCO	2.00E+20	-3.5	1309
CO+H2O2=HOCO+OH	3.60E+04	2.5	28660
HOCO(+M)=CO2+H(+M) Límite de baja presión: Parámetros de TROE: 0.39 1.0E-30 1.0E30	8.20E+11 6.0E26	0.4 -3.148	35335 37116
HOCO+H=CO2+H2	3.10E+17	-1.3	555
HOCO+H=CO+H2O	6.00E+15	-0.5	2125
HOCO+O=CO2+OH	9.00E+12	0	0
HOCO+OH=CO2+H2O DUP	4.60E+12	0	-89
HOCO+OH=CO2+H2O DUP	9.50E+06	2	-89
HOCO+HO2=CO2+H2O2	4.00E+13	0	0

HOCO+O2=CO2+HO2	4.00E+09	1	0
CH2O+H=H+CO+H2	5.11E+07	2.2	11524
CH2O+O=H+CO+OH	2.51E+21	-1.9	22674
CH2O+O2=H+CO+HO2	1.44E+15	0	56388.3
CH2O+OH=H+CO+H2O	7.24E+10	0.9	9310
CH2O+HO2=H+CO+H2O2	2.45E+14	0	30120
CH2O+CH3=H+CO+CH4	1.92E+11	0.9	24224
CH3+OH=CH3OH	6.20E+13	0	-33.3
CH3+OH=H2+HCOH	6.5E11	0.11155	932
CH2+M=CH+H+M	5.6E15	0.000	89000
CH2+M=C+H2+M	5.8E12	0.500	68500
CH2(S)+O2=CH2+O2	3.1E13	0.000	0
CH+OH=H+CO+H	1.796E+23	-2.473	19927.3
CH+O2=H+CO+O	1.975E+23	-2.473	19927.3
CH+CO2=H+CO+CO	5.268E+16	-0.723	18887.3
CH3OH+HO2=CH3O+H2O2	1.5E-3	4.61	15828
CH3O+HO2=CH3OH+O2	1.4E+11	0.00	0
CH2OH+O2=CH2O+HO2	7.2E13	0.000	3736
CH2OH+O2=CH2O+HO2	2.9E16	-1.500	0
CH2OH+CH3=C2H4+H2O	7.2E29	-5.0344	9245

CH3OH+H+CO=CH2OH+CH2O	8.316E-05	5.095	14283.2
CH3OH+CH2(S)=CH2OH+CH3	3.54E-04	4.1900	3600.4
CH3OH+CH2(S)=CH3O+CH3	1.36E-04	4.2600	5626.0
CH3OH+H+CO=CH3O+CH2O	2.049E+06	2.065	27598.5
CH3OOH+H=CH2OOH+H2	5.4E10	0.000	1860
CH3OOH+O=CH2OOH+OH	1.6E13	0.000	4750
CH3OOH+OH=CH2OOH+H2O	7.2E11	0.000	-258
CH3O2+HCO=CH3O+H+CO2	3.0E13	0.000	0
CH3O2+CO=CH3O+CO2	1.6E05	2.180	17940
CH3O2+CH2O=CH3OOH+H+CO	2.454E+14	0.027	30133.3
CH2OOH=CH2O+OH	2.4E12	-0.925	1567
HCOH=CO+H2	6.560E+13	0.000	49465
HCOH=CH2O	5.150E+13	0.000	32109
HCOH+H=CH2O+H	1.0E14	0.000	0
HCOH+H=HCO+H2	2.0E13	0.000	0
HCOH+H=H+CO+H2	1.0E13	0.000	0
HCOH+O=CO2+2H	3.0E13	0.000	0
HCOH+OH=HCO+H2O	2.0E13	0.000	0
HCOH+OH=H+CO+H2O	1.0E13	0.000	0
C2H6+CH3O2=CH3OOH+C2H5	1.9E01	3.640	17100

C2H5+HO2=CH3CH2O+OH	3.1E13	0.000	0
C2H5+O2(+M)=CH3CH2OO(+M) Límite de baja presión: Parámetros de TROE: 1E-30 540 1E30 1E-30	1.5E15 3.3E31	-1.000 -4.90	0 0
C2H5+CH3O2=CH3O+CH3CH2O	5.1E12	0.000	-1410
C2H4(+M)=H2CC+H2(+M) Límite de baja presión: Parámetros de TROE: 0.735 180 1035 5417 Eficiencias de 3er cuerpo: H2O/6/ AR/0.7/	8.0E12 7.0E50	0.440 -9.31	88800 99900
C2H4+OH=CH3+CH2O	1.8E05	1.68	2061
C2H4+OH=CH3CHO+H	2.4E-2	3.91	1723
C2H4+OH=CH2CHOH+H	3.2E05	2.19	5256
C2H4+OH=CH2CH2OH DUP	5.91E+41	-10.43	4832.
C2H4+OH=CH2CH2OH DUP	7.29E+31	-6.91	2855
C2H4+HO2=cC2H4O+OH	1.796E+06	1.809	14760.59
C2H4+HO2=CH3CH2OO	6.596E+47	-12.159	20887.07

C2H4+HO2=CH2CH2OOH	1.438E+05	0.878	7815.54
C2H4+CH2(S)=C2H3+CH3 DUP	4.92E+09	1.02	600
C2H4+CH2(S)=C2H3+CH3 DUP	4.92E+09	1.02	600
C2H3+HO2=CH2CHO+OH	3.0E13	0.000	0
C2H3+O2=CH2CHOO	4.07E+27	-4.67	5222.0
C2H3+O2=CHCHO+OH	2.84E+14	-0.80	7232.0
C2H3+O2=CH2CO+OH	1.17E+03	2.43	7074.0
C2H3+O2=OCHCHO+H	3.08E+12	-0.26	3277.0
C2H3+O2=CH2O+H+CO	1.29E+16	-1.13	3791.0
C2H3+O2=CH3O+CO	3.09E+13	-0.89	3682.0
C2H3+O2=CO2+CH3	6.16E+13	-1.05	3743.0
C2H3+CH3OH=C2H4+CH3O	1.03E6	1.51	26630
C2H3+CH3OH=C2H4+CH2OH	1.75E-2	4.02	23370
C2H2(+M)=H2CC(+M) Límite de baja presión: Parámetros de TROE: 0.5 1.E-30 1.E30	1.8E04 2.5E15	3.510 -0.640	43300 49700
C2H2+OH=CHCHOH	3.5E31	-6.200	6635
C2H2+HO2=CH2CHOO	7.11E+20	-3.15	15650.0

C2H2+HO2=CHCHO+OH	3.24E+09	1.05	16950.0
C2H2+HO2=CH2CO+OH	5.16E-04	3.99	18890.0
C2H2+HO2=CH2CHO+O	1.41E+05	1.86	15460.0
C2H2+HO2=OCHCHO+H	3.94E+04	1.68	13980.0
C2H2+HO2=CH2O+HCO	8.66E+07	0.87	14170.0
C2H2+HO2=CH2O+H+CO	8.66E+07	0.87	14170.0
C2H2+HO2=CO+CH3O	3.06E+05	1.07	14220.0
C2H2+HO2=CO2+CH3	4.13E+05	0.96	14140.0
C2H2+O2=HCO+H+CO DUP	6.661E+33	-5.633	82336.1
C2H2+O2=HCO+H+CO DUP	1.069E+26	-3.525	73959.1
C2H2+O2=H+CO+H+CO	1.218E+32	-4.869	93010.6
H2CC+H=C2H2+H	1.0E14	0.000	0
H2CC+OH=CH2CO+H	2.0E13	0.000	0
H2CC+O2=CH2+CO2	1.0E13	0.000	0
C2+M=C+C+M	1.5E16	0.000	142300
C2+O=C+CO	1.0E14	0.000	0
CH3CH2OH=CH2OH+CH3	5.6E64	-14.470	107039
CH3CH2OH=C2H5+OH	1.5E65	-14.89	112282

CH3CH2OH=C2H4+H2O	5.2E43	-8.900	81461
CH3CHOH+H=CH3CH2OH	1.2E53	-12.330	14505
CH3CH2O+H(+M)=CH3CH2OH(+M) Límite de baja presión:	3.1E11 3.8E51	0.894 -15.550	13 11101
CH3CH2OH+H=CH3CHOH+H2	8.8E03	2.680	2913
CH3CH2OH+H=CH2CH2OH+H2	5.3E03	2.810	7491
CH3CH2OH+H=CH3CH2O+H2	9.5E02	3.140	8696
CH3CH2OH+O=CH2CH2OH+OH	9.7E02	3.230	4660
CH3CH2OH+O=CH3CHOH+OH	1.5E05	2.470	876
CH3CH2OH+O=CH3CH2O+OH	1.5E-3	4.700	1730
CH3CH2OH+OH=CH3CHOH+H2O	4.5E02	3.110	-2666
CH3CH2OH+OH=CH2CH2OH+H2O	9.4E03	2.670	-1004
CH3CH2OH+OH=CH3CH2O+H2O DUP	2.4E03	2.820	-691
CH3CH2OH+OH=CH3CH2O+H2O DUP	7.9E07	1.180	-303
CH3CH2OH+HO2=CH3CHOH+H2O2	8.2E03	2.550	10750
CH3CH2OH+HO2=CH2CH2OH+H2O2	1.2E04	2.550	15750
CH3CH2OH+HO2=CH3CH2O+H2O2	2.5E12	0.000	24000
CH3CH2OH+CH3=CH3CHOH+CH4	2.0E01	3.370	7630

CH3CH2OH+CH3=CH2CH2OH+CH4	2.0E00	3.570	7717
CH3CH2OH+CH3=CH3CH2O+CH4	3.3E02	3.300	12283
CH3CHOH(+M)=CH3CHO+H(+M) Límite de baja presión: Parámetros de TROE: 0.187 65.2 2568 41226	6.2E09 1.8E16	1.310 0.00	33778 20782
CH3CHOH(+M)=CH2CHOH+H (+M) Límite de baja presión: Parámetros de TROE: 0.473 10 2218 2615	6.4E09 8.2E14	1.330 0.00	35974 21517
CH3CHOH(+M)=CH3+CH2O(+M) Límite de baja presión: Parámetros de TROE: 0.124 1 1729 50000	2.2E09 5.9E15	1.180 0.000	33987 21333
CH3CHOH+H=CH2CHOH+H2	3.1E12	0.2728	-334
CH3CHOH+H=C2H4+H2O	1.8E17	-1.216	386
CH3CHOH+H=CH3+CH2OH	2.3E20	-1.795	5893
CH3CHOH+H=C2H5+OH	1.6E16	-0.697	6677
CH3CHOH+O=CH3CHO+OH	1.0E14	0.000	0
CH3CHOH+OH=CH3CHO+H2O	5.0E12	0.000	0
CH3CHOH+HO2=CH3CHO+OH+OH	4.0E13	0.000	0
CH3CHOH+O2=CH3CHO+HO2	5.3E17	-1.638	839

CH3CHOH+O2=CH2CHOH+HO2	7.6E02	2.450	-296
CH2CH2OH=CH2CHOH+H	3.3E28	-5.260	35583
CH2CH2OH+H=C2H4+H2O	2.6E22	-2.599	5235
CH2CH2OH+H=CH3+CH2OH	1.9E22	-2.300	7693
CH2CH2OH+H=C2H5+OH	9.2E17	-1.15762	8193
CH2CH2OH+H(+M)=CH3CH2OH(+M) Límite de baja presión: Parámetros de TROE: 0.8422 125 2219 6882	5.2E17 2.0E41	-0.990 -7.080	1580 6685
CH2CH2OH+O=CH2O+CH2OH	4.0E13	0.000	0
CH2CH2OH+OH=CH2CHOH+H2O	4.6961E+18	-1.5805	7999.2
CH2CH2OH+HO2=CH3CH2OH+O2	1.0E12	0.000	0
CH2CH2OH+HO2=>CH2OH+CH2O+OH	3.0E13	0.000	0
CH2CH2OH+O2=CH2CHOH+HO2	3.6E13	-0.880	3074.0
CH2CH2OH+O2=HOCH2CH2OO	6.4E38	-8.770	5859
CH2CH2OH+O2=CH2O+CH2O+OH	4.4E24	-4.360	4396
CH3CHO+H=CH3CH2O	4.6E07	1.710	7090
CH3CH2O+H(+M)=CH2OH+CH3(+M) Límite de baja presión:	2.6E18 3.0E11	-1.050 0.893	5128 17
CH3CH2O+H=CH3CHO+H2	7.5E09	1.150	673
CH3CH2O+OH=CH3CHO+H2O	3.0E13	0.000	0

CH3CH2O+O2=CH3CHO+HO2	1.5E10	0.000	645
CH3CHO=CH2CO+H2	8.5E44	-9.770	90905
CH3CHO=CH4+CO	1.9E45	-9.430	89415
CH3CHO=CH2CHOH	1.1E46	-9.760	81964
CH3CHO+H=CH3CO+H2	1.3E05	2.580	1219
CH3CHO+O=CH3CO+OH	5.8E12	0.000	1808
CH3CHO+OH=CH3CO+H2O	2.8E12	0.000	-709
CH3CHO+OH=CH2CHO+H2O	8.5E13	0.000	5313
CH3CHO+HO2=CH3CO+H2O2	1.7E13	0.000	16293
CH3CHO+HO2=CH2CHO+H2O2	1.1E13	0.000	23248
CH3CHO+O2=CH3CO+HO2	1.2E05	2.500	37554
CH3CHO+O2=CH2CHO+HO2	1.5E07	1.900	49548
CH3CHO+CH3=CH3CO+CH4	3.5E-8	6.210	1629
CH3CHO+CH3=CH2CHO+CH4	1.8E-1	3.440	10384
CH3CHO+CH3O=CH3CO+CH3OH	1.0E11	0.000	2981
CH3CHO+CH3O=CH2CHO+CH3OH	1.2E11	0.000	7100
CH3CHO+CH3O2=CH3CO+CH3OOH	1.7E13	0.000	16293
CH3CHO+CH3O2=CH2CHO+CH3OOH	1.1E13	0.000	23248
cC2H4O=CH2CHO+H	1.8E13	0.200	71780
cC2H4O=CH3+HCO	5.6E13	0.400	61880

cC2H4O=CH3CO+H	2.4E13	0.250	65310
cC2H4O=CH2CO+H2	3.6E12	-0.200	63030
cC2H4O=CH3CHO	3.2E12	-0.750	46424
cC2H4O=C2H2+H2O	7.6E12	0.060	69530
cC2H4O+H=CH3CHO+H	5.6E13	0.000	10950
cC2H4O+H=cC2H3O+H2	2.0E13	0.000	8310
cC2H4O+H=C2H3+H2O	5.0E09	0.000	5000
cC2H4O+H=C2H4+OH	9.5E10	0.000	5000
cC2H4O+O=cC2H3O+OH	1.9E12	0.000	5250
cC2H4O+OH=cC2H3O+H2O	1.8E13	0.000	3610
cC2H4O+HO2=cC2H3O+H2O2	4.0E12	0.000	17000
cC2H4O+O2=cC2H3O+HO2	4.0E13	0.000	61500
cC2H4O+CH3=cC2H3O+CH4	1.1E12	0.000	11830
CH2CHOH(+M)=CH3CHO(+M)	9.7E23	-3.290	59994
CH2CHOH+H=CH2CHO+H2	1.5E03	3.077	7230
CH2CHOH+H=CHCHOH+H2	2.5E07	2.030	15180
CH2CHOH+O=CH2OH+HCO DUP	3.9E12	0.000	1494
CH2CHOH+O=CH2OH+HCO DUP	-2.335E+22	-2.473	21421.3

CH2CHOH+O=CH2OH+HCO DUP	6.2E13	0.000	6855
CH2CHOH+O=CH2OH+HCO DUP	-3.711E+23	-2.473	26782.3
CH2CHOH+O=CH2OH+H+CO DUP	3.711E+23	-2.473	26782.3
CH2CHOH+O=CH2OH+H+CO DUP	2.335E+22	-2.473	21421.3
CH2CHOH+O=CH2CHO+OH	1.6E07	2.000	4400
CH2CHOH+OH=CHCHOH+H2O	1.3E-1	4.200	-860
CH2CHOH+OH=CH2CHO+H2O DUP	2.372E+03	2.82	-691.48
CH2CHOH+OH=CH2CHO+H2O DUP	7.905E+07	1.18	-303.17
CH2CHOH+HO2=CH2CHO+H2O2	1.6E12	0.000	16293
CH2CHOH+HO2=CH3CHO+HO2	1.5E05	1.670	6810
CH2CHOH+O2=>CH2O+HCO+OH DUP	3.5E07	1.800	39000
CH2CHOH+O2=>CH2O+HCO+OH DUP	-2.095E+17	-0.673	58927.3
CH2CHOH+O2=>CH2O+H+CO+OH	2.095E+17	-0.673	58927.3

CHCHOH=HCCOH+H	1.1E31	-6.153	51383
CHCHOH+H=CH2CHO+H	5.0E13	0.000	0
CHCHOH+H=HCCOH+H2	4.5E13	0.000	0
CHCHOH+O=OCHCHO+H	5.0E13	0.000	0
CHCHOH+OH=HCCOH+H2O	2.0E13	0.000	0
CHCHOH+O2=OCHCHO+OH	1.8E12	0.000	-187
CHCHOH+O2=HOCHO+HCO	2.848E+14	-0.586	1237.3
CHCHOH+O2=HOCHO+H+CO	1.112E+22	-2.498	20265.6
CHCHOH+CH2O=CH2CHOH+HCO DUP	1.549E+11	0.413	8163.9
CHCHOH+CH2O=CH2CHOH+HCO DUP	5.117E+13	-0.005	14641.6
CHCHOH+CH2O=CH2CHOH+H+CO	3.232E+13	0.337	25787.3
CHCHOH+HCO=CH2CHOH+CO	9.0E13	0.000	0
CHCHOH+CH3=HCCOH+CH4	2.1E13	0.000	0
cC2H3O=CH2CHO	8.7E31	-6.900	14994
cC2H3O=CH2CO+H	5.0E13	0.000	14863
cC2H3O=CH3+CO	7.1E12	0.000	14280
CH3CO=CH3+CO	6.5E18	-2.520	16436
CH2CO+H=CH3CO	2.3E08	1.610	2627

CH3CO+H=CH3+H+CO	1.257E+23	-2.473	19927.3
CH3CO+O2=CH3C(O)OO	2.8E34	-7.210	6060
CH3CO+O2=CH2CO+HO2	3.6E10	0.544	3721
CH3CO+O2=CH2O+CO+OH	4.9E23	-3.712	5895
CH3CO+CH3=C2H6+CO	3.3E13	0.000	0
CH3CO+CH3=CH2CO+CH4	5.3E13	0.000	0
CH3CO+CH3O2=CH3+CO2+CH3O	2.4E13	0.000	0
CH2CHO=CH2CO+H	1.3E34	-6.570	49454
CH2CHO=CH3+CO	6.5E34	-6.870	47191
CH2CHO+H=CH3+H+CO	1.137E+32	-4.773	27620.3
CH2CHO+H=CH3CO+H	9.2E17	-1.15762	8193
CH2CHO+O=CH2O+HCO DUP	5.0E13	0.000	0
CH2CHO+O=CH2O+HCO DUP	-2.993E+23	-2.473	19927.3
CH2CHO+O=CH2O+H+CO	2.993E+23	-2.473	19927.3
CH2CHO+OH=CH2OH+H+CO	5.986E+22	-2.473	19927.3
CH2CHO+HO2=CH2O+HCO+OH	3.1E13	0.000	0
CH2CHO+CH2=C2H4+HCO DUP	5.0E13	0.000	0

CH2CHO+CH2=C2H4+HCO DUP	-2.993E+23	-2.473	19927.3
CH2CHO+CH2=C2H4+H+CO	2.993E+23	-2.473	19927.3
CH2CHO+CH=C2H3+HCO DUP	1.0E14	0.000	0
CH2CHO+CH=C2H3+HCO DUP	-5.986E+23	-2.473	19927.3
CH2CHO+CH=C2H3+H+CO	5.986E+23	-2.473	19927.3
CHCHO+H=CH2CO+H	1.0E14	0.000	0
CHCHO+O2=CO2+H+HCO	2.1E09	0.9929	-269
CHCHO+O2=OCHCHO+O	1.3E06	2.4202	1604
HCCO+OH=HCOH+CO DUP	3.032E+16	-0.935	659.4
HCCO+OH=HCOH+CO DUP	8.694E+19	-1.792	5994.3
HCCO+OH=HCOH+CO DUP	2.873E+12	0.370	-24
HCCO+OH=CH2O+CO	1.187E+21	-2.459	2527.6
HCCO+OH=OCHCO+H	2.638E+08	1.410	849
HCCO+OH=CO2+CH2 DUP	7.292E+27	-5.023	2468.0

HCCO+OH=CO2+CH2 DUP	-5.348E+18	-1.740	2024
HCCO+OH=CO2+CH2 DUP	7.106E+19	-2.300	824
HCCO+O2=HCO+CO+O DUP	2.2E02	2.690	3540
HCCO+O2=HCO+CO+O DUP	-1.317E+12	0.217	23467.3
HCCO+O2=H+CO+CO+O	1.317E+12	0.217	23467.3
C2O+M=C+CO+M	2.0E15	0.000	44200
C2O+O2=CO+CO2	1.0E13	0.000	2600
C2O+C=CO+C2	1.0E14	0.000	0
CH3CH2OOH=CH3CH2O+OH	9.26E52	-11.91	53378
CH3CH2OOH+H=CH3CHOOH+H2	6.5E10	0.000	1860
CH3CH2OOH+H=CH3CH2OO+H2	4.3E10	0.000	1860
CH3CH2OOH+H=CH3CH2O+H2O	1.2E10	0.000	1860
CH3CH2OOH+O=CH3CHOOH+OH	1.6E13	0.000	4750
CH3CH2OOH+O=CH3CH2OO+OH	8.7E12	0.000	4750
CH3CH2OOH+OH=CH3CHOOH+H2O	7.2E11	0.000	-258
CH3CH2OOH+OH=CH3CH2OO+H2O	1.1E12	0.000	-437
CH3CH2OOH+HO2=CH3CH2OO+H2O2	4.1E04	2.500	10206

CH3CHOOH=CH3CHO+OH	3.50E12	-0.947	979
CH3CH2OO=CH2CH2OOH	7.32E-03	2.96	20660
CH3CH2OO+H=CH3CH2O+OH	9.6E13	0.000	0
CH3CH2OO+O=CH3CH2O+O2	2.850E+10	1.0	-724
CH3CH2OO+OH=CH3CH2OH+O2	1.7E14	0	0
CH3CH2OO+HO2=CH3CH2OOH+O2	4.5E11	0.000	-1391
CH3CH2OO+CO=CH3CH2O+CO2	1.6E05	2.180	17940
CH3CH2OO+CH3=CH3CH2O+CH3O	5.1E12	0.000	-1411
CH3CH2OO+CH4=CH3CH2OOH+CH3	4.7E04	2.500	21000
CH3CH2OO+CH3OH=CH3CH2OOH+CH2OH	4.0E13	0.000	19400
CH3CH2OO+CH2O=CH3CH2OOH+HCO DUP	4.1E04	2.500	10206
CH3CH2OO+CH2O=CH3CH2OOH+HCO DUP	-2.454E+14	0.027	30133.3
CH3CH2OO+CH2O=CH3CH2OOH+H+CO	2.454E+14	0.027	30133.3
CH3CH2OO+C2H5=CH3CH2O+CH3CH2O	5.1E12	0.000	-1411
CH3CH2OO+C2H6=CH3CH2OOH+C2H5	8.6E00	3.760	17200
CH3CH2OO+CH3CHO=CH3CH2OOH+CH3CO	2.4E19	-2.200	14030
CH3CH2OO+CH3CHO=CH3CH2OOH+CH2CHO	2.3E11	0.400	14864
CH3CH2OO+CH3CH2OO=CH3CH2O+CH3CH2O +O2	2.9E11	-0.270	408

CH3CH2OO+CH3CH2OO=CH3CHO+CH3CH2OH+O2	4.3E09	0.000	-850
CH2CH2OOH=cC2H4O+OH	4.361E+28	-5.830	17202.08
CH2CHOOH=CH2CHO+OH	2.0E35	-6.700	47450
CH2CHOOH+H=CH2CHOO+H2	4.3E10	0.000	1860
CH2CHOOH+H=CH2CHO+H2O	1.2E10	0.000	1860
CH2CHOOH+O=CH2CHOO+OH	8.7E12	0.000	4750
CH2CHOOH+OH=CH2CHOO+H2O	1.1E12	0.000	-437
CH2CHOOH+HO2=CH2CHOO+H2O2	4.1E04	2.500	10206
CH2CHOO=CHCHO+OH	5.89E+36	-7.10	51440.0
CH2CHOO=CH2CHO+O	1.22E+29	-4.71	42340.0
CH2CHOO=OCHCHO+H	4.72E+20	-2.69	32320.0
CH2CHOO=CH2CO+OH	1.55E+24	-3.87	49850.0
CH2CHOO=CH2O+HCO	1.19E+20	-2.29	30170.0
CH2CHOO=CH2O+H+CO	1.19E+20	-2.29	30170.0
CH2CHOO=CO+CH3O	1.16E-01	3.16	18420.0
CH2CHOO=CO2+CH3	6.03E-03	3.46	17420.0
CH2CHOO+H=CH2CHO+OH	9.6E13	0.000	0
CH2CHOO+O=CH2CHO+O2	1.6E13	0.000	-145
CH2CHOO+OH=CH2CHOH+O2	2.0E15	-0.600	0

CH2CHOO+OH=CH2CHO+HO2	4.0E11	0.600	0
CH2CHOO+HO2=CH2CHOOH+O2	4.5E11	0.000	-1391
CH2CHOO+CO=CH2CHO+CO2	1.6E05	2.180	17940
CH2CHOO+CH3=CH2CHO+CH3O	5.1E12	0.000	-1411
CH2CHOO+CH4=CH2CHOOH+CH3	4.7E04	2.500	21000
CH2CHOO+CH3OH=CH2CHOOH+CH2OH	4.0E13	0.000	19400
CH2CHOO+CH2O=CH2CHOOH+HCO DUP	4.1E04	2.500	10206
CH2CHOO+CH2O=CH2CHOOH+HCO DUP	-2.454E+14	0.027	30133.3
CH2CHOO+CH2O=CH2CHOOH+H+CO	2.454E+14	0.027	30133.3
CH2CHOO+C2H6=CH2CHOOH+C2H5	8.6E00	3.760	17200
OCHCHO=CH2O+CO	8.0E55	-12.600	76713
OCHCHO=HCOH+CO	2.6E57	-13.200	79754
OCHCHO=CO+CO+H2	6.1E57	-13.100	80147
OCHCHO=HCO+HCO	1.9E57	-12.800	84321
OCHCHO+H=CH2O+H+CO	3.232E+23	-2.473	24227.3
OCHCHO+O=OCHCO+OH	4.2E11	0.570	2760
OCHCHO+OH=OCHCO+H2O	4.0E06	2.000	-1630
OCHCHO+HO2=HOCHO+CO+OH	3.3E-4	3.995	300

OCHCHO+HO2=OCHCO+H2O2	4.1E04	2.500	10206
OCHCHO+O2=OCHCO+HO2	2.4E05	2.500	36461
OCHCO=HCO+CO	4.100E+14	0.000	8765.0
OCHCO=H+CO+CO	2.454E+24	-2.473	28692.3
OCHCO+O2=CO+CO2+OH	3.3E14	0.000	2075
CH2O+OH=HOCH2O	6.3E06	1.63	4282
HOCH2O=HOCHO+H	1.000E+14	0.00	1.490E+04
HOCHO(+M)=CO+H2O(+M) Límite de baja presión:	7.5E14 4.1E15	0.000 0.00	68710 52980
HOCHO(+M)=CO2+H2(+M) Límite de baja presión:	4.5E13 1.7E15	0.000 0.000	68240 51110
HOCHO+H=HOCO+H2	2.3E02	3.272	4858
HOCHO+H=OCHO+H2	4.2E05	2.255	14091
HOCHO+O=HOCO+OH	5.1E01	3.422	4216
HOCHO+O=OCHO+OH	1.7E05	2.103	9880
HOCHO+OH=HOCO+H2O	7.8E-6	5.570	-2365
HOCHO+OH=OCHO+H2O	4.9E-5	4.910	-5067
HOCHO+HO2=HOCO+H2O2	4.7E-1	3.975	16787
HOCHO+HO2=OCHO+H2O2	3.9E01	3.080	25206
HOCO+HO2=HOCHO+O2	4.0E11	0.000	0

HOCHO+O2=OCHO+HO2	3.0E13	0.000	63000
OCHO=CO2+H	1.0E10	0.000	0
OCHO+O2=CO2+HO2	5.0E13	0.000	0
CH3C(O)OOH=CH3C(O)O+OH	5.0E14	0.000	40142
CH3C(O)OOH+H=CH3C(O)OO+H2	5.4E10	0.000	1860
CH3C(O)OOH+O=CH3C(O)OO+OH	8.7E12	0.000	4750
CH3C(O)OOH+OH=CH3C(O)OO+H2O	1.1E12	0.000	-437
CH3C(O)OOH+HO2=CH3C(O)OO+H2O2	4.1E04	2.500	10206
CH3C(O)OO+H=CH3C(O)O+OH	1.0E14	0.000	0
CH3C(O)OO+O=CH3+CO2+O2	5.0E12	0.000	0
CH3C(O)OO+O=CH3O+CO+O2	1.5E13	0.000	0
CH3C(O)OO+OH=CH3C(O)O+HO2	4.0E11	0.600	0
CH3C(O)OO+HO2=CH3C(O)O+OH+O2	1.9E11	0.000	-1950
CH3C(O)OO+HO2=CH3C(O)OOH+O2	1.2E11	0.000	-1950
CH3C(O)OO+CH3O2=CH3C(O)O+CH3O+O2	1.1E12	0.000	-1000
CH3CHO+CH3C(O)OO=CH3CO+CH3C(O)OOH	1.7E13	0.000	16293
CH3CHO+CH3C(O)OO=CH2CHO+CH3C(O)OOH	1.1E13	0.000	23248
CH3C(O)O=CH3+CO2	2.2E11	0.290	4579
HOCH2CH2OO=CH2O+CH2O+OH	2.0E15	-2.030	15913.0
HOCH2CH2OO=CH2CHOH+HO2	1.4E10	-0.780	14836

HOCH2CH2OO+HO2=>CH2OOH+CH2OH+O2	2.5E11	0.000	-1490
HOCH2CH2OO+CH2O=>CH2OOH+CH2OH+HCO	4.1E04	2.500	10206
HOCH2CH2OO+C2H4=>CH2O+CH2OH+CH3CHO	2.2E12	0.000	17200

Tabla C.3.6 Parámetros cinéticos de las reacciones involucradas en el submecanismo de CH_4+H_2S de J.R. Petherbridge et al. [21]. Unidades: mol, cm, s, cal, K.

Reacción	A	β	Ea
SH+CH3=CH2S+H2	1.018E+12	0.00	0.00
H+CH3S=CH2S+H2	1.988E13	0.00	0.00
H+CH2S=HCS+H2	5.252E12	1.77	2989.29
H+HCS=H2+CS	1.211E14	0.00	0.00
SH+SH=H2+S2	3.012E10	0.00	0.00

C.4 Reacciones modificadas

En este apartado se van a incluir todas aquellas reacciones que se han modificado por valores más recientes en el mecanismo final del presente trabajo, ya que estaban agregadas en el mecanismo base y tenían valores antiguos. Se van a incluir los parámetros cinéticos que se han estado utilizando en las simulaciones.

Tabla C.4.1 Parámetros cinéticos de las reacciones involucradas en el submecanismo de CH_4+H_2S modificadas. Unidades mol,cm,s,cal, K.

Reacción	A	β	Ea	Fuente
$CH_4+OH=CH_3+H_2O$	1E+06	2.183	2300.000	[12]
$CH_4+O=CH_3+OH$	4.39E5	2.5	6578.	[12]
$CH_3+O_2=CH_2O+OH$	6.38E11	0.0	13515	[12]
$CH_3+O_2=CH_3O+O$	2.7E12	0.0	25000	[12]
$CH_3+OH=CH_2+H_2O$	7.8E+12	0.000	0.0	[12]
$CH_3O+H=CH_3+OH$	1.2E+9	1.010	12000.000	[12]
$CH_2OH+H=CH_3+OH$	6.600E+9	1.000	3200.000	[12]
$C_2H_6+OH=C_2H_5+H_2O$	6.62E13	0.0	5042	[12]
$C_2H_6+H=C_2H_5+H_2$	9.8E013	0.00	9220	[12]
$C_2H_6+O=C_2H_5+OH$	1.8E05	2.80	5802	[12]
$C_2H_6+HO_2=C_2H_5+H_2O_2$	1.1E5	2.50	16850	[12]
$C_2H_6+O_2=C_2H_5+HO_2$	7.29E5	2.5	49160	[12]
$C_2H_6+CH_3=C_2H_5+CH_4$	5.6E10	0.00	9418	[12]

DUP				
$C_2H_6+CH_3=C_2H_5+CH_4$ DUP	8.4E14	0.00	22250	[12]
$C_2H_4+H(+M)=C_2H_5(+M)$ Límite de baja presión: Eficiencias de 3er cuerpo: H_2/2/ CO/2/ CO_2/3/ H_2O/5/	3.97E9 4.71E18	1.28 0.0	1292. 755.0	[12]
$C_2H_4+OH=C_2H_3+H_2O$	2.23E4	2.745	2216	[12]
$C_2H_4+H=C_2H_3+H_2$	2.35E2	3.62	11266	[12]
$CH_3+NO=HCN+H_2O$	1.50E11	0.0	15000	[12]
$CH_3+NO=H_2CN+OH$	4.50E11	0.0	15000	[12]
$CH_3+NO(+M)=CH_3NO(+M)$ Límite de baja presión: Parámetros de TROE: 5.0 1.0E-30 120 1E30	9.0E12 2.5E16	0.0 0.0	192 -2841	[12]
$CH_2+NO=HCN+OH$	3.9E11	0.0	378	[12]
$CH_2+NO=HCNO+H$	3.1E12	0.0	378	[12]
HCO+NO=CO+HNO	7.0E21	0.0	0	[12]
$NH_3+O=NH_2+OH$	2.8E2	3.29	4471	[12]
$NH_2+O=HNO+H$	6.6E13	0.0	0	[12]
$NH_2+O=NH+OH$ DUP	7.0E12	0.0	0	[12]

$NH_2+O=NH+OH$ DUP	8.6E-1	4.01	1673	[12]
$H_2NO+O = NH_2+O_2$	2.6E11	0.4872	29050	[12]
$NH_2+NO=N_2+H_2O$	2.8E20	-2.654	1258	[12]
$NH_2+NO=NNH+OH$	2.3E10	0.425	-814	[12]
$NNH=N_2+H$	1.0E9	0.0	0	[12]
$NNH+O=N_2+OH$	1.2E13	0.145	-217	[12]
$NNH+O=N_2O+H$	1.9E14	-0.274	-22	[12]
NNH+O=NH+NO	5.2E11	0.388	-409	[12]
$NNH+O_2=N_2+HO_2$	5.6E14	-0.385	13	[12]
$NH+NO=N_2O+H$	18E14	-0.351	-244	[12]
$NH+NO=N_2+OH$	2.7E12	-0.0721	-512	[12]
HCN+O=NCO+H	7.6E10	0.48	7810	[12]
HCN+O=NH+CO	4.0E14	-0.65	8514	[12]
HCN+O=CN+OH	4.2E10	0.40	20665	[12]
$HNCO+OH=NCO+H_2O$	3.3E6	1.5	3597	[12]
HNCO+CN=NCO+HCN	5.0E12	0.0	0	[12]
$NCO+NCO=N_2+CO+CO$	3.6E13	0.0	0	[12]
HCO(+M)=H+CO(+M) Límite de baja presión:	4.93E+16 7.43E21	-0.9 -2.36	19724 19383	[13]

Parámetros de TROE: 0.103 139. 10900. 4550 Eficiencias de 3er cuerpo: N_2/1.5/ O_2/1.5/ CO/1.5/ H_2/2.0/ CH_4/5.0/ CO_2/3. / H_2O/15. /				
$CH_2+O_2=CO_2+H+H$	2.1E09	0.9929	-269	[13]
$CH_4+O_2=CH_3+HO_2$	2.03E+05	2.7	51714	[13]
$CH_3+HO_2=CH_3O+OH$	6.8E12	0.0	0.0	[16]
$CH_4+H=CH_3+H_2$	4.1E03	3.156	8755	[17]
$CH_3+H(+M)=CH_4(+M)$ Límite de baja presión: Parámetros de TROE: 0.783 74.0 2941.0 6964.0 Eficiencias de 3er cuerpo: H_2/2.86/ H_2O/8.57/ CH_4/2.86/ CO/2.14/ CO_2/2.86/ C_2H_6/4.29/ N_2/1.43/	5.54E24 1.75E33	-2.17 -4.76	0 2440.0	[18]
$CH_3+CH_3(+M)=C_2H_6(+M)$ Límite de baja presión: Parámetros de TROE: 0.62 73 1180 1E30	9.5E14 1.269E39	-0.538 -7.0	179 2762	[9]
$H+O_2=O+OH$	1.0E14	0.000	15286	[9]
$OH+H_2=H_2O+H$ DUP	2.14E14	0.00	9900	[19]

$OH+H_2=H_2O+H$ DUP	8.31E5	2.34	3500	[19]
$O+H_2=OH+H$ DUP	3.80E+12	0	7948	[13]
$O+H_2=OH+H$ DUP	8.80E+14	0	19175	[13]
$HO_2+H=OH+OH$	7.10E+13	0	295	[13]
H2O2(+M) = OH+OH(+M) Límite de baja presión: Parámetros de TROE: 0.43 1E-30 1E+30 Eficiencias de 3er cuerpo: AR/1.0/ H2O/7.5/ CO2/1.6/ N2/1.5/ O2/1.2/ H2O2/7.7/ H2/3.7/ CO/2.8/	2.00E+12 2.49E+24	0.90 2.30	4.8749E+04 4.8749E+04	[9]
CH3+SH=CH3SH	7.3E12	0.230	-139	[9]
CH3+CH3(+M)=C2H6(+M) Límite de baja presión: Parámetros de TROE: 0.62 73 1180 1E30	9.5E14 1.269E39	-0.538 -7.0	179 2762	Estimada en el presente trabajo

C.5 Mecanismo final del presente trabajo

En este apartado se va a insertar el mecanismo final desarrollado en el presente trabajo de final de grado.

```
!                                                    !
!      MSR MODIFIED M1A MECHANISM FROM POPE AND MILLER                !
!                                                    !
!=============================================================================
! !
!Modified and updtated: Abián M., Millera A., Bilbao R., Alzueta M.U.,
!                       Impact of SO2 on the formation of soot from ethylene pyrolysis.
!                                FUEL 159 (2015) 550-558
!
!*****************************************************
!
! *** 8 November 2017: Mmo preparado por Juan Manuel Colom.
!
!*****************************************************
!
!
ELEMENTS
H O C N S AR
END
SPECIES
!!!ordenadas en el mec
H2S
CH2SH
SO2
SH
H
OH
O
H2              ! m=     2
S2
O3
```

```
CO
CO2
COS
CS2
CS
SO
C2H4
C2H2
CH4
!
!!!CO              ! m=    28
!!!CO2             ! m=    44
!!!!C2H4           ! m=    28
!!!!CH4            ! m=    16
C2H6             ! m=    30
!!!!C2H2           ! m=    26
CH2O             ! m=    30
CH               ! m=    13
CH2              ! m=    14
CH2(S)           ! m=    14
CH3              ! m=    15
H2O              ! m=    18
C2               ! m=    24
C2H              ! m=    25
C2H3             ! m=    27
HCO              ! m=    29
N2               ! m=    28
C2H5             ! m=    29
CH2OH            ! m=    31
CH3O             ! m=    31
O2               ! m=    32
CH3OH            ! m=    32
HO2              ! m=    33
H2O2             ! m=    34
C3H2             ! m=    38
H2CCCH           ! m=    39
C2H2OH
AR               ! m=    40
```

C2O ! m= 40
HCCO ! m= 41
CH2CHCH2 ! m= 41
CH3CCH2 ! m= 41
CH3CHCH ! m= 41
CH2CO ! m= 42
HCCOH ! m= 42
OCHCHO ! m= 58
CH2HCO
!
! ESPECIES INCLUIDAS EN EL MECANISMO DE ETANOL
!
C2H5OH
C2H4OH
CH3CH2O
CH3HCO
CH3CO
C2H5CHO
C2H5CO
HCOO
NO
HCN
C
NO2
NO3
HNO
HONO
H2NO
HNOH
NH3
NH2
NH
N
N2H2
NNH
N2O
CN
NCO

HNCO
HOCN
HCNO
C2N2
NCN
CH3CN
CH2CN
H2CN
CH3NO
HONO2
CH3CHOH
!
!Nuevas especies incluidas
!
CH3O2
CH2CHCHCH2
CH2CHCHCH
C4H2
HCCHCCH
CH2CHCCH
CH2CHCCH2
H2CCCCH
C4H
H2CCCCCH
HCCCHCCH
C6H2 ! m= 74
C5H2 ! m= 62
C5H5 ! m= 65
H2C4O ! m= 66
!
!S Species:
!!!SO2
SO2* SO3
!SO
SO(S) HSO HOS HOSO HSO2 HOSO2 HOSOH HOSHO H2SO HSOH S HSOO OSSO SSO2 HS2O
!S2
HS2 H2S2 HSSO2 H2S3O HSSSOH H2S2O2 VDW1 S4 S5 S6 S7 S8
!COS CS2 CS

CH3S CH3SH CH2S CH3CHO CH3SO2 CH3OSO S2O S3 H2SO4 CH3SO HCS

CH3CH2S CH3SCH3 CH2CH2SH CS2OH

!!!COS2

!Mercaptanos:

CH3OOH

!Formacion de CS2

CHS

CH2S2

CH2SH

!

!Mecanismo Jorge

C6H6

C3H4

!nUEVAS

HOCO

!Gri mech 3.0

C3H7 C3H8 CH2CHO HCNN

!Gersen 2017

CS3 COS2 CH3SSH C2H6S C2H6S(1) C2H5S C2H5S(1) C2H5S(2) C2H5S(3) C2H6S2 C2H5S2 C2H5S2(1) C2H5S2(2) C2H3S2 C2H3S2(2)

CH3S2 CH3S2(1) CHS2 HSSO

CH2OOH HCOH CH2CHOO CHCHO H2CC CHCHOH cC2H4O CH3CH2OO CH2CH2OH CH2CHOH CH2CH2OOH

CH3CH2OH HOCH2CH2OO cC2H3O

HOCHO OCHO CH3C(O)OO CH3C(O)O OCHCO CH2CHOOH CH3CH2OOH CH3CHOOH CH3C(O)OOH HOCH2O

!

END

!

!

THERMO

300.000 1000.000 5000.000

C2H4 121286C 2H 4 G 0300.00 5000.00 1000.00 1

0.03528418E+02 0.11485185E-01-0.04418385E-04 0.07844600E-08-0.05266848E-12 2

0.04428288E+05 0.02230389E+02-0.08614880E+01 0.02796162E+00-0.03388677E-03 3

0.02785152E-06-0.09737879E-10 0.05573046E+05 0.02421148E+03 4

CO 121286C 1O 1 G 0300.00 5000.00 1000.00 1

0.03025078E+02 0.14426885E-02-0.05630827E-05 0.10185813E-09-0.06910951E-13 2

-0.14268350E+05 0.06108217E+02 0.03262451E+02 0.15119409E-02-0.03881755E-04 3

0.05581944E-07-0.02474951E-10-0.14310539E+05 0.04848897E+02 4
CO2 121286C 1O 2 G 0300.00 5000.00 1000.00 1
0.04453623E+02 0.03140168E-01-0.12784105E-05 0.02393996E-08-0.16690333E-13 2
-0.04896696E+06-0.09553959E+01 0.02275724E+02 0.09922072E-01-0.10409113E-04 3
0.06866686E-07-0.02117280E-10-0.04837314E+06 0.10188488E+02 4
CH4 121286C 1H 4 G 0300.00 5000.00 1000.00 1
0.01683478E+02 0.10237236E-01-0.03875128E-04 0.06785585E-08-0.04503423E-12 2
-0.10080787E+05 0.09623395E+02 0.07787415E+01 0.01747668E+00-0.02783409E-03 3
0.03049708E-06-0.12239307E-10-0.09825229E+05 0.13722195E+02 4
CH2O 121286C 1H 2O 1 G 0300.00 5000.00 1000.00 1
0.02995606E+02 0.06681321E-01-0.02628954E-04 0.04737153E-08-0.03212517E-12 2
-0.15320369E+05 0.06912572E+02 0.16527311E+01 0.12631439E-01-0.01888168E-03 3
0.02050031E-06-0.08413237E-10-0.14865404E+05 0.13784820E+02 4
H 120186H 1 G 0300.00 5000.00 1000.00 1
0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2
0.02547162E+06-0.04601176E+01 0.02500000E+02 0.00000000E+00 0.00000000E+00 3
0.00000000E+00 0.00000000E+00 0.02547162E+06-0.04601176E+01 4
H2 121286H 2 G 0300.00 5000.00 1000.00 1
0.02991423E+02 0.07000644E-02-0.05633828E-06-0.09231578E-10 0.15827519E-14 2
-0.08350340E+04-0.13551101E+01 0.03298124E+02 0.08249441E-02-0.08143015E-05 3
-0.09475434E-09 0.04134872E-11-0.10125209E+04-0.03294094E+02 4
C 121086C 1 G 0300.00 5000.00 1000.00 1
0.02602087E+02-0.01787081E-02 0.09087041E-06-0.11499333E-10 0.03310844E-14 2
0.08542154E+06 0.04195177E+02 0.02498584E+02 0.08085776E-03-0.02697697E-05 3
0.03040729E-08-0.11066518E-12 0.08545878E+06 0.04753459E+02 4
CH 121286C 1H 1 G 0300.00 5000.00 1000.00 1
0.02196223E+02 0.02340381E-01-0.07058201E-05 0.09007582E-09-0.03855040E-13 2
0.07086723E+06 0.09178373E+02 0.03200202E+02 0.02072875E-01-0.05134431E-04 3
0.05733890E-07-0.01955533E-10 0.07045259E+06 0.03331587E+02 4
CH2(S) 83194H 2C 1 0 0G 300.000 4000.000 1400.00 0 1
0.40752106E+01 0.15779120E-02-0.10806129E-06-0.84592437E-10 0.14033284E-13 2
0.50007492E+05-0.15480316E+01 0.35932946E+01 0.13151238E-02 0.30756846E-06 3
0.42637904E-09-0.34178712E-12 0.50451547E+05 0.17780241E+01 4
CH2 83194H 2C 1 0 0G 300.000 4000.000 1400.00 0 1
0.39737520E+01 0.16097502E-02-0.10785119E-06-0.86399922E-10 0.14301196E-13 2
0.45608973E+05 0.75549729E-01 0.36872995E+01 0.15066403E-02 0.69679857E-07 3
0.23537297E-09-0.19397147E-12 0.45863672E+05 0.20267601E+01 4
CH3 121286C 1H 3 G 0300.00 5000.00 1000.00 1

0.02844051E+02 0.06137974E-01-0.02230345E-04 0.03785161E-08-0.02452159E-12 2
0.16437809E+05 0.05452697E+02 0.02430442E+02 0.11124099E-01-0.01680220E-03 3
0.16218288E-07-0.05864952E-10 0.16423781E+05 0.06789794E+02 4
O 120186O 1 G 0300.00 5000.00 1000.00 1
0.02542059E+02-0.02755061E-03-0.03102803E-07 0.04551067E-10-0.04368051E-14 2
0.02923080E+06 0.04920308E+02 0.02946428E+02-0.16381665E-02 0.02421031E-04 3
-0.16028431E-08 0.03890696E-11 0.02914764E+06 0.02963995E+02 4
CH4 121286C 1H 4 G 0300.00 5000.00 1000.00 1
0.01683478E+02 0.10237236E-01-0.03875128E-04 0.06785585E-08-0.04503423E-12 2
-0.10080787E+05 0.09623395E+02 0.07787415E+01 0.01747668E+00-0.02783409E-03 3
0.03049708E-06-0.12239307E-10-0.09825229E+05 0.13722195E+02 4
OH 121286O 1H 1 G 0300.00 5000.00 1000.00 1
0.02882730E+02 0.10139743E-02-0.02276877E-05 0.02174683E-09-0.05126305E-14 2
0.03886888E+05 0.05595712E+02 0.03637266E+02 0.01850910E-02-0.16761646E-05 3
0.02387202E-07-0.08431442E-11 0.03606781E+05 0.13588605E+01 4
H2O 20387H 2O 1 G 0300.00 5000.00 1000.00 1
0.02672145E+02 0.03056293E-01-0.08730260E-05 0.12009964E-09-0.06391618E-13 2
-0.02989921E+06 0.06862817E+02 0.03386842E+02 0.03474982E-01-0.06354696E-04 3
0.06968581E-07-0.02506588E-10-0.03020811E+06 0.02590232E+02 4
C2 121286C 2 G 0300.00 5000.00 1000.00 1
0.04135978E+02 0.06531618E-03 0.01837099E-05-0.05295085E-09 0.04712137E-13 2
0.09967272E+06 0.07472923E+01 0.06996045E+02-0.07400601E-01 0.03234703E-04 3
0.04802535E-07-0.03295917E-10 0.09897487E+06-0.13862268E+02 4
C2H 83194H 1C 2 0 0G 300.000 4000.000 1400.00 0 1
0.52086663E+01 0.12875765E-02-0.10398387E-06-0.67526325E-10 0.11751871E-13 2
0.64697773E+05-0.53721781E+01 0.39396334E+01 0.32114412E-02-0.39412765E-06 3
-0.74782530E-09 0.27493521E-12 0.65224684E+05 0.17814000E+01 4
C2H2 121386C 2H 2 G 0300.00 5000.00 1000.00 1
0.04436770E+02 0.05376039E-01-0.01912816E-04 0.03286379E-08-0.02156709E-12 2
0.02566766E+06-0.02800338E+02 0.02013562E+02 0.15190446E-01-0.16163189E-04 3
0.09078992E-07-0.01912746E-10 0.02612444E+06 0.08805378E+02 4
C2H3 83194H 3C 2 0 0G 300.000 4000.000 1400.00 0 1
0.71861677E+01 0.34552682E-02-0.29435373E-06-0.20681942E-09 0.36797774E-13 2
0.32229627E+05-0.15977573E+02 0.24955740E+01 0.10269993E-01-0.10226917E-05 3
-0.27594382E-08 0.96919825E-12 0.34232813E+05 0.10614626E+02 4
CO 121286C 1O 1 G 0300.00 5000.00 1000.00 1
0.03025078E+02 0.14426885E-02-0.05630827E-05 0.10185813E-09-0.06910951E-13 2
-0.14268350E+05 0.06108217E+02 0.03262451E+02 0.15119409E-02-0.03881755E-04 3

0.05581944E-07-0.02474951E-10-0.14310539E+05 0.04848897E+02 4
C2H4 121286C 2H 4 G 0300.00 5000.00 1000.00 1
0.03528418E+02 0.11485185E-01-0.04418385E-04 0.07844600E-08-0.05266848E-12 2
0.04428288E+05 0.02230389E+02-0.08614880E+01 0.02796162E+00-0.03388677E-03 3
0.02785152E-06-0.09737879E-10 0.05573046E+05 0.02421148E+03 4
HCO 121286H 1C 1O 1 G 0300.00 5000.00 1000.00 1
0.03557271E+02 0.03345572E-01-0.13350060E-05 0.02470572E-08-0.01713850E-12 2
0.03916324E+05 0.05552299E+02 0.02898329E+02 0.06199146E-01-0.09623084E-04 3
0.10898249E-07-0.04574885E-10 0.04159922E+05 0.08983614E+02 4
N2 121286N 2 G 0300.00 5000.00 1000.00 1
0.02926640E+02 0.14879768E-02-0.05684760E-05 0.10097038E-09-0.06753351E-13 2
-0.09227977E+04 0.05980528E+02 0.03298677E+02 0.14082404E-02-0.03963222E-04 3
0.05641515E-07-0.02444854E-10-0.10208999E+04 0.03950372E+02 4
C2H5 83194H 5C 2 0 0G 300.000 4000.000 1400.00 0 1
0.87349157E+01 0.54537677E-02-0.37647177E-06-0.31297920E-09 0.52844000E-13 2
0.10265269E+05-0.23104086E+02 0.24398923E+01 0.13747212E-01-0.85500653E-06 3
-0.31469924E-08 0.93754355E-12 0.13158588E+05 0.13099146E+02 4
CH2O 121286C 1H 2O 1 G 0300.00 5000.00 1000.00 1
0.02995606E+02 0.06681321E-01-0.02628954E-04 0.04737153E-08-0.03212517E-12 2
-0.15320369E+05 0.06912572E+02 0.16527311E+01 0.12631439E-01-0.01888168E-03 3
0.02050031E-06-0.08413237E-10-0.14865404E+05 0.13784820E+02 4
C2H6 121686C 2H 6 G 0300.00 4000.00 1000.00 1
0.04825938E+02 0.13840429E-01-0.04557258E-04 0.06724967E-08-0.03598161E-12 2
-0.12717793E+05-0.05239506E+02 0.14625388E+01 0.15494667E-01 0.05780507E-04 3
-0.12578319E-07 0.04586267E-10-0.11239176E+05 0.14432295E+02 4
CH2OH 120186H 3C 1O 1 G 0250.00 4000.00 1000.00 1
0.06327520E+02 0.03608270E-01-0.03201547E-05-0.01938750E-08 0.03509704E-12 2
-0.04474509E+05-0.08329365E+02 0.02862628E+02 0.10015273E-01-0.05285435E-05 3
-0.05138539E-07 0.02246041E-10-0.03349678E+05 0.10397938E+02 4
CH3O 121686C 1H 3O 1 G 0300.00 3000.00 1000.00 1
0.03770799E+02 0.07871497E-01-0.02656384E-04 0.03944431E-08-0.02112616E-12 2
0.12783252E+03 0.02929575E+02 0.02106204E+02 0.07216595E-01 0.05338472E-04 3
-0.07377636E-07 0.02075610E-10 0.09786011E+04 0.13152177E+02 4
O2 121386O 2 G 0300.00 5000.00 1000.00 1
0.03697578E+02 0.06135197E-02-0.12588420E-06 0.01775281E-09-0.11364354E-14 2
-0.12339301E+04 0.03189165E+02 0.03212936E+02 0.11274864E-02-0.05756150E-05 3
0.13138773E-08-0.08768554E-11-0.10052490E+04 0.06034737E+02 4
CH3OH 121686C 1H 4O 1 G 0300.00 5000.00 1000.00 1

0.04029061E+02 0.09376593E-01-0.03050254E-04 0.04358793E-08-0.02224723E-12 2
-0.02615791E+06 0.02378195E+02 0.02660115E+02 0.07341508E-01 0.07170050E-04 3
-0.08793194E-07 0.02390570E-10-0.02535348E+06 0.11232631E+02 4
HO2 20387H 1O 2 G 0300.00 5000.00 1000.00 1
0.04072191E+02 0.02131296E-01-0.05308145E-05 0.06112269E-09-0.02841164E-13 2
-0.15797270E+03 0.03476029E+02 0.02979963E+02 0.04996697E-01-0.03790997E-04 3
0.02354192E-07-0.08089024E-11 0.01762273E+04 0.09222724E+02 4
H2O2 120186H 2O 2 G 0300.00 5000.00 1000.00 1
0.04573167E+02 0.04336136E-01-0.14746888E-05 0.02348903E-08-0.14316536E-13 2
-0.01800696E+06 0.05011369E+01 0.03388753E+02 0.06569226E-01-0.14850125E-06 3
-0.04625805E-07 0.02471514E-10-0.01766314E+06 0.06785363E+02 4
C3H2 102193H 2C 3 G 0150.00 4000.00 1000.00 1
0.07670981E+02 0.02748749E-01-0.04370942E-05-0.06455599E-09 0.16638874E-13 2
0.06259722E+06-0.12368903E+02 0.03166713E+02 0.02482571E+00-0.04591637E-03 3
0.04268019E-06-0.14821524E-10 0.06350421E+06 0.08869446E+02 4
H2CCCH 032599C 3H 3 G 0300.00 4000.00 1000.00 1
0.08831047E+02 0.04357194E-01-0.04109066E-05-0.02368723E-08 0.04376520E-12 2
0.39983875E+05-0.22559194E+02 0.04754199E+02 0.11080277E-01 0.02793323E-05 3
-0.05479212E-07 0.01949629E-10 0.41398515E+05-1.94548824E-01 4
AR 120186AR 1 G 0300.00 5000.00 1000.00 1
0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2
-0.07453750E+04 0.04366000E+02 0.02500000E+02 0.00000000E+00 0.00000000E+00 3
0.00000000E+00 0.00000000E+00-0.07453750E+04 0.04366000E+02 4
C2O 121286C 2O 1 G 0300.00 5000.00 1000.00 1
0.04849809E+02 0.02947585E-01-0.10907286E-05 0.01792562E-08-0.11157585E-13 2
0.03282055E+06-0.06453225E+01 0.03368850E+02 0.08241803E-01-0.08765145E-04 3
0.05569262E-07-0.15400086E-11 0.03317081E+06 0.06713314E+02 4
C3H4 101993H 4C 3 G 0300.00 4000.00 1400.00 1
0.09776256E+02 0.05302137E-01-0.03701117E-05-0.03026385E-08 0.05089581E-12 2
0.01954972E+06-0.03077061E+03 0.02539830E+02 0.16334371E-01-0.01764950E-04 3
-0.04647365E-07 0.01729130E-10 0.02251242E+06 0.09935702E+02 4
C3H4P 101993H 4C 3 G 0300.00 4000.00 1400.00 1
0.09768102E+02 0.05219151E-01-0.03753140E-05-0.02992191E-08 0.05107878E-12 2
0.01860277E+06-0.03020678E+03 0.03029730E+02 0.14989613E-01-0.13985000E-05 3
-0.03969619E-07 0.13882165E-11 0.02148408E+06 0.08004594E+02 4
HCCO 32387H 1C 2O 1 G 0300.00 4000.00 1000.00 1
0.06758073E+02 0.02000400E-01-0.02027607E-05-0.10411318E-09 0.01965164E-12 2
0.01901513E+06-0.09071262E+02 0.05047965E+02 0.04453478E-01 0.02268282E-05 3

-0.14820945E-08 0.02250741E-11 0.01965891E+06 0.04818439E+01 4
CH2CHCH2 82489C 3H 5 G 0300.00 4000.00 1000.00 1
0.09651539E+02 0.08075596E-01-0.07965424E-05-0.04650696E-08 0.08603281E-12 2
0.15300955E+05-0.02686773E+03 0.02276486E+02 0.01985564E+00 0.11238421E-05 3
-0.10145757E-07 0.03441342E-10 0.01789496E+06 0.13725151E+02 4
CH3CCH2 82489C 3H 5 G 0300.00 4000.00 1000.00 1
0.09101018E+02 0.07964167E-01-0.07884945E-05-0.04562036E-08 0.08529212E-12 2
0.02670680E+06-0.02150559E+03 0.03385811E+02 0.14045337E-01 0.03204127E-04 3
-0.03824120E-07-0.09053742E-11 0.02909066E+06 0.11266487E+02 4
CH3CHCH 82489C 3H 5 G 0300.00 4000.00 1000.00 1
0.09209764E+02 0.07871412E-01-0.07724522E-05-0.04497357E-08 0.08377272E-12 2
0.02853967E+06-0.02232369E+03 0.03161863E+02 0.15180997E-01 0.02722659E-04 3
-0.05177112E-07 0.05435286E-12 0.03095547E+06 0.11979733E+02 4
CH2CO 121686C 2H 2O 1 G 0300.00 5000.00 1000.00 1
0.06038817E+02 0.05804840E-01-0.01920953E-04 0.02794484E-08-0.14588676E-13 2
-0.08583402E+05-0.07657581E+02 0.02974970E+02 0.12118712E-01-0.02345045E-04 3
-0.06466685E-07 0.03905649E-10-0.07632636E+05 0.08673553E+02 4
HCCOH 32387H 2C 2O 1 G 0300.00 4000.00 1000.00 1
0.07328324E+02 0.03336416E-01-0.03024705E-05-0.01781106E-08 0.03245168E-12 2
0.07598258E+05-0.14012140E+02 0.03899465E+02 0.09701075E-01-0.03119309E-05 3
-0.05537732E-07 0.02465732E-10 0.08701190E+05 0.04491874E+02 4
C3H6 120186C 3H 6 G 0300.00 5000.00 1000.00 1
0.06732257E+02 0.14908336E-01-0.04949899E-04 0.07212022E-08-0.03766204E-12 2
-0.09235703E+04-0.13313348E+02 0.14933071E+01 0.02092517E+00 0.04486794E-04 3
-0.16689121E-07 0.07158146E-10 0.10748264E+04 0.16145340E+02 4
C2H2OH HCCO TRAN 121196H 3C 2O 1 0G 300.000 3000.000 1000.00 0 1
0.57206843E+01 0.10704185E-01-0.50358494E-05 0.11324499E-08-0.10086621E-12 2
0.12849424E+05-0.47081776E+01 0.81498282E-01 0.31640644E-01-0.34085361E-04 3
0.18978838E-07-0.41950165E-11 0.14060783E+05 0.22908977E+02 4
CH2HCO 110393O 1H 3C 2 G 0300.00 5000.00 1000.00 1
0.05975670E+02 0.08130591E-01-0.02743624E-04 0.04070304E-08-0.02176017E-12 2
0.04903218E+04-0.05045251E+02 0.03409062E+02 0.10738574E-01 0.01891492E-04 3
-0.07158583E-07 0.02867385E-10 0.15214766E+04 0.09558290E+02 4
CH3CO 120186C 2H 3O 1 G 0300.00 5000.00 1000.00 1
0.05612279E+02 0.08449886E-01-0.02854147E-04 0.04238376E-08-0.02268403E-12 2
-0.05187863E+05-0.03274949E+02 0.03125278E+02 0.09778220E-01 0.04521448E-04 3
-0.09009462E-07 0.03193717E-10-0.04108507E+05 0.11228854E+02 4
CO2 121286C 1O 2 G 0300.00 5000.00 1000.00 1

0.04453623E+02 0.03140168E-01-0.12784105E-05 0.02393996E-08-0.16690333E-13 2
-0.04896696E+06-0.09553959E+01 0.02275724E+02 0.09922072E-01-0.10409113E-04 3
0.06866686E-07-0.02117280E-10-0.04837314E+06 0.10188488E+02 4
CH3HCO 120186C 2O 1H 4 G 0300.00 5000.00 1000.00 1
0.05868650E+02 0.10794241E-01-0.03645530E-04 0.05412912E-08-0.02896844E-12 2
-0.02264568E+06-0.06012946E+02 0.02505695E+02 0.13369907E-01 0.04671953E-04 3
-0.11281401E-07 0.04263566E-10-0.02124588E+06 0.13350887E+02 4
CH3O2 BUR95 H 3C 1O 2 0G 200.000 6000.000 1000.000 0 1
0.66812963E 01 0.80057271E-02-0.27188507E-05 0.40631365E-09-0.21927725E-13 2
0.52621851E 03-0.99423847E 01 0.20986490E 01 0.15786357E-01 0.75683261E-07 3
-0.11274587E-07 0.56665133E-11 0.20695879E 04 0.15007068E 02 0.33715510E+04 4
CH3OOH BUR95 H 4C 1O 2 00G 200.000 6000.000 1000.000 1
0.61600316E+01 0.10239957E-01-0.36101507E-05 0.57550301E-09-0.34178147E-13 2
-0.17654526E+05-0.61911544E+01 0.49652507E+01 0.92343510E-03 0.34455956E-04 3
-0.44469600E-07 0.17456120E-10-0.16726970E+05 0.29880275E+01-0.14980760E+05 4
C4H 121686C 4H 1 G 0300.00 5000.00 1000.00 1
0.06242882E+02 0.06193682E-01-0.02085931E-04 0.03082203E-08-0.16364826E-13 2
0.07568019E+06-0.07210806E+02 0.05023247E+02 0.07092375E-01-0.06073762E-07 3
-0.02275752E-07 0.08086994E-11 0.07623812E+06-0.06942594E+00 4
C4H2 121686C 4H 2 G 0300.00 5000.00 1000.00 1
0.09031407E+02 0.06047252E-01-0.01948788E-04 0.02754863E-08-0.13856080E-13 2
0.05294735E+06-0.02385067E+03 0.04005191E+02 0.01981000E+00-0.09865877E-04 3
-0.06635158E-07 0.06077413E-10 0.05424065E+06 0.01845736E+02 4
H2CCCCH 82489C 4H 3 G 0300.00 4000.00 1000.00 1
0.11314095E+02 0.05014414E-01-0.05350444E-05-0.02825309E-08 0.05403279E-12 2
0.05181211E+06-0.03062434E+03 0.06545799E+02 0.12424768E-01 0.05603226E-05 3
-0.05631141E-07 0.16652183E-11 0.05352502E+06-0.04264082E+02 4
HCCHCCH 82489C 4H 3 G 0300.00 4000.00 1000.00 1
0.10752738E+02 0.05381153E-01-0.05549637E-05-0.03052266E-08 0.05761740E-12 2
0.06121419E+06-0.02973025E+03 0.04153881E+02 0.01726287E+00-0.02389374E-05 3
-0.10187000E-07 0.04340504E-10 0.06338070E+06 0.06036506E+02 4
CH2CHCCH 82489C 4H 4 G 0300.00 4000.00 1000.00 1
0.10697773E+02 0.06982014E-01-0.06567747E-05-0.03884517E-08 0.07200946E-12 2
0.03034803E+06-0.03128430E+03 0.03233893E+02 0.01865634E+00 0.12703205E-05 3
-0.09410096E-07 0.02956110E-10 0.03301097E+06 0.09922676E+02 4
CH2CHCCH2 82489C 4H 5 G 0300.00 4000.00 1000.00 1
0.11997762E+02 0.07990580E-01-0.08098172E-05-0.04568733E-08 0.08636911E-12 2
0.03228493E+06-0.03528494E+03 0.03879443E+02 0.01997663E+00 0.01872777E-04 3

-0.09306953E-07 0.02386116E-10 0.03526859E+06 0.09842152E+02 4
CH2CHCHCH 82489C 4H 5 G 0300.00 4000.00 1000.00 1
0.12865971E+02 0.07943369E-01-0.08626466E-05-0.04655635E-08 0.08951131E-12 2
0.03783552E+06-0.04182502E+03 0.02995240E+02 0.02288456E+00 0.01975471E-04 3
-0.11482454E-07 0.03197823E-10 0.04142218E+06 0.12894539E+02 4
CH2CHCHCH2 120189C 4H 6 G 0300.00 4000.00 1000.00 1
0.12544366E+02 0.09596525E-01-0.09187012E-05-0.05429640E-08 0.10053636E-12 2
0.08597330E+05-0.04217450E+03 0.01931624E+02 0.02479030E+00 0.03018071E-04 3
-0.11546856E-07 0.02586623E-10 0.12554682E+05 0.01701999E+03 4
OCHCHO 120596H 2C 2O 2 0G 300.000 3000.000 1000.00 0 1
0.49087462E+01 0.13182673E-01-0.71416730E-05 0.18461316E-08-0.18525858E-12 2
-0.27116386E+05 0.59148768E+00 0.25068862E+01 0.18899139E-01-0.10302623E-04 3
0.62607508E-09 0.88114253E-12-0.26427374E+05 0.13187043E+02 4
C5H2 20587C 5H 2 G 0300.00 5000.00 1000.00 1
0.11329175E+02 0.07424056E-01-0.02628188E-04 0.04082541E-08-0.02301332E-12 2
0.07878706E+06-0.03617117E+03 0.03062321E+02 0.02709998E+00-0.10091697E-04 3
-0.12727451E-07 0.09167219E-10 0.08114969E+06 0.07071078E+02 4
H2CCCCCH 101993H 3C 5 G 0300.00 4000.00 1400.00 1
0.14407361E+02 0.04424058E-01-0.03618244E-05-0.02456408E-08 0.04327859E-12 2
0.05896103E+06-0.04775144E+03 0.07441420E+02 0.15851654E-01-0.02219895E-04 3
-0.04928037E-07 0.01984559E-10 0.06162266E+06-0.09047891E+02 4
HCCCHCCH 101993H 3C 5 G 0300.00 4000.00 1400.00 1
0.14122474E+02 0.04593411E-01-0.03738175E-05-0.02574328E-08 0.04539160E-12 2
0.06249257E+06-0.04722335E+03 0.06854796E+02 0.01699404E+00-0.02582284E-04 3
-0.05488764E-07 0.02281480E-10 0.06515364E+06-0.07133854E+02 4
C5H5 101993H 5C 5 G 0300.00 4000.00 1400.00 1
0.15310937E+02 0.07473806E-01-0.05837457E-05-0.04386651E-08 0.07696839E-12 2
0.02525889E+06-0.05951593E+03 0.10073161E+01 0.03189880E+00-0.04748189E-04 3
-0.11023903E-07 0.04584680E-10 0.03047390E+06 0.01934167E+03 4
H2C4O 120189H 2C 4O 1 G 0300.00 4000.00 1000.00 1
0.10268878E+02 0.04896164E-01-0.04885080E-05-0.02708566E-08 0.05107013E-12 2
0.02346902E+06-0.02815985E+03 0.04810971E+02 0.13139988E-01 0.09865073E-05 3
-0.06120720E-07 0.16400028E-11 0.02545803E+06 0.02113424E+02 4
C6H2 121686C 6H 2 G 0300.00 5000.00 1000.00 1
0.12756519E+02 0.08034381E-01-0.02618215E-04 0.03725060E-08-0.01878850E-12 2
0.08075469E+06-0.04041262E+03 0.05751085E+02 0.02636719E+00-0.11667596E-04 3
-0.10714498E-07 0.08790297E-10 0.08262012E+06-0.04335532E+02 4
C6H4 111293H 4C 6 G 0300.00 4000.00 1000.00 1

0.14016253E+02 0.08242769E-01-0.08099663E-05-0.04654132E-08 0.08748122E-12 2
0.04410395E+06-0.05139376E+03 0.15200236E+01 0.02876611E+00 0.14177245E-05 3
-0.16505889E-07 0.05873156E-10 0.04844894E+06 0.01719033E+03 4
C6H5 82489C 6H 5 G 0300.00 4000.00 1000.00 1
0.15775887E+02 0.09651109E-01-0.09429416E-05-0.05469111E-08 0.10265216E-12 2
0.03302698E+06-0.06176280E+03 0.11435567E+00 0.03627324E+00 0.11582856E-05 3
-0.02196964E-06 0.08463556E-10 0.03836054E+06 0.02380117E+03 4
C6H6 20387C 6H 6 G 0300.00 5000.00 1000.00 1
0.12910740E+02 0.01723296E+00-0.05024210E-04 0.05893497E-08-0.01947521E-12 2
0.03664511E+05-0.05002699E+03-0.03138012E+02 0.04723103E+00-0.02962207E-04 3
-0.03262819E-06 0.01718691E-09 0.08890031E+05 0.03657573E+03 4
CH3CN 111596H 3C 2N 1 0G 300.000 3000.000 1000.00 0 1
0.23924046E+01 0.15618873E-01-0.79120497E-05 0.19372333E-08-0.18611956E-12 2
0.84999377E+04 0.11145236E+02 0.25197531E+01 0.13567523E-01-0.25764077E-05 3
-0.30893967E-08 0.14288692E-11 0.85533762E+04 0.10920868E+02 4
CH2CN 111596H 2C 2N 1 0G 300.000 3000.000 1000.00 0 1
0.46058146E+01 0.94485160E-02-0.47116329E-05 0.11389957E-08-0.10828942E-12 2
0.29171486E+05 0.10084415E+01 0.25296724E+01 0.18114138E-01-0.18960575E-04 3
0.11944583E-07-0.32544142E-11 0.29592293E+05 0.10993441E+02 4
HNO pg9601H 1N 1O 1 G 0300.00 5000.00 1000.00 1
0.03615144E+02 0.03212486E-01-0.01260337E-04 0.02267298E-08-0.01536236E-12 2
0.11769108E+05 0.04810264E+02 0.02784403E+02 0.06609646E-01-0.09300223E-04 3
0.09437980E-07-0.03753146E-10 0.12025976E+05 0.09035629E+02 4
HCN 110193H 1C 1N 1 G 0300.00 4000.00 1000.00 1
0.03426457E+02 0.03924190E-01-0.01601138E-04 0.03161966E-08-0.02432850E-12 2
0.01485552E+06 0.03607795E+02 0.02417787E+02 0.09031856E-01-0.01107727E-03 3
0.07980141E-07-0.02311141E-10 0.01501044E+06 0.08222891E+02 4
HNCO 110193H 1C 1N 1O 1G 0300.00 4000.00 1400.00 1
0.06545307E+02 0.01965760E-01-0.01562664E-05-0.01074318E-08 0.01874680E-12 2
-0.01664773E+06-0.01003880E+03 0.03858467E+02 0.06390342E-01-0.09016628E-05 3
-0.01898224E-07 0.07651380E-11-0.01562343E+06 0.04882493E+02 4
HOCN 110193H 1C 1N 1O 1G 0300.00 4000.00 1400.00 1
0.06022112E+02 0.01929530E-01-0.01455029E-05-0.01045811E-08 0.01794814E-12 2
-0.04040321E+05-0.05866433E+02 0.03789424E+02 0.05387981E-01-0.06518270E-05 3
-0.01420164E-07 0.05367969E-11-0.03135335E+05 0.06667052E+02 4
NCO 110193C 1N 1O 1 G 0300.00 4000.00 1400.00 1
0.06072346E+02 0.09227829E-02-0.09845574E-06-0.04764123E-09 0.09090445E-13 2
0.01359820E+06-0.08507293E+02 0.03359593E+02 0.05393239E-01-0.08144585E-05 3

-0.01912868E-07 0.07836794E-11 0.01462809E+06 0.06549694E+02 4

NO* dummy O 1N 1 0 G 0300.00 4000.00 1400.00 1

0.06072346E+02 0.09227829E-02-0.09845574E-06-0.04764123E-09 0.09090445E-13 2

0.01359820E+06-0.08507293E+02 0.03359593E+02 0.05393239E-01-0.08144585E-05 3

-0.01912868E-07 0.07836794E-11 0.01462809E+06 0.06549694E+02 4

!

!VALORES TERMODINAMICOS DEL MECANISMO DE ETANOL

!

C2H5OH BUR 8/88C 2H 6O 1 G 200.000 6000.000 1000.00 1

0.65624365E+01 0.15204222E-01-0.53896795E-05 0.86225011E-09-0.51289787E-13 2

-0.31525621E+05-0.94730202E+01 0.48586957E+01-0.37401726E-02 0.69555378E-04 3

-0.88654796E-07 0.35168835E-10-0.29996132E+05 0.48018545E+01-0.28257829E+05 4

C2H4OH MARI99C 2H 5O 1 0G 200.000 4000.000 1000.00 1

0.74564000E+00 0.02930200E-00-2.18510000E-05 8.85746000E-09-1.38170000E-12 2

-0.54736000E+04 0.22235000E+02 0.74564000E+00 0.02930200E-00-2.18510000E-05 3

8.85746000E-09-1.38170000E-12-0.54736000E+04 0.22235000E+02 4

C2H5CHO BURC92C 3H 6O 1 0G 273.150 5000.000 1000.00 1

0.33137982E+01 0.26619606E-01-0.10475596E-04 0.18815334E-08-0.12761310E-12 2

-0.25459603E+05 0.96608447E+01 0.76044596E+01-0.86403564E-02 0.73930097E-04 3

-0.79687398E-07 0.28004927E-10-0.25489789E+05-0.67643691E+01-0.23097645E+05 4

C2H5CO BURC92C 3H 5O 1 0G 298.150 5000.000 1000.00 1

0.30445698E+01 0.23236429E-01-0.86317936E-05 0.14799550E-08-0.96860829E-13 2

-0.61787211E+04 0.13122302E+02 0.67368294E+01-0.26945299E-02 0.49927017E-04 3

-0.50025808E-07 0.15011503E-10-0.65703366E+04-0.23398732E+01-0.43321855E+04 4

HCOO BOZELLI C 1H 1O 2 0G 300.000 5000.000 1453.000 01

6.40920688E+00 3.28189026E-03-1.18710674E-06 1.91323635E-10-1.13932748E-14 2

-2.20542060E+04-1.04575060E+01 1.52482282E+00 1.26249843E-02-6.61406757E-06 3

7.72750880E-10 2.09088864E-13-2.02040511E+04 1.64205770E+01 4

CH2SH BUR 8/88C 1H 3S 1 G 300.000 5000.000 1000.00 1

0.02560000E+02 0.19780000E-01-0.26780000E-04 2.17600000E-08-0.73490000E-13 2

0.17539000E+05 1.17400000E+01 0.02560000E+02 0.19780000E-01-0.26780000E-04 3

2.17600000E-08-0.73490000E-13 0.17539000E+05 1.17400000E+01 4

!

!

!VALORES TERMODINAMICOS DEL MECANISMO DEL S

!

!SO2 121286S 1O 2 G 0300.00 5000.00 1000.00 1

! 0.05254498E+02 0.01978545E-01-0.08204226E-05 0.01576383E-08-0.01120451E-12 2

!-0.03756886E+06-0.01146056E+02 0.02911439E+02 0.08103022E-01-0.06906710E-04 3
! 0.03329016E-07-0.08777121E-11-0.03687882E+06 0.01111740E+03 4
SO2 tpis89S 1.O 2. 0. 0.G 200.000 6000.000 1000. 1 ! -70.95 59.29
5.38423482E+00 1.67930560E-03-6.32062944E-07 1.08465348E-10-6.66890336E-15 2
-3.76067022E+04-1.83130517E+00 3.67480752E+00 2.28302107E-03 8.46893049E-06 3
-1.36562039E-08 5.76271873E-12-3.69455073E+04 7.96866430E+00-3.56978343E+04 4
! GBR1509
SO2* pg00 S 1O 2 G 0300.00 5000.00 1000.00 1
0.05254498E+02 0.01978545E-01-0.08204226E-05 0.01576383E-08-0.01120451E-12 2
-0.08300578E+04-0.01146056E+02 0.02911439E+02 0.08103022E-01-0.06906710E-04 3
0.03329016E-07-0.08777121E-11-0.01400178E+04 0.01111740E+03 4
!SO3 121286S 1O 3 G 0300.00 5000.00 1000.00 1
! 0.07050668E+02 0.03246560E-01-0.01408897E-04 0.02721535E-08-0.01942365E-12 2
!-0.05020668E+06-0.01106443E+03 0.02575283E+02 0.01515092E+00-0.01229872E-03 3
! 0.04240257E-07-0.05266812E-11-0.04894411E+06 0.01219512E+03 4
SO3 tpis89S 1.O 3. 0. 0.G 200.000 6000.000 1000. 1 ! -94.61 61.30
7.29677572E+00 2.73576437E-03-1.06377755E-06 1.80776031E-10-1.12077527E-14 2
-5.03096739E+04-1.24246659E+01 2.37461122E+00 1.59543297E-02-1.26322543E-05 3
2.81827264E-09 6.23371547E-13-4.89269231E+04 1.31043046E+01-4.76155540E+04 4
! GBR 1509
!SO 121286S 1O 1 G 0300.00 5000.00 1000.00 1
! 0.04021078E+02 0.02584856E-02 0.08948142E-06-0.03580145E-09 0.03228430E-13 2
!-0.07119620E+04 0.03452523E+02 0.03080401E+02 0.01803106E-01 0.06705022E-05 3
!-0.02069005E-07 0.08514657E-11-0.03986163E+04 0.08581028E+02 4
SO tpis89S 1.O 1. 0. 0.G 200.000 6000.000 1000. 1 ! 1.14 53.04
3.96894225E+00 3.77296831E-04 7.67102696E-09-1.37544433E-11 1.37139416E-15 2
-7.28571725E+02 3.73493087E+00 3.61859514E+00-2.32173768E-03 1.16462669E-05 3
-1.42092510E-08 5.60765370E-12-4.80621641E+02 6.36504115E+00 5.72529951E+02 4
! GBR 1509
SO(S) est09 S 1O 1 G 0300.00 5000.00 1000.00 1
0.04309940E+02-0.12150870E-02 2.75383045E-06-2.07106108E-09 5.55106589E-13 2
1.07760928E+04 0.01311757E+02 0.04309940E+02-0.12150870E-02 2.75383045E-06 3
-2.07106108E-09 5.55106589E-13 1.07760928E+04 0.01311757E+02 4
!HSO BOZ/PGH 1O 1S 1 0G 300.000 1500.000 1500.00 0 1
! 0.25807593E+01 0.79910902E-02-0.51535972E-05 0.74202801E-09 0.24445691E-12 2
!-0.37976678E+04 0.12226703E+02 0.25807593E+01 0.79910902E-02-0.51535972E-05 3
! 0.74202801E-09 0.24445691E-12-0.37976678E+04 0.12226703E+02 4
HSO T04/07H 1.S 1.O 1. 0.G 200.000 6000.000 1000. 1! -5.20 57.75

4.34724125E+00 2.53372236E-03-9.51430950E-07 1.58095446E-10-9.65294637E-15 2
-4.20893834E+03 3.15887502E+00 4.13565093E+00-3.69243127E-03 2.05169784E-05 3
-2.40530656E-08 9.17084270E-12-3.82371653E+03 5.88770120E+00-2.61672666E+03 4
! GBR 1509
!HOS BOZ/PGH 1O 1S 1 0G 300.000 1500.000 1500.00 0 1
! 0.26373673E+01 0.78911909E-02-0.81172603E-05 0.42483382E-08-0.85790116E-12 2
!-0.10726887E+04 0.11709682E+02 0.26373673E+01 0.78911909E-02-0.81172603E-05 3
! 0.42483382E-08-0.85790116E-12-0.10726887E+04 0.11709682E+02 4
HOS T04/07S 1.O 1.H 1. 0.G 200.000 6000.000 1000. 1 ! -1.60/57.31
4.37246017E+00 2.01398865E-03-6.50854476E-07 9.74413078E-11-5.52225169E-15 2
-2.28578181E+03 3.13657231E+00 3.69440567E+00 3.94327613E-04 1.10155102E-05 3
-1.63102588E-08 7.03352877E-12-1.99257018E+03 7.31635620E+00-8.05146665E+02 4
! GBR 1509
!HOSO Whe09 H 1O 2S 1 0G 300.000 1500.000 1500.00 0 1
! 0.16711716E+01 0.20882497E-01-0.26138676E-04 0.15816303E-07-0.36463525E-11 2
!-0.30422867E+05 0.19201855E+02 0.16711716E+01 0.20882497E-01-0.26138676E-04 3
! 0.15816303E-07-0.36463525E-11-0.30422867E+05 0.19201855E+02 4
HOSO DAGGLA03 GOUMAR99 H 1O 2S 1 0G 300.000 1500.000 1500.00 0 1 ! -57.70
67.47
0.16184697E+01 0.21164061E-01-0.26690482E-04 0.16272216E-07-0.37779005E-11 2
-0.30255641E+05 0.19477260E+02 0.16184697E+01 0.21164061E-01-0.26690482E-04 3
0.16272216E-07-0.37779005E-11-0.30255641E+05 0.19477260E+02 4
DAG/GLA03 GOU/MAR99
!HSO2 PG00 H 1O 2S 1 0G 300.000 1500.000 1500.00 0 1
! 0.15627374E+01 0.20691389E-01-0.23112073E-04 0.12670203E-07-0.27274176E-11 2
!-0.18214824E+05 0.17556820E+02 0.15627374E+01 0.20691389E-01-0.23112073E-04 3
! 0.12670203E-07-0.27274176E-11-0.18214824E+05 0.17556820E+02 4
HSO2 H 1O 2S 1 0G 300.00 2000.00 1000.00 1 ! -33.80 63.00
0.15627374E+01 0.20691389E-01-0.23112073E-04 0.12670203E-07-0.27274176E-11 2
-0.18214824E+05 0.17556820E+02 0.15627374E+01 0.20691389E-01-0.23112073E-04 3
0.12670203E-07-0.27274176E-11-0.18214824E+05 0.17556820E+02 4
ALZ/GLA01 GOU/MAR99
HOSO2 BOZ/R H 1O 3S 1 0G 300.000 1500.000 1500.00 0 1
0.24358474E+01 0.29991941E-01-0.40650871E-04 0.26047603E-07-0.62778546E-11 2
-0.48803251E+05 0.14364072E+02 0.24358474E+01 0.29991941E-01-0.40650871E-04 3
0.26047603E-07-0.62778546E-11-0.48803251E+05 0.14364072E+02 4
HOSOH BOZ/R H 2O 2S 1 0G 300.000 1500.000 1500.00 0 1
0.17225311E+01 0.25308046E-01-0.30864965E-04 0.18614741E-07-0.42872813E-11 2
-0.39295778E+05 0.16536892E+02 0.17225311E+01 0.25308046E-01-0.30864965E-04 3

0.18614741E-07-0.42872813E-11-0.39295778E+05 0.16536892E+02 4
HOSHO BOZ/R H 2O 2S 1 0G 300.000 1500.000 1500.00 0 1
0.11903822E+01 0.25644735E-01-0.26622842E-04 0.13479665E-07-0.26474629E-11 2
-0.33744886E+05 0.19095494E+02 0.11903822E+01 0.25644735E-01-0.26622842E-04 3
0.13479665E-07-0.26474629E-11-0.33744886E+05 0.19095494E+02 4
H2SO BOZ/R H 2O 1S 1 0G 300.000 1500.000 1500.00 0 1
0.19580519E+01 0.97265201E-02 0.68413170E-06-0.62343720E-08 0.24166577E-11 2
-0.66770889E+04 0.14783451E+02 0.19580519E+01 0.97265201E-02 0.68413170E-06 3
-0.62343720E-08 0.24166577E-11-0.66770889E+04 0.14783451E+02 4
!HSOH BOZ/R H 2O 1S 1 0G 300.000 1500.000 1500.00 0 1
! 0.25676441E+01 0.11380521E-01-0.58667324E-05-0.59470041E-09 0.87438329E-12 2
!-0.15571256E+05 0.11766399E+02 0.25676441E+01 0.11380521E-01-0.58667324E-05 3
!-0.59470041E-09 0.87438329E-12-0.15571256E+05 0.11766399E+02 4
HSOH H 2O 1S 1 0G 300.00 5000.00 1388.00 1 ! -28.52 58.66
0.25676441E+01 0.11380521E-01-0.58667324E-05-0.59470041E-09 0.87438329E-12 2
-0.15571256E+05 0.11766399E+02 0.25676441E+01 0.11380521E-01-0.58667324E-05 3
-0.59470041E-09 0.87438329E-12-0.15571256E+05 0.11766399E+02 4
! GLABOZ96
! Zhou - Leeds University
!S 121286S 1 G 0300.00 5000.00 1000.00 1
! 0.02902148E+02-0.05484546E-02 0.02764576E-05-0.05017115E-09 0.03150685E-13 2
! 0.03249423E+06 0.03838471E+02 0.03187329E+02-0.01595776E-01 0.02005531E-04 3
!-0.01507081E-07 0.04931282E-11 0.03242259E+06 0.02414441E+02 4
S J 9/82S 1. 0. 0. 0.G 200.000 6000.000 1000. 1 ! 66.19/40.11
2.87936498E+00-5.11050388E-04 2.53806719E-07-4.45455458E-11 2.66717362E-15 2
3.25013791E+04 3.98140647E+00 2.31725616E+00 4.78018342E-03-1.42082674E-05 3
1.56569538E-08-5.96588299E-12 3.25068976E+04 6.06242434E+00 3.33128471E+04 4
! GBR 1509
!SH 121286S 1H 1 G 0300.00 5000.00 1000.00 1
! 0.03053810E+02 0.01258884E-01-0.04249169E-05 0.06929591E-09-0.04281691E-13 2
! 0.01588225E+06 0.05973551E+02 0.04133327E+02-0.03787893E-02-0.02777854E-04 3
! 0.05370112E-07-0.02394006E-10 0.01555862E+06 0.01611535E+01 4
SH H 1S 1 0 0G 300.00 5000.00 1000.00 1 ! 34.23 46.73
3.05381000E+00 1.25888400E-03-4.24916900E-07 6.92959100E-11-4.28169100E-15 2
1.63513273E+04 5.97355100E+00 4.13332700E+00-3.78789300E-04-2.77785400E-06 3
5.37011200E-09-2.39400600E-12 1.60276973E+04 1.61153500E-01 4
Zhou: R.C. Shiell, X.K. Hu, Q.J. Hu, J.W. Hepburn, J. Phys. Chem. A 104 (2000) 4339–4342.
!H2S 121286H 2S 1 G 0300.00 5000.00 1000.00 1

! 0.02883147E+02 0.03827835E-01-0.01423398E-04 0.02497999E-08-0.01660273E-12 2
!-0.03480743E+05 0.07258162E+02 0.03071029E+02 0.05578261E-01-0.01030967E-03 3
! 0.01201953E-06-0.04838370E-10-0.03559826E+05 0.05935226E+02 4
H2S g 4/01H 2.S 1. 0. 0.G 200.000 6000.000 1000. 1 ! -4.92 49.18
2.97879430E+00 3.59760372E-03-1.22803151E-06 1.96833209E-10-1.16716162E-14 2
-3.51607638E+03 6.77921228E+00 4.12024455E+00-1.87907426E-03 8.21426650E-06 3
-7.06425730E-09 2.14234860E-12-3.68215173E+03 1.53174068E+00-2.47759639E+03 4
! GBR 1509
HSOO H 1O 2S 1 0G 300.00 5000.00 1000.00 1 ! 32.29 67.63
5.87948232E+00 4.58580173E-03-2.93621833E-06 1.10178148E-09-1.86219122E-13 2
1.41706015E+04-1.04622817E+00 3.04640372E+00 1.52114268E-02-1.84762707E-05 3
1.13862234E-08-2.72421836E-12 1.48073744E+04 1.28748017E+01 4
! Zhou: C. Zhou, K. Sendt, B.S. Haynes, J. Phys. Chem. A 113 (2009) 2975–2981.
!S2 121386S 2 G 0300.00 5000.00 1000.00 1
! 0.03904443E+02 0.06925733E-02-0.01233097E-05 0.08783809E-11 0.01374662E-13 2
! 0.01425693E+06 0.04956834E+02 0.03157673E+02 0.03099480E-01-0.01560746E-04 3
!-0.01357891E-07 0.01137444E-10 0.01439187E+06 0.08596062E+02 4
S2 tpis89S 2 0 0 0G 200.000 6000.000 1 ! 30.73 54.52
3.83249656E+00 8.88970881E-04-2.59080844E-07 3.63847115E-11-1.72606371E-15 2
1.42836134E+04 5.33000845E+00 2.87736627E+00 5.00301430E-03-6.04370732E-06 3
3.04738962E-09-3.87017618E-13 1.44342379E+04 9.79873919E+00 1.54669367E+04 4
! Zhou - Burcat
!HS2 burc94H 1S 2 0 0G 298.150 5000.000 2000.00 0 1
! 0.46552282E+01 0.29202531E-02-0.11010941E-05 0.18878697E-09-0.12318000E-13 2
! 0.16492900E+04 0.27987542E+01 0.40214995E+01 0.31961918E-02 0.21507270E-05 3
!-0.48650943E-08 0.21391804E-11 0.18942796E+04 0.64213003E+01 0.32457475E+04 4
HS2 H 1S 2 0G 300.00 2000.00 1000.00 1 ! 25.84 60.94
3.59075969E+00 4.98506901E-03-3.43045513E-06 1.19341826E-09-1.67403033E-13 2
1.17649789E+04 8.92475572E+00 2.81672268E+00 1.03969679E-02-1.55535096E-05 3
1.24197562E-08-3.90834999E-12 1.18156870E+04 1.21143632E+01 4
! Zhou - K. Sendt, B.S. Haynes, J. Phys. Chem. A 109 (2005) 8180–8186;
! K. Sendt, M. Jazbec, B.S. Haynes, Proc. Combust. Inst. 29 (2003) 2439–2446.
!H2S2 burc94H 2S 2 0 0G 298.150 5000.000 2000.00 0 1
! 0.65731735E+01 0.25619139E-02-0.69109315E-06 0.94286242E-10-0.52907210E-14 2
!-0.24677791E+03-0.72991840E+01 0.21128554E+01 0.21398828E-01-0.33893856E-04 3
! 0.28468801E-07-0.95576325E-11 0.67951055E+03 0.14205983E+02 0.20128667E+04 4
H2S2 H 2S 2 0G 300.00 2000.00 1000.00 1 ! 3.70 61.61
4.69311463E+00 6.01993785E-03-3.01832133E-06 7.52297526E-10-7.91533129E-14 2

1.72179592E+02 2.47728860E+00 2.07852476E+00 1.94742814E-02-2.93966240E-05 3
2.37295586E-08-7.52058161E-12 5.96292301E+02 1.44741864E+01 4
! Zhou - K. Sendt, B.S. Haynes, J. Phys. Chem. A 109 (2005) 8180–8186;
! K. Sendt, M. Jazbec, B.S. Haynes, Proc. Combust. Inst. 29 (2003) 2439–2446.
H2S2O2 H 2O 2S 2 G 300.00 5000.00 1000.00 1 ! -69.74 77.82
1.16213004E+01 3.43806006E-03-5.74448284E-07-3.13293096E-10 1.00662179E-13 2
-3.91048380E+04-2.90177401E+01 8.28112013E-01 4.74477762E-02-6.95648159E-05 3
4.87812487E-08-1.32222441E-11-3.69287907E+04 2.29903159E+01 4
! Zhou - K. Sendt, B.S. Haynes, J. Phys. Chem. A 109 (2005) 8180–8186;
! K. Sendt, M. Jazbec, B.S. Haynes, Proc. Combust. Inst. 29 (2003) 2439–2446.
H2S3O H 2O 1S 3 G 300.00 5000.00 1000.00 1 ! -17.86 80.56
1.18514105E+01 3.33850673E-03-6.86562800E-07-2.02600304E-10 7.47780445E-14 2
-1.28853402E+04-2.85026663E+01 3.67805059E+00 4.07191390E-02-6.67990246E-05 3
5.28547092E-08-1.60811288E-11-1.13979874E+04 9.98571106E+00 4
! Zhou - K. Sendt, B.S. Haynes, J. Phys. Chem. A 109 (2005) 8180–8186;
! K. Sendt, M. Jazbec, B.S. Haynes, Proc. Combust. Inst. 29 (2003) 2439–2446.
HSSSOH H 2O 1S 3 G 300.00 5000.00 1000.00 1 ! -28.04 82.12
1.10809208E+01 3.73387762E-03-2.44411342E-07-6.13453741E-10 1.64649581E-13 2
-1.78355780E+04-2.35331548E+01 2.93988478E+00 4.05695638E-02-6.59918573E-05 3
5.33283075E-08-1.67311298E-11-1.63029028E+04 1.49845285E+01 4
! Zhou - K. Sendt, B.S. Haynes, J. Phys. Chem. A 109 (2005) 8180–8186;
! K. Sendt, M. Jazbec, B.S. Haynes, Proc. Combust. Inst. 29 (2003) 2439–2446.
HSSO2 H 1O 2S 2 0G 300.00 2000.00 1000.00 1 ! -40.89 73.61
7.76282262E+00 7.02637234E-03-4.08428794E-06 1.12459784E-09-1.18489230E-13 2
-2.33271862E+04-9.48284274E+00 3.49856646E+00 2.50749289E-02-3.40614452E-05 3
2.40531480E-08-6.85626593E-12-2.24794312E+04 1.09552126E+01 4
! Zhou: PhD; L.A. Curtiss, K. Raghavachari, P.C. Redfern, V.
! Rassolov, J.A. Pople, J. Chem. Phys. 109 (1998) 7764–7776. ??
S4 tpis89S 4. 0. 0. 0.G 200.000 6000.000 1 ! 32.41 70.15
9.12781762E+00 9.13784446E-04-3.62719239E-07 6.24637076E-11-3.90794764E-15 2
1.33309374E+04-1.74976107E+01 1.62124479E+00 3.69694158E-02-6.92243749E-05 3
6.03240791E-08-1.99529262E-11 1.46879795E+04 1.76312033E+01 1.63127271E+04 4
! Zhou - Burcat
S5 tpis89S 5. 0. 0. 0.G 200.000 6000.000 1 ! 31.78 84.61
1.33325960E+01 2.09782536E-04-3.36431685E-07 8.53311588E-11-6.48294924E-15 2
1.13787913E+04-3.48611560E+01 3.27621083E+00 4.32967838E-02-8.47662885E-05 3
8.12574426E-08-2.97793536E-11 1.36965078E+04 1.41196663E+01 1.59953327E+04 4
! Zhou - Burcat

S6 tpis89S 6. 0. 0. 0.G 200.000 2500.000 1 ! 24.21 85.50
1.34043558E+01 3.42127317E-03-1.12816145E-06 1.46420087E-10-6.61286087E-15 2
8.10860569E+03-3.42545590E+01 2.69715935E+00 6.86818730E-02-1.43788282E-04 3
1.35427080E-07-4.71805554E-11 9.35349932E+03 1.24775267E+01 1.21853457E+04 4
! Zhou - Burcat
S7 tpis89S 7. 0. 0. 0.G 200.000 6000.000 1 ! 26.73 96.74
1.78534018E+01 1.21114205E-03-4.83082305E-07 8.34576672E-11-5.23294619E-15 2
7.80776842E+03-5.40618730E+01 2.91732736E+00 8.29649517E-02-1.73743030E-04 3
1.63959287E-07-5.74388498E-11 1.01380200E+04 1.37221660E+01 1.34572415E+04 4
! Zhou - Burcat
S8 tpis89S 8. 0. 0. 0.G 200.000 6000.000 1 ! 24.20 103.35
2.04307658E+01 5.18092908E-03-2.91895357E-06 5.97574588E-10-4.13758389E-14 2
5.11843364E+03-6.74373075E+01 4.13158109E+00 9.43298552E-02-2.05775943E-04 3
2.05747851E-07-7.51844045E-11 8.20318834E+03 7.83537207E+00 1.21807686E+04 4
! Zhou - Burcat
HS2O H 1O 1S 2 0G 300.00 2000.00 1000.00 1 ! -7.89 68.60
6.11859237E+00 5.59523243E-03-3.70626629E-06 1.22524738E-09-1.62789560E-13 2
-6.05886590E+03-1.97720682E+00 2.70484711E+00 2.32126968E-02-3.77894894E-05 3
3.04178811E-08-9.47692405E-12-5.52811032E+03 1.36259179E+01 4
! Zhou: PhD; L.A. Curtiss, K. Raghavachari, P.C. Redfern, V.
! Rassolov, J.A. Pople, J. Chem. Phys. 109 (1998) 7764–7776. ??
SSO2 O 2S 2 0G 300.00 2000.00 1000.00 1 ! -40.72 68.23
6.34280650E+00 6.05027505E-03-4.24571996E-06 1.40852829E-09-1.81318004E-13 2
-2.27684952E+04-3.78737520E+00 2.80168627E+00 1.99919280E-02-2.56401242E-05 3
1.65559742E-08-4.33620009E-12-2.20225598E+04 1.34189370E+01 4
! Zhou: PhD; L.A. Curtiss, K. Raghavachari, P.C. Redfern, V.
! Rassolov, J.A. Pople, J. Chem. Phys. 109 (1998) 7764–7776. ??
VDW1 H 2O 3S 1 G 300.00 5000.00 1000.00 1 ! -131.26 82.88
1.01262222E+01 3.57132793E-03-7.13009073E-09-5.82222901E-10 1.37375969E-13 2
-6.93881691E+04-1.74036743E+01 8.13179120E+00 8.32444914E-03-2.04192137E-06 3
-2.95153810E-09 1.78217150E-12-6.88287103E+04-6.98378761E+00 4
! H2O...SO2??:
! Zhou - K. Sendt, B.S. Haynes, J. Phys. Chem. A 109 (2005) 8180–8186;
! K. Sendt, M. Jazbec, B.S. Haynes, Proc. Combust. Inst. 29 (2003) 2439–2446.
OSSO O 2S 2 0G 300.00 2000.00 1000.00 1 ! -28.15 71.33
8.06932897E+00 2.78600929E-03-1.65788135E-06 4.55717434E-10-4.76687943E-14 2
-1.68597542E+04-1.12637659E+01 4.27684328E+00 1.71764292E-02-2.30032367E-05 3
1.50850596E-08-3.93335889E-12-1.60275576E+04 7.31095245E+00 4

```
! Zhou: PhD; L.A. Curtiss, K. Raghavachari, P.C. Redfern, V.
! Rassolov, J.A. Pople, J. Chem. Phys. 109 (1998) 7764–7776. ??
HSSO2               H   1O   2S   2    0G    300.00   2000.00 1000.00      1 ! -40.89  73.61
 7.76282262E+00 7.02637234E-03-4.08428794E-06 1.12459784E-09-1.18489230E-13    2
-2.33271862E+04-9.48284274E+00 3.49856646E+00 2.50749289E-02-3.40614452E-05    3
 2.40531480E-08-6.85626593E-12-2.24794312E+04 1.09552126E+01                   4
! Zhou: PhD; L.A. Curtiss, K. Raghavachari, P.C. Redfern, V.
! Rassolov, J.A. Pople, J. Chem. Phys. 109 (1998) 7764–7776. ??
CH3NO BUR0302     T12/92C   1H   3N   1O   1G   200.00   6000.00  1000.        1 !BURCAT
 0.50677397E+01 0.93871079E-02-0.33958317E-05 0.55076729E-09-0.33095301E-13    2 !H298 =
18.88 kcal/mol
 0.71852464E+04-0.10709779E+01 0.52463494E+01-0.68175691E-02 0.46713959E-04    3 !S298 =
62.33 cal/mol/K
-0.53482743E-07 0.19916692E-10 0.79241319E+04 0.18687355E+01 0.95017371E+04    4 !
!
!Termodinamica nuevas especies S/C del sacadas del Burcat
!
COS                 g5/01C   1O   1S   1    0G   200.000  6000.000  1000.       1
 5.37456093E+00 2.10411234E-03-7.76417533E-07 1.29745227E-10-7.92407725E-15    2
-1.89178351E+04-3.78473799E+00 1.77198991E+00 1.71486966E-02-2.73082140E-05    3
 2.25553393E-08-7.34373482E-12-1.81328604E+04 1.36810097E+01-1.70424956E+04    4
CS2                 g6/95C   1S   2    0    0G   200.000  6000.000  1000.       1
 5.94905043E+00 1.69288150E-03-6.74333823E-07 1.16460519E-10-6.37363519E-15    2
 1.20171256E+04-6.17036834E+00 2.17230835E+00 1.81263444E-02-3.08080090E-05    3
 2.65150564E-08-8.92801520E-12 1.28063739E+04 1.19826948E+01 1.40357038E+04    4
CS                  g11/01C   1S   1    0    0G   200.000  6000.000  1000.       1
 3.76959667E+00 7.30980640E-04-2.42920716E-07 2.88070971E-11-5.21956199E-17    2
 3.22498707E+04 3.42022942E+00 3.73124786E+00-3.09803648E-03 1.24828276E-05    3
-1.41633372E-08 5.33370965E-12 3.24420956E+04 4.54855088E+00 3.35016830E+04    4
!
CS2OH               dummy  C   1H   1S   2O   1G   200.000  6000.000  1000.       1
 5.94905043E+00 1.69288150E-03-6.74333823E-07 1.16460519E-10-6.37363519E-15    2
 1.20171256E+04-6.17036834E+00 2.17230835E+00 1.81263444E-02-3.08080090E-05    3
 2.65150564E-08-8.92801520E-12 1.28063739E+04 1.19826948E+01 1.40357038E+04    4
!
!COS2               pG/13  C   1O   1S   2    0G   200.000  6000.000  1000.       1
! 2.82500000E+00 2.02120000E-02-2.87800000E-05 1.86200000E-08-4.55300000E-12    2
! 1.54100000E+03 1.23600000E+01 2.82500000E+00 2.02120000E-02-2.87800000E-05    3
! 1.86200000E-08-4.55300000E-12 1.54100000E+03 1.23600000E+01 2.82500000E+00    4
```

!

!

CH3S IU3/03H 3C 1S 1 0G 200.000 6000.000 1000. 1

4.62809340E+00 7.50242892E-03-2.70631691E-06 4.37671177E-10-2.61526827E-14 2

1.30328459E+04 4.15868210E-02 2.56437070E+00 1.15796385E-02-4.50119584E-06 3

-5.02342418E-10 6.95252997E-13 1.37469790E+04 1.12504946E+01 1.49857923E+04 4

CH3SH T12/08C 1H 4S 1 0G 200.000 6000.000 1000. 1

4.50369870E+00 9.49866516E-03-3.34303841E-06 5.31967412E-10-3.15164389E-14 2

-4.46153406E+03 1.51156041E+00 3.78634471E+00 3.77026048E-03 1.96468694E-05 3

-2.65727342E-08 1.05290360E-11-3.87921543E+03 7.09507940E+00-2.45670376E+03 4

CH2S T11/08C 1H 2S 1 0G 200.000 6000.000 1000. 1

4.19801901E+00 5.14114256E-03-1.90400104E-06 3.33562196E-10-2.14380834E-14 2

1.21202116E+04 1.89538934E+00 3.98890625E+00-4.48093468E-03 3.23152583E-05 3

-3.98564197E-08 1.57804745E-11 1.26210562E+04 5.29851918E+00 1.38253747E+04 4

CH3CHO C 2H 4O 1 0G 200.000 6000.000 1000. 1

0.54041108E+01 0.11723059E-01-0.42263137E-05 0.68372451E-09-0.40984863E-13 2

-0.22593122E+05-0.34807917E+01 0.47294595E+01-0.31932858E-02 0.47534921E-04 3

-0.57458611E-07 0.21931112E-10-0.21572878E+05 0.41030159E+01-0.19987949E+05 4

CH3SO2 (ZHU2006) C 1H 3S 1O 2G 200.00 6000.00 1000. 1

0.28260000E+01 0.25630000E-01-0.21440000E-04 9.25300000E-09-0.15790000E-13 2

-0.28809000E+05 1.32900000E+01 0.28260000E+01 0.25630000E-01-0.21440000E-04 3

9.25300000E-09-0.15790000E-13-0.28809000E+05 1.32900000E+01 0.28260000E+01 4

CH3OSO C 1H 3S 1O 2G 200.000 6000.000 1000. 1

0.22960000E+01 0.25080000E-01-0.19940000E-04 8.14500000E-09-0.13260000E-13 2

-0.29221000E+05 1.92800000E+01 0.22960000E+01 0.25080000E-01-0.19940000E-04 3

8.14500000E-09-0.13260000E-13-0.29221000E+05 1.92800000E+01 0.22960000E+01 4

S2O tpis89S 2O 1 0 0G 200.000 6000.000 1000. 1

6.02401811E+00 1.00035579E-03-3.91923038E-07 6.69240060E-11-4.16275707E-15 2

-8.76531218E+03-2.93690271E+00 3.01869800E+00 1.08575811E-02-1.25419070E-05 3

6.57657832E-09-1.21573834E-12-8.02370855E+03 1.21738889E+01-6.73948254E+03 4

S3 S 3 G 200.000 6000.000 1000. 1

6.53302278E+00 4.89117086E-04-1.94120477E-07 3.34257105E-11-2.09106833E-15 2

1.53186530E+04-4.42378063E+00 2.67426151E+00 1.85725510E-02-3.39241252E-05 3

2.89518256E-08-9.41515882E-12 1.60320458E+04 1.37269667E+01 1.74079204E+04 4

CH3SCH3 C 2H 6S 1 0G 200.000 6000.000 1000. 1

6.46633952E+00 1.55897399E-02-5.49135107E-06 8.74455165E-10-5.18380108E-14 2

-7.34925770E+03-8.01940674E+00 5.28055093E+00 2.44703498E-03 4.47525603E-05 3

-5.76668384E-08 2.25740377E-11-6.22993885E+03 2.04977549E+00-4.25469691E+03 4

CH3CH2S C 2H 5S 1 0G 200.000 6000.000 1000. 1

6.06146203E+00 1.35096776E-02-4.79809612E-06 7.68421362E-10-4.57369490E-14 2

8.87147183E+03-5.21760983E+00 4.12080784E+00 6.77995700E-03 2.82399071E-05 3

-3.90230535E-08 1.53781094E-11 1.00274180E+04 7.80653672E+00 1.17370255E+04 4

CH2CH2SH C 2H 5S 1 0G 200.000 6000.000 1000. 1

6.32502214E+00 1.54070231E-02-5.45709466E-06 8.72281676E-10-5.18467041E-14 2

-8.26561807E+03-5.41769249E+00 5.40529602E+00 2.42610602E-03 4.12377755E-05 3

-5.18768956E-08 1.99031036E-11-7.22408589E+03 3.16335395E+00-5.23345332E+03 4

H2SO4 T 8/03H 2S 1O 4 0G 200.000 6000.000 1000. 1

1.13355392E+01 5.60829109E-03-1.94574192E-06 3.07136054E-10-1.81109544E-14 2

-9.21087435E+04-2.96094003E+01 4.53388173E+00 3.10347679E-02-4.10421795E-05 3

2.95752341E-08-8.81459071E-12-9.05459072E+04 3.93961412E+00-8.81230524E+04 4

CH3SO C 1H 3S 1O 1G 200.00 6000.00 1000. 1

2.49700000E+00 1.79300000E-02-1.24500000E-05 4.60900000E-09-7.05600000E-13 2

-1.09760000E+04 1.51000000E+01 2.49700000E+00 1.79300000E-02-1.24500000E-05 3

4.60900000E-09-7.05600000E-13-1.09760000E+04 1.51000000E+01 2.49700000E+00 4

HCS C 1H 1S 1 0G 200.000 6000.000 1000. 1

4.24664932E+00 2.35823084E-03-8.25468697E-07 1.30882236E-10-7.73500263E-15 2

3.24994581E+04 3.27483332E+00 3.79164958E+00-4.94798913E-04 1.27553978E-05 3

-1.73549729E-08 7.20528315E-12 3.27828773E+04 6.50582055E+00 3.39731635E+04 4

! CS2_Formation:

CHS S 1 C 1 H 1 G 3E+02 2E+03 6E+02 1

2.96088242E+00 5.92410544E-03-3.72132997E-06 1.85807328E-10 5.69493618E-13 2

3.31074004E+04 9.20333175E+00 2.96088242E+00 5.92410544E-03-3.72132997E-06 3

1.85807328E-10 5.69493618E-13 3.31074004E+04 9.20333175E+00 4

CH2S2 S 2 C 1 H 2 G 3E+02 2E+03 6E+02 1

9.28227975E-02 3.78289139E-02-5.94374921E-05 4.69657189E-08-1.44348174E-11 2

1.16888208E+04 2.39888789E+01 9.28227975E-02 3.78289139E-02-5.94374921E-05 3

4.69657189E-08-1.44348174E-11 1.16888208E+04 2.39888789E+01 4

!

!

!Termodinamica para Agregadas nuevas 10/06/18

CH2SH S 1 C 1 H 3 G 3E+02 2E+03 6E+02 1

3.76502431E+00 7.18268533E-03 4.29207685E-06-1.01537669E-08 4.53517374E-12 2

1.76791280E+04 8.44775742E+00 3.76502431E+00 7.18268533E-03 4.29207685E-06 3

-1.01537669E-08 4.53517374E-12 1.76791280E+04 8.44775742E+00 4

HOCO FAB/JAN05C 1O 2H 1 0G 200.000 3000.000 998.402 1 !H298 =-44.33 kcal/mol [FAB/JAN05]

4.63988707E+00 5.66362726E-03-2.67855311E-06 6.17048884E-10-5.60953531E-14 2 !S298 = 60.07 cal/mol/K [FAB/JAN05]

-2.40527335E+04 1.90175132E+00 2.82191157E+00 9.66218175E-03-2.78560177E-06 3 !Cp [FAB/JAN05] (polyfit RAS/GLA07a)

-4.12692493E-09 2.61472072E-12-2.35465218E+04 1.14284719E+01 4 !

!

!!!!Gri-mech 3.0

C3H8 L 4/85C 3H 8 G 300.000 5000.000 1000.000 1

0.75341368E+01 0.18872239E-01-0.62718491E-05 0.91475649E-09-0.47838069E-13 2

-0.16467516E+05-0.17892349E+02 0.93355381E+00 0.26424579E-01 0.61059727E-05 3

-0.21977499E-07 0.95149253E-11-0.13958520E+05 0.19201691E+02 4

C3H7 L 9/84C 3H 7 G 300.000 5000.000 1000.000 1

0.77026987E+01 0.16044203E-01-0.52833220E-05 0.76298590E-09-0.39392284E-13 2

0.82984336E+04-0.15480180E+02 0.10515518E+01 0.25991980E-01 0.23800540E-05 3

-0.19609569E-07 0.93732470E-11 0.10631863E+05 0.21122559E+02 4

HCNN SRI/94C 1N 2H 1 G 300.000 5000.000 1000.000 1

0.58946362E+01 0.39895959E-02-0.15982380E-05 0.29249395E-09-0.20094686E-13 2

0.53452941E+05-0.51030502E+01 0.25243194E+01 0.15960619E-01-0.18816354E-04 3

0.12125540E-07-0.32357378E-11 0.54261984E+05 0.11675870E+02 4

CH2CHO SAND86O 1H 3C 2 G 300.000 5000.000 1000.000 1

0.05975670E+02 0.08130591E-01-0.02743624E-04 0.04070304E-08-0.02176017E-12 2

0.04903218E+04-0.05045251E+02 0.03409062E+02 0.10738574E-01 0.01891492E-04 3

-0.07158583E-07 0.02867385E-10 0.15214766E+04 0.09558290E+02 4

!!Gersen 2017

COS2 1210 C 1S 2N 0O 1G 298.150 3000.000 1000.00 1 ! MC Lin, pw

6.47100147E+00 5.31400384E-03-3.33567524E-06 9.65540977E-10-1.05777415E-13 2

8.81198264E+02-4.89420879E+00 2.82159429E+00 2.13606383E-02-2.95791354E-05 3

1.99101868E-08-5.20419029E-12 1.53862942E+03 1.23498199E+01 4

CS3 1212 C 1S 3N 0O 0G 298.150 3000.000 1000.00 1 ! Marshall 2011

7.44998849E+00 4.09008516E-03-2.66836187E-06 7.91509758E-10-8.81304625E-14 2

2.92863391E+04-8.79780982E+00 3.22895232E+00 2.18033829E-02-3.04820379E-05 3

2.01631135E-08-5.13831964E-12 3.00890887E+04 1.13589615E+01 4

CH3SSH S 2 C 1 H 4 G 3E+02 2E+03 6E+02 1

3.45000658E+00 2.17174498E-02-1.53887364E-05 4.66095130E-09-7.35054971E-14 2

-2.51531482E+03 1.10317640E+01 3.45000658E+00 2.17174498E-02-1.53887364E-05 3

4.66095130E-09-7.35054971E-14-2.51531482E+03 1.10317640E+01

C2H6S S 1 C 2 H 6 G 3E+02 2E+03 6E+02 1

3.54306910E+00 1.80088842E-02 3.44054064E-06-1.43734400E-08 6.54366209E-12 2

-6.43957635E+03 9.02191426E+00 3.54306910E+00 1.80088842E-02 3.44054064E-06 3

-1.43734400E-08 6.54366209E-12-6.43957635E+03 9.02191426E+00 4
C2H6S(1) S 1 C 2 H 6 G 3E+02 2E+03 6E+02 1
4.99715179E+00 5.70327864E-03 3.32666851E-05-4.28900849E-08 1.62517198E-11 2
-7.06596781E+03 4.83895279E+00 4.99715179E+00 5.70327864E-03 3.32666851E-05 3
-4.28900849E-08 1.62517198E-11-7.06596781E+03 4.83895279E+00 4
C2H5S S 1 C 2 H 5 G 3E+02 2E+03 6E+02 1
2.79516200E+00 2.46384962E-02-1.51175319E-05 1.70130260E-09 1.64060449E-12 2
1.53829318E+04 1.08014892E+01 2.79516200E+00 2.46384962E-02-1.51175319E-05 3
1.70130260E-09 1.64060449E-12 1.53829318E+04 1.08014892E+01 4
C2H5S(1) S 1 C 2 H 5 G 3E+02 2E+03 6E+02 1
5.27083512E+00 6.31667773E-03 2.40960966E-05-3.29052296E-08 1.27714380E-11 2
1.34064865E+04 3.28415046E+00 5.27083512E+00 6.31667773E-03 2.40960966E-05 3
-3.29052296E-08 1.27714380E-11 1.34064865E+04 3.28415046E+00 4
C2H5S(2) S 1 C 2 H 5 G 3E+02 2E+03 6E+02 1
6.58767302E+00 3.22579018E-04 3.52303452E-05-4.21351374E-08 1.56477857E-11 2
1.76744307E+04-2.41124835E+00 6.58767302E+00 3.22579018E-04 3.52303452E-05 3
-4.21351374E-08 1.56477857E-11 1.76744307E+04-2.41124835E+00 4
C2H5S(3) S 1 C 2 H 5 G 3E+02 2E+03 6E+02 1
2.96473868E+00 8.19219008E-03 3.16985872E-05-4.53690374E-08 1.81271402E-11 2
1.10017436E+04 1.32736604E+01 2.96473868E+00 8.19219008E-03 3.16985872E-05 3
-4.53690374E-08 1.81271402E-11 1.10017436E+04 1.32736604E+01 4
C2H4S S 1 C 2 H 4 G 3E+02 2E+03 6E+02 1
1.39360773E+00 2.70632189E-02-2.26613880E-05 9.47364684E-09-1.22763230E-12 2
8.15709758E+03 1.90210221E+01 1.39360773E+00 2.70632189E-02-2.26613880E-05 3
9.47364684E-09-1.22763230E-12 8.15709758E+03 1.90210221E+01 4
C2H4S(2) S 1 C 2 H 4 G 3E+02 2E+03 6E+02 1
3.36279363E+00 1.00124420E-02 1.41714693E-05-2.36319248E-08 9.68167734E-12 2
7.05827058E+03 1.05234149E+01 3.36279363E+00 1.00124420E-02 1.41714693E-05 3
-2.36319248E-08 9.68167734E-12 7.05827058E+03 1.05234149E+01
C2H6S2 S 2 C 2 H 6 G 3E+02 2E+03 6E+02 1
3.93422696E+00 2.68676551E-02-4.97220072E-06-1.20006241E-08 6.73998299E-12 2
-5.43790248E+03 1.13997590E+01 3.93422696E+00 2.68676551E-02-4.97220072E-06 3
-1.20006241E-08 6.73998299E-12-5.43790248E+03 1.13997590E+01 4
C2H5S2 S 2 C 2 H 5 G 3E+02 2E+03 6E+02 1
4.20791029E+00 2.74810542E-02-1.41427893E-05-2.01576875E-09 3.25970114E-12 2
1.50345518E+04 9.84495663E+00 4.20791029E+00 2.74810542E-02-1.41427893E-05 3
-2.01576875E-09 3.25970114E-12 1.50345518E+04 9.84495663E+00 4
C2H5S2(1) S 2 C 2 H 5 G 3E+02 2E+03 6E+02 1

5.52474819E+00 2.14869555E-02-3.00854062E-06-1.12456766E-08 6.13604883E-12 2

1.93024961E+04 4.14955781E+00 5.52474819E+00 2.14869555E-02-3.00854062E-06 3

-1.12456766E-08 6.13604883E-12 1.93024961E+04 4.14955781E+00 4

C2H5S2(2) S 2 C 2 H 5 G 3E+02 2E+03 6E+02 1

3.87054035E+00 1.95650836E-02 6.02242267E-06-2.09729265E-08 9.70001155E-12 2

4.36035988E+03 1.15688821E+01 3.87054035E+00 1.95650836E-02 6.02242267E-06 3

-2.09729265E-08 9.70001155E-12 4.36035988E+03 1.15688821E+01 4

C2H3S2 S 2 C 2 H 3 G 3E+02 2E+03 6E+02 1

5.42553300E-01 4.07015859E-02-4.29342945E-05 2.02940495E-08-2.93019531E-12 2

2.92744818E+04 2.38793658E+01 5.42553300E-01 4.07015859E-02-4.29342945E-05 3

2.02940495E-08-2.93019531E-12 2.92744818E+04 2.38793658E+01 4

C2H3S2(2) S 2 C 2 H 3 G 3E+02 2E+03 6E+02 1

2.68966753E+00 2.58978589E-02-1.60282327E-05 7.34530197E-11 2.60908507E-12 2

2.51936310E+04 1.42963022E+01 2.68966753E+00 2.58978589E-02-1.60282327E-05 3

7.34530197E-11 2.60908507E-12 2.51936310E+04 1.42963022E+01 4

CHS2 S 2 C 1 H 1 G 3E+02 2E+03 6E+02 1

1.78227402E+00 1.84266329E-02-2.01226669E-05 1.05813349E-08-2.03753253E-12 2

2.58434267E+04 1.76510876E+01 1.78227402E+00 1.84266329E-02-2.01226669E-05 3

1.05813349E-08-2.03753253E-12 2.58434267E+04 1.76510876E+01 4

CH3S2 S 2 C 1 H 3 G 3E+02 2E+03 6E+02 1

2.70209948E+00 2.83470618E-02-3.39468090E-05 2.07356939E-08-4.97656310E-12 2

1.93071933E+04 1.39099513E+01 2.70209948E+00 2.83470618E-02-3.39468090E-05 3

2.07356939E-08-4.97656310E-12 1.93071933E+04 1.39099513E+01 4

CH3S2(1) S 2 C 1 H 3 G 3E+02 2E+03 6E+02 1

3.38631997E+00 1.44148783E-02-4.39411307E-06-4.31135105E-09 2.88652307E-12 2

7.28294753E+03 1.12008872E+01 3.38631997E+00 1.44148783E-02-4.39411307E-06 3

-4.31135105E-09 2.88652307E-12 7.28294753E+03 1.12008872E+01 4

HSSO H 1O 1S 2 0G 300.00 2000.00 1000.00 1 ! -7.89 68.60

6.11859237E+00 5.59523243E-03-3.70626629E-06 1.22524738E-09-1.62789560E-13 2

-6.05886590E+03-1.97720682E+00 2.70484711E+00 2.32126968E-02-3.77894894E-05 3

3.04178811E-08-9.47692405E-12-5.52811032E+03 1.36259179E+01 4

! Zhou: PhD; L.A. Curtiss, K. Raghavachari, P.C. Redfern, V.

! Rassolov, J.A. Pople, J. Chem. Phys. 109 (1998) 7764–7776. ??

CH2OOH C 1H 3O 2 0G 200.00 2500.00 1000.00 1 !H298 = 15.79 kcal/mol [JAN/ROS04]

6.98746029E+00 9.00484259E-03-3.24366912E-06 5.24324826E-10-3.13587080E-14 2 !S298 = 65.89 cal/mol/K [JAN/ROS04]

5.01257769E+03-1.02619220E+01 5.83126679E+00-3.51771199E-03 4.54550577E-05 3 !Cp(T) scaled Cp[CH3OO](T) to Cp298 = 14.89 cal/mol/K [JAN/ROS04]

-5.66903320E-08 2.21633070E-11 6.06187060E+03-5.79143222E-01 4 !

HOCO FAB/JAN05C 1O 2H 1 0G 200.00 3000.00 998.402 1 !H298 =-44.33 kcal/mol [FAB/JAN05]

4.63988707E+00 5.66362726E-03-2.67855311E-06 6.17048884E-10-5.60953531E-14 2 !S298 = 60.07 cal/mol/K [FAB/JAN05]

-2.40527335E+04 1.90175132E+00 2.82191157E+00 9.66218175E-03-2.78560177E-06 3 !Cp [FAB/JAN05] (polyfit RAS/GLA08a)

-4.12692493E-09 2.61472072E-12-2.35465218E+04 1.14284719E+01 4 !

! Fabian WMF Janoschek R J Mol Struct THEOCHEM 2005, 713, 227–234

! CL Rasmussen J Hansen P Marshall P Glarborg Int J Chem Kinet 40 (2008) 454-480

H2CC Vinylidene T 7/11C 2.H 2. 0. 0.G 200.000 6000.000 1000.0 1

4.27807305E+00 4.75622626E-03-1.63007378E-06 2.54622680E-10-1.48860086E-14 2

4.80140478E+04 6.39978600E-01 3.28154941E+00 6.97642650E-03-2.38527914E-06 3

-1.21077631E-09 9.82041734E-13 4.83191706E+04 5.92035686E+00 4.95846418E+04 4

! E Goos A Burcat B Ruscic Ideal gas thermochemical database with updates from active thermochemical

! http://burcat.technion.ac.il/dir/

! mirrored at http://garfield.chem.elte.hu/burcat/burcat.html.

! Accessed April 2016

CH2CHOH T03/10C 2.H 4.O 1. 0.G 200.000 6000.000 1000.0 1

7.49818166E+00 1.03957000E-02-3.66891058E-06 5.85205827E-10-3.47373827E-14 2

-1.81643092E+04-1.38388104E+01 2.28758479E+00 1.97013262E-02 1.96382662E-06 3

-1.94389758E-08 1.02616778E-11-1.65373421E+04 1.41333462E+01-1.49958566E+04 4

! E Goos A Burcat B Ruscic Ideal gas thermochemical database with updates from active thermochemical

! http://burcat.technion.ac.il/dir/

! mirrored at http://garfield.chem.elte.hu/burcat/burcat.html.

! Accessed April 2016

cC2H4O OXYRANE L 8/88C 2H 4O 1 0G 200.000 6000.000 1000.0 1

0.54887641E+01 0.12046190E-01-0.43336931E-05 0.70028311E-09-0.41949088E-13 2

-0.91804251E+04-0.70799605E+01 0.37590532E+01-0.94412180E-02 0.80309721E-04 3

-0.10080788E-06 0.40039921E-10-0.75608143E+04 0.78497475E+01-0.63304657E+04 4

! E Goos A Burcat B Ruscic Ideal gas thermochemical database with updates from active thermochemical

! http://burcat.technion.ac.il/dir/

! mirrored at http://garfield.chem.elte.hu/burcat/burcat.html.

! Accessed April 2016

CH3CH2OO C 2H 5O 2 0G 200.00 6000.00 1000. 1

8.88872432E+00 1.35833179E-02-4.91116949E-06 7.92343362E-10-4.73525704E-14 2

-7.44107388E+03-1.90789836E+01 4.50099327E+00 6.87965342E-03 4.74143971E-05 3

-6.92287127E-08 2.87395324E-11-5.39547911E+03 7.91490068E+00-3.45206633E+03 4

! E Goos A Burcat B Ruscic Ideal gas thermochemical database with updates from active thermochemical

! http://burcat.technion.ac.il/dir/

! mirrored at http://garfield.chem.elte.hu/burcat/burcat.html.

! Accessed April 2016

CH2CH2OH T05/11C 2.H 5.O 1. 0.G 200.000 6000.000 1000. 1

7.01348674E+00 1.20204391E-02-4.21992012E-06 6.70675981E-10-3.97135273E-14 2

-6.16161779E+03-8.62052409E+00 4.20954137E+00 9.12964578E-03 2.47462263E-05 3

-3.92945764E-08 1.66541312E-11-4.91511371E+03 8.30445413E+00-3.10541451E+03 4

! E Goos A Burcat B Ruscic Ideal gas thermochemical database with updates from active thermochemical

! http://burcat.technion.ac.il/dir/

! mirrored at http://garfield.chem.elte.hu/burcat/burcat.html.

! Accessed April 2016

CHCHO H 2 C 2 O 1 G 200.0 3000.0 1000.0 1

5.96287949E+00 7.99898746E-03-4.30605647E-06 1.11076174E-09-1.11415021E-13 2

2.87255915E+04-5.17392496E+00 2.06863692E+00 1.87233234E-02-1.21318942E-05 3

-3.33726595E-10 2.32881768E-12 2.97393543E+04 1.47865706E+01 4

! Lopez et al., Experimental and Kinetic Modeling Study of C2H2 Oxidation at High Pressure, Int. J. Chem. Kin., 2016

CHCHOH H 3 C 2 O 1 G 298.0 6000.0 1000.0 1

8.78246275E+00 5.24796644E-03-1.71857235E-06 2.59722068E-10-1.48227402E-14 2

1.28836399E+04-2.10851258E+01-1.99180555E+00 4.73233467E-02-6.66058794E-05 3

4.68997052E-08-1.30686109E-11 1.52000823E+04 3.14259422E+01 4

! Goldsmith et al., J. Phys. Chem. A 2012, 116, 3325?3346

CH2CHOO 0C 2H 3O 2 G 300.00 2000.00 1000.00 1

0.14160300E+01 0.29933721E-01-0.26385173E-04 0.11770709E-07-0.20511571E-11 2

0.11361727E+05 0.18969526E+02 0.14146113E+01 0.29754629E-01-0.25839387E-04 3

0.11222085E-07-0.18678097E-11 0.11371249E+05 0.19022561E+02 4

! J Gimenez CL Rasmussen MU Alzueta P Marshall P Glarborg Proc. Combust. Inst. 32 (2009) 367-375

CH2CH2OOH T 4/15C 2.H 5.O 2. 0.G 200.000 6000.000 1000. 1

9.41379980E+00 1.33542122E-02-4.68067639E-06 7.43230845E-10-4.39824231E-14 2

1.98459602E+03-2.24516643E+01 5.07456388E+00 1.32389561E-02 2.53758646E-05 3

-4.38089546E-08 1.89061540E-11 3.71063204E+03 2.72289544E+00 5.95858854E+03 4

! E Goos A Burcat B Ruscic Ideal gas thermochemical database with updates from active thermochemical

! http://burcat.technion.ac.il/dir/

! mirrored at http://garfield.chem.elte.hu/burcat/burcat.html.

! Accessed April 2016

CH3CH2OH L 8/88C 2H 6O 1 0G 200.000 6000.000 1000.0 1

0.65624365E+01 0.15204222E-01-0.53896795E-05 0.86225011E-09-0.51289787E-13 2

-0.31525621E+05-0.94730202E+01 0.48586957E+01-0.37401726E-02 0.69555378E-04 3

-0.88654796E-07 0.35168835E-10-0.29996132E+05 0.48018545E+01-0.28257829E+05 4

! E Goos A Burcat B Ruscic Ideal gas thermochemical database with updates from active thermochemical

! http://burcat.technion.ac.il/dir/

! mirrored at http://garfield.chem.elte.hu/burcat/burcat.html.

! Accessed April 2016

CH3CHOH T06/11C 2.H 5.O 1. 0.G 200.000 6000.000 1000.0 1

6.35842302E+00 1.24356276E-02-4.33096839E-06 6.84530381E-10-4.03713238E-14 2

-9.53018581E+03-6.05106112E+00 4.22283250E+00 5.12174798E-03 3.48386522E-05 3

-4.91943637E-08 2.01183723E-11-8.35622088E+03 8.01675700E+00-6.64945980E+03 4

! E Goos A Burcat B Ruscic Ideal gas thermochemical database with updates from active thermochemical

! http://burcat.technion.ac.il/dir/

! mirrored at http://garfield.chem.elte.hu/burcat/burcat.html.

! Accessed April 2016

HOCH2CH2OO C 2H 5O 3 0G 300.00 2500.00 800.0 1

0.05564182E+01 0.41251869E-01-0.31064687E-04 0.12292960E-07-0.19969071E-11 2

-0.22047390E+05 0.24998308E+02 0.05564182E+01 0.41251869E-01-0.31064687E-04 3

0.12292960E-07-0.19969071E-11-0.22047390E+05 0.24998308E+02 4

! S Olivella A Sole J Phys Chem A 108 (2004) 11651–11663

! J Gimenez CL Rasmussen MU Alzueta P Marshall P Glarborg Proc. Combust. Inst. 32 (2009) 367-375

cC2H3O A 1/05C 2.H 3.O 1. 0.G 200.000 6000.000 1000.0 1

5.60158035E+00 9.17613962E-03-3.28028902E-06 5.27903888E-10-3.15362241E-14 2

1.71446252E+04-5.47228512E+00 3.58349017E+00-6.02275805E-03 6.32426867E-05 3

-8.18540707E-08 3.30444505E-11 1.85681353E+04 9.59725926E+00 1.97814471E+04 4

! E Goos A Burcat B Ruscic Ideal gas thermochemical database with updates from active thermochemical

! http://burcat.technion.ac.il/dir/

! mirrored at http://garfield.chem.elte.hu/burcat/burcat.html.

! Accessed April 2016

OCHO 1104 C 1H 1N 0O 2G 298.150 3000.000 1000.00 1 ! fitted to litt data

4.41052368E+00 7.50888367E-03-4.25889679E-06 1.12761124E-09-1.14144138E-13 2

-1.70297531E+04 3.43148293E+00 3.62860375E+00 8.12496033E-03-1.41560718E-06 3

-3.27951824E-09 1.61553900E-12-1.67477889E+04 7.83169538E+00 4

! Marshall and Glarborg, Proc. Combust. Inst. 35 (2015) 153–160

HOCHO FORMIC ACID A 5/14H 2C 1O 2 0G 200.000 6000.000 1000.00 1

0.46138316E+01 0.64496364E-02-0.22908251E-05 0.36716047E-09-0.21873675E-13 2

-4.53303180E+04 0.84788383E+00 0.38983616E+01-0.35587795E-02 0.35520538E-04 3

-0.43849959E-07 0.17107769E-10-4.67785744E+04 0.73495397E+01-4.55218865E+04 4

! E Goos A Burcat B Ruscic Ideal gas thermochemical database with updates from active thermochemical

! http://burcat.technion.ac.il/dir/

! mirrored at http://garfield.chem.elte.hu/burcat/burcat.html.

! Accessed April 2016

CH3C(O)O 1508 C 2H 3N 0O 2G 298.000 3000.000 1000.00 1 ! Bozzelli 2015; PM

4.15456832E+00 1.68674623E-02-8.75191344E-06 2.18661448E-09-2.13394222E-13 2

-2.52304326E+04 5.95052997E+00 1.30016170E+00 2.37699204E-02-1.23328477E-05 3

5.87354833E-11 1.44736765E-12-2.44337929E+04 2.08501841E+01 4

! in Marshall and Glarborg, Proc. Combust. Inst. 35 (2015) 153–160

CH3C(O)OO 1508 C 2H 3N 0O 3G 298.000 3000.000 1000.00 1

5.76603946E+00 1.88598136E-02-9.95181008E-06 2.52994204E-09-2.50541483E-13 2

-2.21268244E+04-4.84080352E-01 2.12837736E+00 2.94919132E-02-2.00221362E-05 3

5.32494396E-09 3.03452421E-14-2.12033645E+04 1.80451737E+01 4

! Bozzelli 2015; PM

OCHCO 0C 2O 2H 1 G 350.000 2900.000 1000.00 1

0.49499388E+01 0.10163032E-01-0.55772010E-05 0.14572026E-08-0.14743475E-12 2

-0.90965061E+04 0.25798798E+01 0.33940561E+01 0.14362856E-01-0.88413766E-05 3

0.16096129E-08 0.32038938E-12-0.86841442E+04 0.10592041E+02 4

! Marshall and Glarborg, Proc. Combust. Inst. 35 (2015) 153–160

CH2CHOOH 0C 2H 4O 2 G 300.00 2000.00 1000.00 1 !JIM/GLA08

0.28251887E+01 0.27416672E-01-0.20445609E-04 0.77739928E-08-0.11866050E-11 2

-0.63252694E+04 0.89664101E+01 0.27982099E+01 0.27437708E-01-0.20346847E-04 3

0.76212730E-08-0.11267055E-11-0.63155298E+04 0.91182864E+01 4

! J Gimenez CL Rasmussen MU Alzueta P Marshall P Glarborg Proc. Combust. Inst. 32 (2009) 367-375

CH3CHOOH C 2H 5O 2 0G 200.00 2500.00 999.993 1 !

9.10837027E+00 1.52964186E-02-5.54863574E-06 9.02285762E-10-5.44120016E-14 2 !H298 = 6.43 kcal/mol [JAN/ROS04]

-9.32702959E+02-2.03914131E+01 6.26853790E+00 1.11351157E-04 6.15943537E-05 3 !S298 = 74.84 cal/mol/K [JAN/ROS04]

-7.95035384E-08 3.12333450E-11 9.62571275E+02-1.80971233E-01 4 !Cp(T) scaled Cp[CH3CH2OO](T) to Cp298 = 19.70 cal/mol/K [JAN/ROS04]

! Janoschek R Rossi MJ Int J Chem Kinet 2004 36 661–686

! CL Rasmussen JG Jacobsen P Glarborg Int J Chem Kinet 40 (2008) 778-807

CH3CH2OOH T02/10C 2.H 6.O 2. 0.G 200.000 6000.000 1000.0 1

9.58691079E+00 1.48603589E-02-5.29787964E-06 8.47317148E-10-5.03436325E-14 2

-2.38367900E+04-2.28310676E+01 4.14672004E+00 9.78668137E-03 4.91492257E-05 3

-7.42532076E-08 3.11169441E-11-2.14671219E+04 9.84024999E+00-1.94936072E+04 4

! E Goos A Burcat B Ruscic Ideal gas thermochemical database with updates from active thermochemical

! http://burcat.technion.ac.il/dir/

! mirrored at http://garfield.chem.elte.hu/burcat/burcat.html.

! Accessed April 2016

CH3C(O)OOH 1508 C 2H 4N 0O 3G 298.000 3000.000 1000.00 1

5.64132391E+00 2.17230931E-02-1.11238026E-05 2.75682193E-09-2.67754066E-13 2

-4.51408748E+04-1.61172400E+00 1.43747508E+00 3.39384339E-02-2.25467319E-05 3

5.77205354E-09 1.28451673E-13-4.40701023E+04 1.98194302E+01 4

! Bozzelli 2015; PM

HOCH2O 1311 C 1H 3N 0O 2G 298.000 3000.000 1000.00 1

3.64142330E+00 1.46738744E-02-8.24143161E-06 2.24789889E-09-2.38670785E-13 2

-2.22304345E+04 7.15858335E+00-1.97308533E+00 4.26372227E-02-5.84444247E-05 3

4.12218747E-08 -1.13584932E-11-2.13827984E+04 3.28690136E+01 4

!

!

!

!

END

!

!

REACTIONS

C2H3+O2=C2H2+HO2 1.34E6 1.61 -383.5 !

C2H4+O2=CH2HCO+OH 2.0E08 1.500 39000.000 !

C2H4+O2=C2H3+HO2 4.2E13 0.00 57630.000 !

C2H2+O=HCCO+H 1.4E07 2.000 1900.000 !

H+C2H2(+M)=C2H3(+M) 3.64E10 1.09 2640 ! Marinov 1996 xxxxxxxxxxx

LOW/2.254E40 -7.269 6577./

TROE/0.5 675. 675./

H2/2/ CO/2/ CO2/3/ H2O/5/

!CH3+CH3(+M)=C2H6(+M) 2.1E16 -0.97 620. ! GRI2.11

! LOW /1.26E50 -9.67 6220/

! TROE/ 0.5325 151 1038 4970 /

! N2/1.43/ H2O/8.59/ H2/2/ CO/2/ CO2/3/

!#! H2O/8.59/ H2/2/ CO/2/ CO2/3/

```
!CH3+H(+M)=CH4(+M)              1.3E16     -0.63   383.  ! GRI-MECH2.11
!  LOW/1.75E33  -4.76 2440.0/
!  TROE/0.783  74.0 2941.0 6964.0/
! H2/2.86/ H2O/8.57/ CH4/2.86/  CO/2.14/ CO2/2.86/ C2H6/4.29/ N2/1.43/
!CH4+O2=CH3+HO2                 0.790E+14  0.000  56000.000 ! SKINNER ET AL 1972
!CH4+O2=CH3+HO2                 4.000E+13  0.000  57000.000 !  CEC 1994
!CH4+H=CH3+H2                  1.3E4    3.0   8040.  !cec 92
!CH4+OH=CH3+H2O                 0.160E+07  2.100   2460.000 ! TULLY
!CH4+O=CH3+OH                   1.02E9     1.5     8604. !TSANG
CH4+HO2=CH3+H2O2                0.180E+12  0.000  18700.000 ! NBS
!CH3+HO2=CH3O+OH                 8.0E12   0.0  0.0 ! Jam&PG rbn (Troe unpub.)
CH3+O=CH2O+H                    8.0E13   0.0   0.0    !GUTMAN
!CH3+O2=CH3O+O                 2.87E13      0.0   30481  !frenk JPC 1995
!CH3+O2=CH2O+OH                 1.85E12     0.0   20315 !Frenk jpc 1995
!CH2OH+H=CH3+OH                 0.100E+15  0.000      0.000 ! NBS 87
!CH3O+H=CH3+OH                  0.100E+15  0.000      0.000 ! EST JAM
!CH3+OH=CH2+H2O                 0.750E+07  2.000   5000.000 ! JAM
CH3+HCO=CH4+CO                  1.2E14    0.0     0.0   ! NBS 86
CH3+H=CH2+H2                   0.900E+14  0.000  15100.000 ! PG
CH3+OH(+M)=CH3OH(+M)           6.3E13    0.0     0.0   !GRI2.11
  LOW/1.89E38  -6.3   3100/
  TROE/0.2105 83.5 5398 8370/
  N2/1.43/ H2O/8.58/ CO2/3/ CO/2/ H2/2/
!#!  H2O/8.58/ CO2/3/ CO/2/ H2/2/
!CH3OH+OH=CH2OH+H2O             5.30E4    2.53     960.    ! NBS
!cojo la del mecanismo etanol
!CH3OH+OH=CH3O+H2O              1.32E4    2.53     960.    !
!cojo la del mecanismo etanol
CH3OH+O=CH2OH+OH                3.88E5     2.5     3080.    ! NBS
!CH3OH+H=CH2OH+H2               1.7E7      2.1     4868     ! NBS
!cojo la del mecanismo etanol
!CH3OH+H=CH3O+H2                4.24E6     2.1     4868     ! NBS
!cojo la del mecanismo etanol
!CH3OH+HO2=CH2OH+H2O2           9.64E10     0.0   12578.    ! NBS
!cojo la del mecanismo etanol
CH2O+H(+M)=CH3O(+M)            5.4E11  0.454  2600. ! GRI2.11
  LOW/1.54E30  -4.8  5560 /
  TROE/ 0.758 94 1555 4200/
```

```
   N2/1.43/  H2O/8.58/ CO/2/ H2/2/ CO2/3/
!#!  H2O/8.58/ CO/2/ H2/2/ CO2/3/
H+CH2O(+M)=CH2OH(+M)          5.4E11   0.454   3600. ! GRI2.11
    LOW/.91E32 -4.82 6530/
    TROE/0.7187 103 1291 4160/
   N2/1.43/ H2O/8.58/ CO/2/ CO2/3/ H2/2/
!#!  H2O/8.58/ CO/2/ CO2/3/ H2/2/
CH3O+H=CH2O+H2               0.200E+14  0.000      0.000 ! PG
!CH2OH+H=CH2O+H2              0.200E+14  0.000      0.000
!cojo la del mecanismo etanol
CH3O+OH=CH2O+H2O             0.100E+14  0.000      0.000 ! PG
CH2OH+OH=CH2O+H2O            0.100E+14  0.000      0.000
CH3O+O=CH2O+OH               0.100E+14  0.000      0.000 ! PG
!CH2OH+O=CH2O+OH              0.100E+14  0.000      0.000
!cojo la del mecanismo etanol
CH3O+O2=CH2O+HO2             0.630E+11  0.000   2600.000 ! PG
CH2OH+O2=CH2O+HO2            1.57E15    -1.0       0.0   ! EURCOM 1992
 DUP
CH2OH+O2=CH2O+HO2            7.23E13    0.0      3577.  !
 DUP
CH2+H=CH+H2                  0.100E+19 -1.560      0.000 ! THORNE,ET AL
CH2+OH=CH+H2O                0.113E+08  2.000   3000.000 ! JAM
CH2+OH=CH2O+H                0.250E+14  0.000      0.000 ! PG
CH+O2=HCO+O                  0.330E+14  0.000      0.000 ! PG
CH+O=CO+H                    0.570E+14  0.000      0.000 ! PG
CH+OH=HCO+H                  0.300E+14  0.000      0.000 ! PG
CH+CO2=HCO+CO                0.340E+13  0.000    690.000 ! PG
CH+H2O=CH2O+H                5.72E12    0.0     -751.0    !LIN
CH+CH2O=CH2CO+H              0.946E+14  0.000   -515.000 ! THORNE
CH+C2H2=C3H2+H               0.100E+15  0.000      0.000 ! THORNE
CH+CH2=C2H2+H                0.400E+14  0.000      0.000 ! PG
CH+CH3=C2H3+H                0.300E+14  0.000      0.000 ! PG
CH+CH4=C2H4+H                0.600E+14  0.000      0.000 ! PG
CH2+CO2=CH2O+CO              0.110E+12  0.000   1000.000 ! PG
CH2+O=CO+H+H                 0.500E+14  0.000      0.000 ! JAM 2/87
CH2+O=CO+H2                  0.300E+14  0.000      0.000 ! JAM 2/87
CH2+O2=CO+H2O     2.20E22   -3.3  2867. ! DOMBROWSKY(HGGW) BER.BUN.1992
!CH2+O2=CO2+H+H    3.29E21   -3.3  2867.  !
```

```
CH2+O2=CH2O+O     3.29E21   -3.3  2867. !
CH2+O2=CO2+H2     2.63E21   -3.3  2867. !
CH2+O2=CO+OH+H    1.64E21   -3.3  2867. !
CH2+CH2=C2H2+H+H              0.400E+14  0.000      0.000 ! BRAUN,ET AL
CH2+HCCO=C2H3+CO              0.300E+14  0.000      0.000 ! JAM,1/11/82
CH2+C2H2=H2CCCH+H             0.120E+14  0.000   6600.000 ! BOHLAND ET AL,21S
CH2+CH4=CH3+CH3               4.3E12    0.0     10030. ! PG 86
CH2O+OH=HCO+H2O               0.343E+10  1.180   -447.000 ! NBS
CH2O+H=HCO+H2                 1.3E8     1.62    2166. ! CEC 94
CH2O+M=HCO+H+M                0.331E+17  0.000  81000.000 ! DEAN,C 1980
    H2/2/ CO/2/ CO2/3/  H2O/5/
CH2O+O=HCO+OH                 0.180E+14  0.000   3080.000 ! NBS
CH2O+CH3=HCO+CH4              7.8E-8      6.1     1967. ! CEC 1994
CH2O+HO2=HCO+H2O2             3.0E12    0.0     13000.  !CEC 1994
CH2O+O2=HCO+HO2               6.0E13     0.0      40660 ! CEC 94
HCO+OH=H2O+CO                 0.100E+15  0.000      0.000 ! TEMPS
!HCO+M=H+CO+M                 3.48E17   -1.0    17010.0  ! Timoen et al 1987
!    CO/1.87/   H2/1.87/  CH4/2.81/ CO2/3./ H2O/5./
HCO+H=CO+H2                   0.119E+14  0.250    0.000 ! HARD.. 21ST, JAM
HCO+O=CO+OH                   0.300E+14  0.000      0.000 ! PG
HCO+O=CO2+H                   0.300E+14  0.000      0.000 ! PG
HCO+O2=HO2+CO                 7.58E12    0.0    406. !TIMONEN(GUTMAN)JPC 1988
CO+O+M=CO2+M                  0.617E+15  0.000   3000.000 ! NBS
    H2/2/ CO/2/ CO2/3/  H2O/16/
CO+OH=CO2+H                   1.51E7     1.3     -758   ! BAULCH&DRYSDALE
CO+O2=CO2+O                   2.53E12    0.0     47688. !TSANG,BAULCH
!HO2+CO=CO2+OH                0.580E+14  0.000  22934.000 ! ATRI ET AL ,C 197
HO2+CO=CO2+OH                 1.570E5    2.18    17900.000 ! YOU/WANG,2007
!C2H4+H=C2H3+H2               5.42E14    0.0     14902    ! EURCOM 1992
C2H4+O=CH3+HCO                8.1E6      1.88     180. ! CEC 94
C2H4+O=CH2CO+H2               6.8E5      1.88     180  !
!C2H4+OH=C2H3+H2O             0.202E+14  0.000   5955.000 ! TULLY 1987
C2H4+CH3=C2H3+CH4             5.0E11     0.0     15000 !JAM&Pg rbn (Zhang 1990)
CH2+CH3=C2H4+H                0.400E+14  0.000      0.000 ! JAM
!C2H4+H(+M)=C2H5(+M)           1.081E12   0.454    1822.  ! MARINOV
!   LOW/1.112E34  -5.0   4448.0/
!  TROE/0.5 95.0  95.0    200./
!    H2/2/ CO/2/ CO2/3/ H2O/5/
```

```
C2H3+H=C2H2+H2              0.400E+14  0.000      0.000 ! HOYERMANN
C2H3+O=CH2CO+H              0.300E+14  0.000      0.000 ! HOYERMANN 21ST
C2H3+O2=CH2O+HCO              4.58E16    -1.39   1015 !  Mebel,et al.
C2H3+OH=C2H2+H2O               2.0E13    0.0     0.0   ! JAM
C2H3+C2H=C2H2+C2H2          0.300E+14  0.000      0.000 ! MMSK
C2H3+CH3=C2H2+CH4             2.1E13   0.0     0.0 ! NBS, Fahr 91(rbn PG)
C2H3+CH2O=C2H4+HCO              5.4E3   2.81   5860 ! NBS 86
C2H3+HCO=C2H4+CO              9.0E13    0.0    0.0  ! NBS 86
C2H3+C2H3=H2CCCH+CH3            1.8E13  0.0   0.0 ! CJP 091699 adj
C2H3+C2H3=C2H4+C2H2             6.3E13  0.0   0.0 ! CJP 091699 adj
C2H3+CH=CH2+C2H2              0.500E+14  0.000      0.000 ! JAM
OH+C2H2=C2H+H2O               3.37E7    2.0   14000. ! MILLER
OH+C2H2=HCCOH+H               5.04E5    2.3   13500. ! MILLER
OH+C2H2=CH2CO+H               2.18E-4   4.5   -1000. ! MILLER
OH+C2H2=CH3+CO                4.83E-4   4.0   -2000. ! MILLER
!OH+C2H2(+M)=C2H2OH(+M)          1.52E8  1.7    1000. ! MILLER&MELIUS!
!
!   LOW/1.81E23  -2.0   0.0 /                ! Atkinson(cited in CEC 92)/PG
!  H2/2/  CO/2/   CO2/3/   H2O/5/
!           HO2+C2H2=CH2HCO+O              1.0E12   0.0   10000 ! JAM           xxxxxx
!           HO2+C2H2=CH2O+HCO              1.0E12   0.00   10000 ! JAM           xxxxxx
! last 2 k's crudely based on calculations of Mebel,Morokuma,Lin,et al(C2H3+O2)
HCCOH+H=HCCO +H2              3.0E7   2.0     1000. ! JAM
HCCOH+OH=HCCO+H2O             1.0E7   2.0     1000. !JAM
HCCOH+O=HCCO+OH               2.0E7  3.0     1900. !JAM(O+C2H2)
C2H2+O=C2H+OH               0.316E+16 -0.600  15000.000 !MMSK
C2H2OH+O=OCHCHO+H             5.0E13   0.0     0.0  ! JAM 1996
C2H2OH+O2=OCHCHO+OH            1.0E12   0.0    5000. ! JAM 1996
OCHCHO+M=HCO+HCO+M             1.0E17    0.0  25000. ! JAM
xxxxxxxxxx
OCHCHO+H=CH2O+HCO             3.0E13    0.0   0.0  !JAM
CH2CO+O=CO2+CH2             0.175E+13  0.000   1350.000 ! SEE WAGNER,TEMPS ET
CH2CO+H=CH3+CO               5.93E6   2.0    1300. ! CEC 92 / JAM
CH2CO+H=HCCO+H2              3.0E7     2.0  10000.000 ! JAM 1996
CH2CO+O=HCCO+OH              2.0E7  2.0   10000.000 !
CH2CO+OH=HCCO+H2O             1.0E7   2.0   3000.000 !
CH2CO+OH=CH2OH+CO             7.2E12   0.0   0.0 ! Temps,HggW,et al 1992
CH2CO+OH=CH3+CO2              3.0E12  0.0   0.0 ! Grussdorf 94 (PG rbn)
CH2+CO(+M)=CH2CO(+M)          8.1E11    0.5  4510. ! GRI2.11
```

```
 LOW/ 1.88E33 -5.11 7095./
 TROE/ 0.5907 275 1226 5185/
   H2/2/ CO/2/ CO2/3/  H2O/8.58/  N2/1.43/
C2H+O2=CO+CO+H          2.52E13    0.0    0.0   ! GLASS&CURL(STEPHENS)JPC1987
C2H+CH4=CH3+C2H2             7.23E12   0.0    976 ! Leone JPC 1996
CH+CO(+M)=HCCO(+M)          5.0E13   0.0    0.0  ! GRI2.11
 LOW/ 1.88E28  -3.74 1936 /
 TROE/ 0.5757 237  1652 5069 /
  N2/1.43/ H2O/8.58/ CO/2/ CO2/3/ H2/2/
!#!  H2O/8.58/ CO/2/ CO2/3/ H2/2/
HCCO+C2H2=H2CCCH+CO          1.0E11   0.0     3000. ! JAM
H+HCCO=CH2(S)+CO             0.100E+15  0.000      0.000 ! PEETERS 1985
O+HCCO=H+CO+CO               0.100E+15  0.000      0.000 ! PEETERS 1985
HCCO+O2=CO2+CO+H              1.4E7    1.7        1000. ! HGGW.Peeters,JAM
HCCO+O2=CO +CO +OH           2.88E7     1.7       1000. !
CH+HCCO=C2H2+CO              0.500E+14  0.000      0.000 ! JAM EST
HCCO+HCCO=C2H2+CO+CO          0.100E+14  0.000      0.000 ! MMSK
HCCO+OH=C2O+H2O              6.0E13     0.0    0.0    ! JAM
C2O+H=CH+CO                  1.0E13    0.0     0.0    ! JAM
C2O+O=CO+CO                  5.0E13    0.0      0.0   ! JAM
C2O+OH=CO+CO+H               2.0E13    0.0     0.0    ! JAM
C2O+O2=CO+CO+O               2.0E13  0.0   0.0  ! JAM
C2H+O=CH+CO                  0.500E+14  0.000      0.000 ! BROWNE
C2H+OH=HCCO+H                0.200E+14  0.000      0.000 ! JAM,12/22
C2H+OH=C2+H2O           4.0E7    2.0     8000.   !  JAM
C2+H2=C2H+H              4.0E5    2.4     1000.   !  JAM
C2+O2=CO+CO              5.0E13    0.0     0.0   ! JAM
C2+OH=C2O+H              5.0E13    0.0     0.0   ! JAM
!C2H2+O2=HCCO+OH              0.200E+09  1.500  30100.000 ! MMSK
C2H2+O2=HCO+HCO              0.200E+09  1.500  30100.000 ! MMSK/Benson 1996
C2H2+M=C2H+H+M               9.08E30    -3.7  127138. !TSANG&HAMP(TAN&GARD)
    H2/2/ CO/2/ CO2/3/  H2O/5/
C2H4+M=C2H2+H2+M             3.50E+16  0.000  71500. ! CEC 94
     N2/1.5/  H2O/10/
!#!     H2O/10/
C2H3+H(+M)=C2H4(+M)              6.1E12  0.27  280.000 !   GRI2.11
     LOW /0.98E30 -3.86 3320./
     TROE /0.7820 207.50 2663.00 6095.00/
```

```
 H2/2.85/ CO/2.1/ CO2/2.85/  H2O/7.14/ CH4/2.85/ C2H6/4.29/  N2/1.43/
!
!
!
!REACCIONES MECANISMO REBURNING
!
!
!
 ! ****************************************
 ! *   H2/O2 Subset                       *
 ! ****************************************
 !
!O+OH=O2+H                  2.0E14 -0.40      0
H+O2=O+OH     1.0E14   0.000     15286
!O+H2=OH+H                  5.0E04  2.67   6290
O+H2=OH+H 3.80E+12   0           7948
DUP
O+H2=OH+H 8.80E+14   0           19175
DUP
OH+H2=H2O+H                2.1E08  1.52   3450
2OH=O+H2O                  4.3E03  2.70  -2486
H+H+M=H2+M                 1.0E18 -1.00      0
   H2O/0/
H+H+H2O=H2+H2O             6.0E19 -1.25      0
H+O+M=OH+M                 6.2E16 -0.60      0
   H2O/5/
H+OH+M=H2O+M               1.6E22 -2.00      0
   H2O/5/
O+O+M=O2+M                 1.9E13  0.00  -1788
   H2O/5/
!
!Pruebas reacción H+O2+M
!
!H+O2(+M)=HO2(+M)           1.48E+12  0.6    0.0
!    LOW /3.50E+16 -0.41 -1116.0/
!    TROE /0.5 100000 10/
! AR/0.0/ H2O/10.6/ H2/1.5/ CO2/2.4/
!H+O2(+AR)=HO2(+AR)         1.480E+12  0.6    0.0
```

```
!    LOW /7.00E+17 -0.8  0.0/
!    TROE /0.45 10 100000/
!H+O2(+M)=HO2(+M)              4.66E12  0.44      0 ! (Konnov/C&F 2008)
!     LOW /5.70E19 -1.4 0/
!    TROE/ 0.5 1.0E-30 1.0E30 /
!     H2O/0/  N2/0/  H2/1.5/   O2/0/  AR/0/
!H+O2(+AR)=HO2(+AR)            4.66E12  0.44      0 ! (Konnov/C&F 2008)
!     LOW /7.43E18 -1.2 0/
!    TROE/ 0.5 1.0E-30 1.0E30 /
!H+O2(+O2)=HO2(+O2)            4.66E12  0.44      0 ! (Konnov/C&F 2008)
!     LOW /5.69E18 -1.094 0/
!    TROE/ 0.5 1.0E-30 1.0E30 /
!H+O2(+H2O)=HO2(+H2O)          9.06E12  0.2       0 ! (Konnov/C&F 2008)
!     LOW /3.67E19 -1.0 0/
!    TROE/ 0.8 1.0E-30 1.0E30 /
!H+O2+M=HO2+M                  4.5E18  0.00       0 ! (Glarborg 1995 CST, basada en Atkinson et
al.1992)
!     H2O/10/  N2/0/
!H+O2+M=HO2+M                   4.5E18  0.00      0 ! (Glarborg 1995 CST, basada en Atkinson et
al.1992)
    !H2O/10/  N2/0/
!H+O2+M=HO2+M                  5.69E18 -1.09      0 ! (Michael 2002 J.Phis.Chem, 2002)
   ! H2O/16/  N2/0/
!!!!!!!
!!!!!!
!H+O2=HO2                     1E11    0.00       0 ! (Para sacar K para una Temp dada)
!!!!!!!!
!H+O2+M=HO2+M                  1E11 -1.00        0! (la que había)
   !H2O/16/  N2/0/
H+O2+M=HO2+M                  8E17   -0.80       0 ! (Dagaut 2009 E&F)
    H2O/20/  N2/0/  CO2/4/                                  !
H+O2+N2 = HO2+N2              6.7E19 -1.42       0 ! *
H+HO2=H2+O2                   4.3E13  0.00   1411
!H+HO2=OH+OH                   1.7E14  0.00    874
HO2+H=OH+OH                        7.10E+13           0           295
H+HO2=O+H2O                   3.0E13  0.0    1721
O+HO2=O2+OH                   3.3E13  0.0       0
OH+HO2=H2O+O2                 1.9E16 -1.0       0
HO2+HO2=H2O2+O2               4.2E14  0.0   11982
```

```
 DUP
HO2+HO2=H2O2+O2              1.3E11  0.0   -1629
 DUP
!H2O2+M=OH+OH+M               1.3E17  0.0   45500
!   H2O/5/
H2O2(+M) = OH+OH(+M)          2.00E+12   0.90  4.8749E+04
 LOW/2.49E+24 -2.30 4.8749E+04/
 TROE/0.43 1E-30 1E+30/
 AR/1.0/ H2O/7.5/ CO2/1.6/ N2/1.5/ O2/1.2/ H2O2/7.7/ H2/3.7/ CO/2.8/
! Troe, Combust. Flame 158:594-601 (2011)
! Efficiencies for H2 and CO taken from Li et al., Int. J. Chem. Kinet. 36:566-575 (2004)
H2O2+H=HO2+H2                1.7E12  0.0    3755
H2O2+H=OH+H2O                1.0E13  0.0    3576
H2O2+O=OH+HO2                6.6E11  0.0    3974
H2O2+OH=H2O+HO2              7.8E12  0.0    1330
 DUP
H2O2+OH=H2O+HO2              5.8E14  0.0    9560 ! +
 DUP
!*****NUEVAS O3*****
O+O2+M=O3+M 1.88E+21 -2.8 0.0 !private communication
O+O3=O2+O2 4.80E+12 0.0 4090.0 !Atkinson et al. (2004)
H+O3=OH+O2 8.43E+13 0.0 950.0 !Atkinson et al. (2004)
OH+O3=HO2+O2 1.14E+12 0.0 2000.0 !Atkinson et al. (2004)
HO2+O3=OH+O2+O2 8.43E+09 0.0 1200.0 !Zahniser et al. (1980)
  ! ********************************************
  ! *   CH4/CH3/CH2/CH/C Subset                *
  ! ********************************************
  !
CH2(S)+H2=CH3+H              7.2E13  0.0       0 !
!CH2(S)+H2O=CH3+OH            3.0E15 -0.6       0 !
CH2(S)+N2=CH2+N2             1.3E13  0.0     430 !
CH2(S)+AR=CH2+AR             1.5E13  0.0     884 !
CH2(S)+H=CH2+H               2.0E14  0.0       0 !
CH2(S)+H2O=CH2+H2O           3.0E13  0.0       0 !
CH2(S)+H=CH+H2               3.0E13  0.0       0 !
CH2(S)+O=CO+H+H              3.0E13  0.0       0 !
CH2(S)+OH=CH2O+H             3.0E13  0.0       0 !
CH2(S)+O2=CO+OH+H            7.0E13  0.0       0 !
```

```
CH2(S)+CO2=CH2O+CO            3.0E12  0.0       0 !
CH2(S)+CH4=CH3+CH3            4.3E13  0.0       0 !
CH2(S)+CH3=C2H4+H             2.0E13  0.0       0 !
CH2(S)+CH2CO=C2H4+CO          1.6E14  0.0       0 !
CH2(S)+C2H6=CH3+C2H5          1.2E+14 0.0       0 !
CH+H=C+H2                     1.5E14  0.0       0 !
CH+OH=C+H2O                   4.0E7   2.0    3000 !
C+OH=CO+H                     5.0E13  0.00      0 !
C+O2=CO+O                     2.0E13  0.00      0 !
C+CH3=C2H2+H                  5.0E13  0.00      0 !
C+CH2=C2H+H                   5.0E13  0.00      0 !
 !
 ! *********************************************
 ! *   CH3OH/CH2OH/CH2O subset                 *
 ! *********************************************
CH2OH+O2=CH2O+HO2             1.6E15 -1.0       0 !
 DUP
CH2OH+O2=CH2O+HO2             7.2E13  0.0    3577 !
 DUP
 !
 ! *********************************************
 ! *   C2H6/C2H5/C2H4/C2H3/C2H2/C2H/C2 subset *
 ! *********************************************
 !
!C2H6+H=C2H5+H2                5.4E02  3.50   5210 !
!C2H6+O=C2H5+OH                3.0E07  2.00   5115 !
!C2H6+OH=C2H5+H2O              7.2E6   2.0     864 !
!C2H6+HO2 = C2H5+H2O2          1.3E13  0.00  20460 !
!C2H6+O2=C2H5+HO2              5.0E13  0.0   55000 !
!C2H6+CH3=C2H5+CH4             5.5E-1  4.00   8300 !
C2H5+H(+M) = C2H6(+M)      5.2E17 -0.99   1580 !
  LOW  /  2.0E41 -7.08 6685/
  TROE/  0.8422 125 2219 6882 /
  N2/1.0/ H2O/6/  AR/0.7/
C2H5+H=CH3+CH3                4.9E12  0.35      0 !
C2H5+O = CH3+CH2O             4.2E13  0.00      0 !
C2H5+O = CH3HCO+H             5.3E13  0.00      0 !
C2H5+O = C2H4+OH              3.0E13  0.00      0 !
```

```
C2H5+OH = C2H4+H2O         2.4E13  0.00      0 !
C2H5+O2 = C2H4+HO2         1.0E10  0.00  -2190 !
C2H5+CH2O = C2H6+HCO       5.5E03  2.81   5860 !
C2H5+HCO = C2H6+CO         1.2E14  0.00      0 !
C2H5+CH3 = C2H4+CH4        1.1E12  0.00      0 !
C2H5+C2H5 = C2H6+C2H4      1.5E12  0.00      0 !
C2H4+O = CH2HCO+H           4.7E06  1.88    180 !
C2H4+HO2=CH3HCO+OH           2.2E12  0.0   17200 !
C2H3+O2 = CH2HCO+O           3.03E11 -0.29 10.73 !
H2+C2H=C2H2+H               4.1E05  2.39    864 !
C2H2+O=CH2+CO               6.1E6   2.00   1900 !
OH+C2H2(+M)=C2H2OH(+M)        1.5E8   1.7    1000 !
  LOW/1.81E23  -2.0   0.0 /                  !
 H2/2/  CO/2/   CO2/3/   H2O/5/
!HO2+C2H2=CH2HCO+O           1.0E12  0.0   10000 !
!HO2+C2H2=CH2O+HCO           1.0E12  0.0   10000 !
 !
 ! *****************************************************
 ! *   CH3HCO/CH2HCO/CH3CO/CH2CO/HCCOH/HCCO/C2O subset *
 ! *****************************************************
 !
CH3HCO = CH3+HCO             7.1E15  0.00  81280 !
CH3HCO+H = CH3CO+H2          4.1E09  1.16   2400 !
CH3HCO+O = CH3CO+OH          5.8E12  0.00   1800 !
CH3HCO+OH=CH3CO+H2O          2.3E10  0.73  -1110 !
CH3HCO+HO2 = CH3CO+H2O2       3.0E12  0.00  12000 !
CH3HCO+O2 = CH3CO+HO2        3.0E13  0.00  39000 !
CH3HCO+CH3=CH3CO+CH4         2.0E-6  5.6    2464 !
CH2HCO=CH3+CO               1.0E13  0.0   42000 !
!CH2HCO+M=CH3+CO+M           2.0E16  0.0   42000 !
!    H2/2/ CO/2/ CO2/3/  H2O/5/
CH2HCO+H=CH3+HCO             1.0E14  0.0       0 !
CH2HCO+H=CH3CO+H             3.0E13  0.0       0 !
CH2HCO+O=CH2O + HCO          5.0E13  0.0       0 !
CH2HCO+OH=CH2CO+H2O          2.0E13  0.0       0 !
CH2HCO+OH=CH2OH+HCO          1.0E13  0.0       0 !
CH2HCO+O2 = CH2O+CO+OH       2.2E11  0.0    1500 !
CH2HCO+CH3=C2H5CHO           5.0E13  0.0       0 !
```

```
CH2HCO+CH2=C2H4+HCO          5.0E13  0.0      0 !
CH2HCO+CH =C2H3+HCO          1.0E14  0.0      0 !
C2H5+HCO = C2H5CHO           1.8E13  0.0      0 !
C2H5CHO+H = C2H5CO+H2        8.0E13  0.0      0 !
C2H5CHO+O = C2H5CO+OH        7.8E12  0.0   1730 !
C2H5CHO+OH = C2H5CO+H2O      1.2E13  0.0      0 !
C2H5+CO = C2H5CO             1.5E11  0.0   4800 !
C2H2OH+H=CH2HCO+H            5.0E13  0.0      0 !
CH3CO(+M)=CH3+CO(+M)         2.8E13  0.0  17100 !
 LOW/2.1E15  0.0  14000./
 TROE/ 0.5 1.0E-30 1.0E30 /
   H2/2/ CO/2/ CO2/3/  H2O/5/
CH3CO+H = CH3+HCO            2.1E13  0.00     0 !
CH3CO+H = CH2CO+H2           1.2E13  0.00     0 !
CH3CO+O = CH3+CO2            1.5E14  0.00     0 !
CH3CO+O = CH2CO+OH           4.0E13  0.00     0 !
CH3CO+OH = CH2CO+H2O         1.2E13  0.00     0 !
 !
 ! *****************************************************
 ! *   H/N/O subset                                    *
 ! *   taken from [nh2no2] except where noted          *
 ! *****************************************************
 !
H+NO+M=HNO+M                 4.0E20 -1.75     0 ! a (GLA 1998, se ha quitado la eficacia del tercer
cuerpo para el N2 ya que se tiene en cuenta en la siguiente reacción)
   H2O/10/  O2/1.5/ H2/2/ CO2/3/ N2/0/
H+NO+N2=HNO+N2               7.0E19 -1.50     0 !
NO+O+M=NO2+M                 7.5E19 -1.41     0 !
 N2/1.7/   O2/1.5/  H2O/10/
!!!!OH+NO+M=HONO+M           5.1E23 -2.51    -68 !
!!!!  H2O/5/
!HO2+NO=NO2+OH               2.1E12  0.00   -479 !
HO2+NO=NO2+OH                          2.32E10  0.58     1433 ! (actualizada)
!NO2+OH=NO+HO2                         1.35E13  0.0    7613 !
!NO2+OH=NO+HO2                 1.02E13  0.0        5962 !
NO2+H=NO+OH                  8.85E13  0.0      0 ! (actualizada)
NO2+O=NO+O2                  3.9E12  0.0    -238 !
!NO2+O=NO+O2                           1.050E14  -0.520   0 ! (actualizar?) Juanma JUnio
NO2+SO=SO2+NO                        8.43E12   0.0   0 ! (Prueba juanma junio)
```

```
NO2+SO2=SO3+NO                  6.31E12   0.0  2.7E4 ! (Prueba juanma junio)
NO2+O(+M)=NO3(+M)            1.3E13  0.0       0 !
   LOW/1.0E28  -4.08 2470./
  N2/1.5/ O2/1.5/  H2O/18.6/
NO2+NO2=NO+NO+O2             1.6E12  0.0   26123 !
NO2+NO2=NO3+NO               9.6E09  0.73  20900 !
NO3+H=NO2+OH                 6.0E13  0.0       0 !
NO3+O=NO2+O2                 1.0E13  0.0       0 !
NO3+OH=NO2+HO2               1.4E13  0.0       0 !
NO3+HO2=NO2+O2+OH            1.5E12  0.0       0 !
NO3+NO2=NO+NO2+O2            5.0E10  0.0    2940 !
HNO+H=H2+NO                  4.5E11  0.72    655 !
HNO+O=NO+OH                  1.0E13  0.0       0 !
HNO+OH=NO+H2O                3.6E13  0.0       0 !
!!!!!!!HNO+O2=HO2+NO              1.0E13  0.0   25000 !
HNO+NO2=HONO+NO              6.0E11  0.0    2000 !
HNO+HNO=N2O+H2O              9.0E08  0.0    3100 !
HNO+NH2=NH3+NO               3.63E6  1.63  -1252 !
H2NO+M=HNO+H+M               2.5E15  0.0   50000 !
  H2O/5/  N2/2/
H2NO+H=HNO+H2                3.0E7   2.0    2000 !
H2NO+H=NH2+OH                5.0E13  0.0       0 !
H2NO+O=HNO+OH                3.0E7   2.0    2000 !
!H2NO+O = NH2+O2              2.0E14   0        0 !
H2NO+OH=HNO+H2O              2.0E7   2.0    1000 !
H2NO+NO=HNO+HNO              2.0E04  2.0   13000 !
H2NO+NO2=HNO+HONO            6.0E11  0.0    2000 !
HONO+H=H2+NO2                1.2E13  0.0    7352 !
HONO+O=OH+NO2                1.2E13  0.0    5961 !
HONO+OH=H2O+NO2              4.0E12  0.0       0 !
NH3+M = NH2+H+M              2.2E16   0    93470 !
NH3+H=NH2+H2                 6.4E05  2.39  10171 !
!NH3+O=NH2+OH                9.4E06  1.94   6460 !
NH3+OH=NH2+H2O               2.0E06  2.04    566 !
NH3+HO2=NH2+H2O2             3.0E11  0.0   22000 !
NH2+H=NH+H2                  4.0E13  0.00   3650 !
!NH2+O=HNO+H                 6.6E14 -0.50      0 !
!NH2+O=NH+OH                 6.8E12  0.        0 !
```

```
NH2+OH=NH+H2O               4.0E06  2.     1000 !
NH2+HO2=H2NO+OH              5.0E13  0.0       0 !
NH2+HO2=NH3+O2              1.0E13  0.0       0 !
!NH2+NO=NNH+OH               8.9E12 -0.35      0 !
!NH2+NO=N2+H2O               1.3E16 -1.25      0 !
! DUP
!NH2+NO=N2+H2O              -8.9E12 -0.35      0 !
! DUP
NH2+NO2=N2O+H2O              3.2E18 -2.2       0 !
NH2+NO2=H2NO+NO              3.5E12  0.        0 !
NH2+H2NO=NH3+HNO             3.0E12  0.0    1000 !
HONO+NH2=NO2+NH3              71.1    3.02  -4941 !
NH2+NH2=N2H2+H2              8.5E11  0.        0 !
NH2+NH=N2H2+H                5.0E13  0.        0 !
NH2+N=N2+H+H                 7.2E13  0.        0 !
NH+H=N+H2                   3.0E13  0.        0
NH+O=NO+H                    9.2E13  0.        0
NH+OH=HNO+H                  2.0E13  0.        0
NH+OH=N+H2O                  5.0E11  0.50   2000
NH+O2=HNO+O                  4.6E05  2.     6500 !
NH+O2=NO+OH                  1.3E06  1.5     100 !
!NH+NO=N2O+H                 2.9E14 -0.4       0 !
! DUP
!NH+NO=N2O+H                -2.2E13 -0.23      0
! DUP
!NH+NO=N2+OH                 2.2E13 -0.23      0
NH+NO2=N2O+OH                1.0E13  0.        0
NH+NH=N2+H+H                 2.5E13  0.        0
NH+N=N2+H                   3.0E13  0.        0
N+OH=NO+H                    3.8E13  0.        0
N+O2=NO+O                   6.4E09  1.     6280
N+NO=N2+O                   3.3E12  0.30      0
N2H2+M=NNH+H+M               5.0E16  0.    50000
   H2O/15/ O2/2/ N2/2/ H2/2/
N2H2+H=NNH+H2                5.0E13  0.     1000
N2H2+O=NH2+NO                1.0E13  0.        0
N2H2+O=NNH+OH                2.0E13  0.     1000
N2H2+OH=NNH+H2O              1.0E13  0.     1000
```

```
N2H2+NO=N2O+NH2              3.0E12  0.       0
N2H2+NH2=NH3+NNH             1.0E13  0.    1000
N2H2+NH=NNH+NH2              1.0E13  0.    1000
!NNH=N2+H                   1.0E7   0.       0 !
NNH+H=N2+H2                  1.0E14  0.       0
!NNH+O=N2+OH                 8.0E13  0.       0
!NNH+O=N2O+H                 1.0E14  0.       0
!NNH+O=NH+NO                 5.0E13  0.       0
NNH+OH=N2+H2O                5.0E13  0.       0
!NNH+O2=N2+HO2                2.0E14  0.       0 !
NNH+O2=N2+O2+H               5.0E13  0.       0 !
NNH+NO=N2+HNO                5.0E13  0.       0
NNH+NH2=N2+NH3               5.0E13  0.       0
NNH+NH=N2+NH2                5.0E13  0.       0
N2O+M=N2+O+M                 4.0E14  0.    56100
 N2/1.7/   O2/1.4/ H2O/12/ CO/1.5/  CO2/3/
N2O+H=N2+OH                  3.3E10  0.    4729
 DUP
N2O+H=N2+OH                  4.4E14  0.    19254
 DUP
N2O+O=NO+NO                  6.6E13  0.    26630 !
N2O+O=N2+O2                 1.0E14  0.    28000 !
N2O+OH=N2+HO2                1.3E-2  4.72  36561 !
N2O+OH=HNO+NO                1.2E-4  4.33  25081 !
!HNO+NO = N2O+OH              2.0E12  0.0   26000 !
N2O+NO=NO2+N2                5.3E05  2.23  46281 !
 !
 ! ****************************************************
 ! *  cyanide subset                          *
 ! ****************************************************
 !
CN+H2=HCN+H                  3.0E05  2.45   2237 !
!HCN+O=NCO+H                  1.4E04  2.64   4980
!HCN+O=NH+CO                  3.5E03  2.64   4980
!HCN+O=CN+OH                  2.7E09  1.58  29200
HCN+OH = CN+H2O              3.9E06  1.83  10300 !
HCN+OH=HOCN+H                5.9E04  2.40  12500
HCN+OH=HNCO+H                2.0E-3  4.     1000
```

HCN+OH=NH2+CO 7.8E-4 4. 4000
HCN+CN=C2N2+H 1.5E07 1.71 1530 !
CN+O=CO+N 7.7E13 0. 0 !
CN+OH=NCO+H 4.0E13 0. 0 !
CN+O2=NCO+O 7.5E12 0. -389 !
CN+CO2=NCO+CO 3.7E06 2.16 26884 !
CN+NO2=NCO+NO 5.3E15 -0.752 344 !
CN+NO2=CO+N2O 4.9E14 -0.752 344 !
CN+NO2=N2+CO2 3.7E14 -0.752 344 !
CN+HNO=HCN+NO 1.8E13 0.00 0
CN+HONO=HCN+NO2 1.2E13 0.00 0
CN+N2O=NCN+NO 3.9E03 2.6 3696 !
!CN+HNCO=HCN+NCO 1.5E13 0. 0 !
CN+NCO=NCN+CO 1.8E13 0. 0 !
HNCO=NH+CO 1.1E16 0. 86000 !
HNCO+H=NH2+CO 2.2E07 1.7 3800 !
HNCO+O=HNO+CO 1.5E08 1.57 44012 !
HNCO+O=NH+CO2 9.8E7 1.41 8524 !
HNCO+O=NCO+OH 2.2E6 2.11 11425 !
!HNCO+OH=NCO+H2O 6.4E05 2. 2563 !
HNCO+HO2=NCO+H2O2 3.0E11 0. 22000 !
HNCO+O2=HNO+CO2 1.0E12 0. 35000 !
HNCO+NH2=NH3+NCO 5.0E12 0. 6200 !
HNCO+NH=NH2+NCO 3.0E13 0. 23700 !
HOCN+H=NCO+H2 2.0E07 2. 2000 !
HOCN+O=NCO+OH 1.5E04 2.64 4000 !
HOCN+OH=NCO+H2O 6.4E05 2. 2563 !
HCNO+H=HCN+OH 1.0E14 0 12000 !
HCNO+O=HCO+NO 2.0E14 0. 0 !
HCNO+OH=CH2O+NO 4.0E13 0. 0 !
NCO+M=N+CO+M 3.1E16 -0.50 48000 !
NCO+H=NH+CO 5.0E13 0. 0 !
NCO+O=NO+CO 4.7E13 0. 0 !
NCO+OH=NO+HCO 5.0E12 0. 15000 !
NCO+O2=NO+CO2 2.0E12 0. 20000 !
NCO+H2=HNCO+H 7.6E02 3. 4000 !
NCO+HCO=HNCO+CO 3.6E13 0. 0 !
NCO+NO=N2O+CO 6.2E17 -1.73 763 !

```
NCO+NO=N2+CO2                7.8E17 -1.73    763 !
NCO+NO2=CO+NO+NO             2.5E11  0.     -707 !
NCO+NO2=CO2+N2O              3.0E12  0.     -707 !
NCO+HNO=HNCO+NO              1.8E13  0.        0 !
NCO+HONO=HNCO+NO2            3.6E12  0.        0 !
NCO+N=N2+CO                 2.0E13  0.        0 !
!NCO+NCO=N2+CO+CO             1.8E13  0.        0 !
C2N2+O=NCO+CN                4.6E12  0.     8880 !
C2N2+OH=HOCN+CN              1.9E11  0.     2900 !
NCN+O=CN+NO                 1.0E14  0.        0 !
NCN+OH=HCN+NO                5.0E13  0.        0 !
NCN+H=HCN+N                 1.0E14  0.        0 !
NCN+O2=NO+NCO                1.0E13  0.        0 !
H+CH3CN=HCN+CH3              4.0E7   2.     2000 !
H+CH3CN=CH2CN+H2             3.0E7   2.     1000 !
O+CH3CN=NCO+CH3              1.5E4   2.64   4980 !
OH+CH3CN=CH2CN+H2O           2.0E7   2.     2000 !
CH2CN+O=CH2O+CN              1.0E14    0.   0.   !
CN+CH2OH=CH2CN+OH            5.0E13  0.        0 !
H2CN+M=HCN+H+M               3.0E14  0.    22000 !
 !
 ! *****************************************************
 ! *  subset for CxHyOz+nitrogen species reactions     *
 ! *****************************************************
 !
CO+NO2 = CO2+NO              9.0E13  0.    33779 !
CO+N2O=N2+CO2                3.2E11  0.    20237 !
CO2+N=NO+CO                 1.9E11  0.     3400 !
CH2O+NCO=HNCO+HCO            6.0E12  0.        0 !
CH2O+NO2 = HCO+HONO          8.0E02  2.77  13730 !
!!!!!HCO+NO=HNO+CO             7.2E12  0.        0 !
HCO+NO2 = CO+HONO            1.2E23 -3.29   2355 !
HCO+NO2 = H+CO2+NO           8.4E15 -0.75   1930 !
HCO+HNO=CH2O+NO              6.0E11  0.     2000 !
CH4+CN=CH3+HCN               6.2E04  2.64   -437 !
NCO+CH4 = CH3+HNCO           9.8E12  0.00   8120 !
!CH3+NO=HCN+H2O               1.5E-1  3.523  3950 !
!CH3+NO=H2CN+OH               1.5E-1  3.523  3950 !
```

```
CH3+N=H2CN+H                7.1E13  0.       0 !
CH3+CN=CH2CN+H              1.0E14  0.       0 !
CH3+HOCN=CH3CN+OH           5.0E12  0.    2000 !
!CH2+NO=HCN+OH              2.2E12  0.    -378 !
!CH2+NO=HCNO+H              1.3E12  0.    -378 !
CH2+NO2=CH2O+NO             5.9E13  0.       0 !
CH2+N=HCN+H                 5.0E13  0.       0 !
CH2+N2=HCN+NH               1.0E13  0.   74000 !
H2CN+N=N2+CH2               2.0E13  0.       0 !
CH2(S)+NO=HCN+OH            2.0E13  0.       0 !
CH2(S)+NO=CH2+NO            1.0E14  0.       0 !
CH2(S)+HCN=CH3+CN           5.0E13  0.       0 !
CH+NO2=HCO+NO               1.0E14  0.       0 !
CH+NO = HCN+O               4.8E13  0.00     0 !
CH+NO = HCO+N               3.4E13  0.00     0 !
CH+NO = NCO+H               1.9E13  0.00     0 !
CH+N=CN+H                   1.3E13  0.       0 !
CH+N2=HCN+N                 3.7E07  1.42  20723 !
CH+N2O=HCN+NO               1.9E13  0.    -511 !
C+NO=CN+O                   2.0E13  0.       0 !
C+NO=CO+N                   2.8E13  0.       0 !
C+N2=CN+N                   6.3E13  0.   46019 !
C+N2O=CN+NO                 5.1E12  0.       0 !
C2H6+CN=C2H5+HCN            1.2E05  2.77  -1788 !
C2H6+NCO = C2H5+HNCO        1.5E-9  6.89  -2910 !
C2H4+CN = C2H3+HCN          5.9E14 -0.24     0 !
C2H3+NO=C2H2+HNO            1.0E12  0.    1000 !
C2H3+N=HCN+CH2              2.0E13  0.       0 !
C2H2+NCO = HCCO+HCN         1.4E12  0.00  1815 !
!!!!!C2H+NO=CN+HCO          2.1E13  0.       0 !
CH2CO+CN=HCCO+HCN           2.0E13  0.       0 !
HCCO+NO=HCNO+CO             7.2E12  0.       0 !
HCCO+NO=HCN+CO2             1.6E13  0.       0 !
HCCO+NO2=HCNO+CO2           1.6E13  0.       0 !
HCCO+N=HCN+CO               5.0E13  0.       0 !
!
!
! REACCIONES MECANISMO ETANOL
```

```
!
!
! *****************************************************
! *   C2H6OH subset                                   *
! *****************************************************
!
C2H5OH(+M) = CH2OH+CH3(+M)      5.9E23  -1.68   91163! MAR99 *
  LOW /2.9E85 -18.9 109914/
  TROE/ 0.5 200 890 4600 /
  H2O/5.0/ H2/2/ CO/2/ CO2/3/
C2H5OH(+M) = C2H5+OH(+M)        1.2E23  -1.54   96005! MAR99 *
  LOW /3.2E85 -18.8 114930/
  TROE/ 0.5 300 900 5000 /
  H2O/5.0/ H2/2/ CO/2/ CO2/3/
C2H5OH(+M) = C2H4+H2O(+M)       2.8E13   0.09   66136! MAR99 *
  LOW /2.6E83 -18.8 86452/
  TROE/ 0.7 350 800 3800 /
  H2O/5.0/
C2H5OH(+M) = CH3HCO+H2(+M)      7.2E11   0.09   91007! MAR99 *
  LOW /4.5E87 -19.4 115586/
  TROE/ 0.9 900 1100 3500 /
  H2O/5.0/
C2H5OH+OH = C2H4OH+H2O          1.7E11   0.27     600! MAR99  * overall
!C2H5OH+OH = CH3CHOH+H2O        2.6E06   2.00   -1373! DRY
!C2H5OH+OH = CH3CHOH+H2O        4.6E11   0.15       0! MAR99
C2H5OH+OH = CH3CH2O+H2O         7.5E11   0.30    1634! MAR99
C2H5OH+H = C2H4OH+H2            1.2E07   1.80    5098! MAR99  * fit
!C2H5OH+H = CH3CHOH+H2          2.6E07   1.65    2827! MAR99
C2H5OH+H = CH3CH2O+H2           1.5E07   1.60    3038! MAR99
C2H5OH+O = C2H4OH+OH            9.4E07   1.70    5459! MAR99  * overall
!C2H5OH+O = CH3CHOH+OH          1.9E07   1.85    1824! MAR99
C2H5OH+O = CH3CH2O+OH           1.6E07   2.00    4448! MAR99
C2H5OH+CH3 = C2H4OH+CH4         2.2E02   3.18    9622! MAR99  * fit
!C2H5OH+CH3 = CH3CHOH+CH4       7.3E02   2.99    7948! MAR99
C2H5OH+CH3 = CH3CH2O+CH4        1.4E02   2.99    7649! MAR99
C2H5OH+HO2 = C2H4OH+H2O2        1.2E04   2.55   15750! MAR99
C2H4OH+O2 = CH2O+CH2O+OH        6.0E10   0.00   24500! MAR99
!C2H5OH+HO2 = CH3CHOH+H2O2      8.2E03   2.55   10750! MAR99
```

```
C2H5OH+HO2 = CH3CH2O+H2O2       2.5E12   0.00   24000! MAR99
!
CH3CH2O+M = CH3HCO+H+M          1.2E35  -5.89   25274! MAR99
CH3CH2O+M = CH3+CH2O+M          1.3E38  -6.96   23800! MAR99
CH3CH2O+CO = C2H5+CO2           4.7E02   3.16    5380! MAR99  * anal to ch3o+co
CH3CH2O+O2 = CH3HCO+HO2         4.0E10   0.00    1100! HAR90
CH3CH2O+H = CH3+CH2OH           3.0E13   0.00       0! MAR99 *
CH3CH2O+H = C2H4+H2O            3.0E13   0.00       0! MAR99 *
CH3CH2O+OH = CH3HCO+H2O         1.0E13   0.00       0! MAR99 *
!
!CH3CHOH+O2 = CH3HCO+HO2         4.8E14   0.00    5017! MAR99 * anal to ch2oh+o2
! DUP
!CH3CHOH+O2 = CH3HCO+HO2         8.4E15  -1.20       0! MAR99 *
! DUP
!CH3CHOH+CH3 = C3H6+H2O          2.0E13   0.00       0! MAR99 *
!CH3CHOH+O = CH3HCO+OH           1.0E14   0.00       0! MAR99 *
!CH3CHOH+H = CH3+CH2OH           3.0E13   0.00       0! MAR99 *
!CH3CHOH+H = C2H4+H2O            3.0E13   0.00       0! MAR99 *
!CH3CHOH+HO2 = CH3HCO+OH+OH      4.0E13   0.00       0! MAR99 *
!CH3CHOH+OH = CH3HCO+H2O         5.0E12   0.00       0! MAR99 *
!CH3CHOH+M = CH3HCO+H+M          1.0E14   0.00   25000! MAR99 *
!!CH3HCO+OH = CH3CO+H2O          9.2E06   1.50    -962! TAY96 *
!!CH3HCO+OH = CH2HCO+H2O         1.7E05   2.40     815! TAY96 *
!
!*****************************************************
! ***   CH2O/HCO Subset
!*****************************************************
!
HCO+HCO=CO+CH2O                 3.0E13  0.00      0 ! cec94 (300)
!
!*****************************************************
! *** CH3OH/CH2OH/CH2O Subset ***
!*****************************************************
!
!CH3OH(+M)=CH3+OH(+M)            1.9E16  0.0   91730 !TSA87+Held98
!  LOW/2.95E44  -7.35 95640/
!  TROE/0.414 279 5459/
!  N2/1.43/ H2O/8.58/
```

```
CH3OH(+M)=CH2OH+H(+M)          2.7E16 -0.08  98940 !TSA87+Held98
  LOW/2.34E40  -6.33 103100/
  TROE/0.773 693 5333/
CH3OH+H=CH2OH+H2              1.7E7   2.1    4868
CH3OH+H=CH3O+H2               4.2E6   2.1    4868
!CH3OH+H=CH2OH+H2             1.67E7   2.0    4520 ! LI/WILL96
!CH3OH+H=CH3O+H2              3.8E7   2.0    5860 ! LI/WILL96
!CH3OH+O=CH2OH+OH             3.9E5   2.5    3080
!CH3OH+OH=CH2OH+H2O           5.30E4  2.53    960
!CH3OH+OH=CH2OH+H2O           7.1E06  1.80   -600 ! BOT/COH91
!CH3OH+OH=CH3O+H2O            1.32E4  2.53    960
!CH3OH+OH=CH3O+H2O            1.0E06  2.10    500 ! BOT/COH91
CH3OH+OH=CH2OH+H2O            1.4E06  2.00   -3510 ! LI/WILL96
CH3OH+OH=CH3O+H2O             6.3E06  2.00    6300 ! LI/WILL96
!CH3OH+HO2=CH2OH+H2O2          9.6E10  0.0   12578 ! nbs87
!CH3OH+HO2=CH2OH+H2O2          3.0E12  0.0   12578 !
! A factor fit to ch3oh oxidation data
CH3OH+HO2=CH2OH+H2O2          1.0E12  0.0   10040 ! 81tsu
CH3OH+O2=CH2OH+HO2            2.1E13  0.00  44900 ! nbs87
CH3OH+CH3=CH2OH+CH4           3.2E01  3.17   7170 ! nbs87
CH3OH+CH3=CH3O+CH4            1.5E01  3.10   6940 ! nbs87
CH3O+HO2=CH2O+H2O2            3.0E11  0.00      0 ! nbs86
CH3O+CO=CH3+CO2               1.6E13  0.00  11800 ! nbs86
CH3O+CH3=CH2O+CH4             2.4E13  0.00      0 ! nbs86
CH3O+CH2O=CH3OH+HCO           1.0E11  0.00   3000 ! nbs86
CH3O+HCO=CH3OH+CO             9.0E13  0.00      0 ! nbs86
CH3O+CH3OH=CH3OH+CH2OH        3.0E11  0.00   4100 ! nbs86
CH3O+CH3O=CH3OH+CH2O          6.0E13  0.00      0 ! nbs86
!CH2OH+H=CH2O+H2              2.0E13  0.00      0
! PG98: removed
CH2OH+H=CH2O+H2               4.8E13  0.00      0 ! DOB/WAG94
!CH2OH+O=CH2O+OH              1.0E13  0.00      0
! PG98: removed
CH2OH+O=CH2O+OH               6.5E13  0.00   -700 ! SEE/GUT94
CH2OH+O2=CH2O+HO2             1.6E15 -1.0       0
 DUP
CH2OH+O2=CH2O+HO2             7.2E13  0.0    3577
 DUP
```

```
CH2OH+HO2=CH2O+H2O2          3.6E13  0.0      0 ! Grotheer ea 85
CH2OH+HCO=CH3OH+CO           1.2E14  0.0      0 ! nbs87
CH2OH+HCO=CH2O+CH2O          1.8E14  0.0      0 ! nbs87
CH2OH+CH2O=CH3OH+HCO         5.5E03  2.8    5860 ! nbs87
CH2OH+CH2OH=CH3OH+CH2O       5.0E12  0.0      0 ! nbs87
CH2OH+CH3O=CH3OH+CH2O        2.4E12  0.0      0 ! nbs87
!
!*****************************************************
! *** H/N/O Subset ***
!*****************************************************
!
HONO2+OH=NO3+H2O             1.0E10  0.0   -1240 ! LAM/BEN84
H2NO+O2=HNO+HO2              3.0E12  0.0   25000 ! a (JAM 6/98)
HONO+HONO=>NO+NO2+H2O        3.5E-1  3.64  12100 ! MEB/LIN98
H2NO+HO2=HNO+H2O2            2.9E04  2.69   1600 ! a (BOZ/DEA98)
HNOH+H=NH2+OH                4.0E13  0.0       0 ! a (BOZ/DEA98)
HNOH+H=HNO+H2                4.8E8   1.5     378 ! a (BOZ/DEA98)
HNOH+O=HNO+OH                7.0E13  0.0       0 ! a (BOZ/DEA98)
DUP
HNOH+O=HNO+OH                3.3E08  1.5    -358 ! a (BOZ/DEA98)
DUP
HNOH+OH=HNO+H2O              2.4E6   2.0   -1192 ! a (BOZ/DEA98)
HNOH+NH2=NH3+HNO             1.8E6   1.94  -1152 ! a (BOZ/DEA98)
HNOH+HO2=HNO+H2O2            2.9E4   2.69  -1600 ! a (BOZ/DEA98)
HNOH+M=HNO+H+M               2.0E24 -2.84  58934 ! a (BOZ/DEA98)
  H2O/10/
HNOH+O2=HNO+HO2              3.0E12  0.0   25000 ! a (JAM 10/98)
HNOH+NO2=HONO+HNO            6.0E11  0.0    2000 ! a (JAM 98)
!
!*****************************************************
! ***  Subset for CxHyOz+nitrogen species reactions ***
!*****************************************************
!
CH3OH+NO2=CH2OH+HONO         3.7E11  0.0   21400 ! ANA/HAN88
CH2OH+NO=CH2O+HNO            1.3E12  0.0       0 ! NES/STI89/p (300)
CH2OH+NO2=CH2O+HONO          5.0E12  0.0       0 ! NES/STI89/p (300)
CH2OH+HNO=CH3OH+NO           3.0E12  0.0       0 ! PG98 est.
CH3O+NO=CH2O+HNO             1.3E14 -0.7       0 ! ATK92
```

```
CH3O+NO2=CH2O+HONO            6.0E12  0.0    2285 ! MCC/KAU85
CH3O+HNO=CH3OH+NO             3.2E13  0.0       0 ! HE/LIN88
!CH3+NO(+M)=CH3NO(+M)          9.0E12  0.0     119 ! DAV/PIL91
!LOW/3.2E23  -1.87 0/
! H2O/10/ N2/1.5/
CH3+NO2=CH3O+NO               4.0E13 -0.20      0 ! PG98
CH3+HONO=CH4+NO2              1.0E12  0.0       0 ! PG98 est.
! analogy NH2+HONO
CH3NO=HCN+H2O                 3.0E13  0.0   50000 ! LIF93 est.
!
!NUEVAS REACCIONES AÑADIDAS
!
CH3+O2(+M)=CH3O2 (+M)                7.8E8   1.2       0
LOW/5.8E25  -3.3  0/
CH3O2+O=CH3O+O2               2.59E13   0       0
CH3O2+H=CH3O+OH               9.64E13   0       0
CH3O2+NO=CH3O+NO2             3.10E12   0    -358
CH3O2+CH3=CH3O+CH3O           3.24E13   0       0
!
!
!
C2H+NO=CN+HCO                 6.03E13  0.       570
!
!
!
!
!
!
!!!!**************Mecanismo NO-NO2 (articulo P. Glarborg et al., Combustion and Flame 132, 629-638, 2003
!
OH+NO+M=HONO+M                5.1E23 -2.51    -68 ! Cambio en las eficacias de tercer cuerpo antes: H2O/5/ Ahora en relación cn NO+O+M=NO2+M
N2/1.7/   O2/1.5/  H2O/10/
!!!!!!H2O/5/
!
!
NO2+HO2=HONO+O2                      6.3E08   1.25     5000 !Hori et al., 1998
HNO+O2=NO+HO2                              2.0E13   0.0         16000 !Dean et al., 2000
```

```
!HCO+NO=CO+HNO                    7.0E13   -0.40      0 ! Veyret et al., 1981
!
!!!HO2+NO+M=HONO2+M               2.23E12  -3.5   2200 !
!!!NO2+H+M=HONO+M                 1.40E18 -1.5       900
!!!NO3+M=O2+NO+M                  2.05E8   1          12122
!!!   NO2/0/
!
!
!SON REACCIONES DEL ARTI DE GLARBORG 2003, ACTUALIZANDO VALORES, DEJO LOS ANTERIORES EXCEPTO LAS QUE NO ESTABAN ANTERIORMENTE
!!!CH2O+M=HCO+H+M             6.1E+15  0.000  76900 ! Kumaran, 1998 (Glarborg 2003)
!!!     H2O/5/
!!!!H2/2/ CO/2/ CO2/3/  H2O/5/
CH2O+M=CO+H2+M                    2.8E15   0          63800    !KUMARAN, 1998 (GLARBORG 2003)
              H2O/5/
!!!H2/2/ CO/2/ CO2/3/  H2O/5/
!!!CH2O+H=HCO+H2               5.7E07     1.90    2740 ! JUST 1981 (GLARBORG 2003)
!!!!CH2O+HO2=HCO+H2O2            4.1E04    2.5     10200  ! EITENEER 1998 (GLARBORG 2003)
!!!!CH2O+O2=HCO+HO2              5.0E04     3.0      39000 ! GLARBORG 2003
!!!HCO+M=H+CO+M                4.8E17   -1.20    17700.0  ! fRIEDRICHS, 2002 (GLARBORG 2003)
!!!!         H2O/5./
!!!!CO/1.87/   H2/1.87/  CH4/2.81/ CO2/3./ H2O/5./
HCO+HO2=CO2+OH+H              3.0E13   0           0          ! TSANG 1986 (GLARBORG 2003)
!!!!!HCO+O2=HO2+CO              7.58E12    0.0    406. !DESAIN 2001 (GLARBORG 2003)
!
!!!!*********************************************************************************
**
!!
!!  sulphur subset: Alzueta 2001
!!  a: ref: Glarborg, Kubel, Dam-Johansen, Chiang, *
!!         Bozzelli, IJCK 28:773 (1996)
!!
!!*******************************************************************************
*
!!
! ******** H2S subset: taken from Song ea 2013. 24/Sept:JM   *********
!
! ******* H2S reactions *******
```

```
!
H2S+M = S+H2+M          1.6E24  -2.613   89100 ! Shiina+98 (9911)
   N2/1.5/ SO2/10/ H2O/10/
H2S+S = SH+SH           7.4E6    2.3     9007 ! Gao ea 2011
DUP
H2S+S = SH+SH           4.7E7    1.33    -436 !
DUP
H2S+H = SH+H2           3.5E07   1.94     904 ! Peng eaJPCA1999
!H2S+H = SH+H2       1.2E07  2.10   700 ! a (Yoshimura+92)
H2S+O = SH+OH           7.5E07   1.75    2900 ! Goumri ea 95
H2S+OH = SH+H2O         8.7E13  -0.7        0 ! Ellingson ea, JACS2007 /Zhou ea 2013
DUP
H2S+OH = SH+H2O         4.1E7   1.77        0 ! Ellingson ea, JACS2007
DUP
SH+H2O2=H2S+HO2      5E12    0.0    0 ! ESTIMATED PRESENT WORK
!SH+H2O2=H2S+HO2     5.6E4    2.823    8668 ! Zhou TST (2009)
!H2S+HO2=SH+H2O2              3.16E12    0.0    16890 ! Marwan 2011 PRUEBA
H2S+HO2=HSO+H2O      1.0E0    3.29     6224 ! Zhou (Molina Sendt TST) 2009
SH+HO2=H2S+O2           3.8E4    2.78    -1529 ! Zhou TST (2009)
!H2S+O2=HO2+SH       9.53E5   2.13   39124 ! (Prueba JM O2 singlet)
!SH+HO2=H2S+O2                3.5E16    -1.84    -2758 ! Prueba chinos
H2S+O2=HSO+OH           1.0E11   0.0     49100 ! Zhou est (2009)
H2S+O3=SO2+H2O          5.3E8    1.66    11665 ! MOU/MORJPCA2013
H2S+O3=HOSO+OH          1.1E3    2.77    11369 ! MOU/MORJPCA2013
!H2S+SO=SH+HSO          5.4E3    3.21    26824 ! Zhou TST (2009) (Glarborg dice: rv too fast; la
suprime) y utiliza la siguiente
H2S+SO(S)=HSO+SH        1.0E13   0.000   11000 ! (NUEVA) Zhou est 2009
H2S+SO=SH+HOS           1.0E13   0.0     36500 ! Zhou est (2009)
H2S+SO2=S2O+H2O         1.7E6    1.86    37740 ! Sendt ea 2005
!H2S+M=H+SH+M           1.8E14   0.0     64000 ! (NUEVA) Frenklach 1981
H2S+S(+M)=H2S2(+M)   6.4E7    1.28     -478 ! Zhou 2009
   LOW /2.4E21 -1.612 1670/
   TROE /0.5 726 726/
H2S+SO2=H2S2O2          3.5E18  -2.12    33530 ! (NUEVA) Sendt ea 2005
H2S+HSO=SH+HSOH         1E13     0.0     17300 ! (NUEVA) Zhou est 2009
H2S+HOS=SH+HSOH         1E13     0.0     12500 ! (NUEVA) Zhou est 2009
H2S+S2O=H2S3O                 2.4E19  -2.3     30450 ! (NUEVA) Sendt ea 2005
H2S+S2O=S3+H2O                8E7      1.51    34010 ! (NUEVA) Sendt ea 2005
H2S+S2O=HSSSOH                2.9      3.64    22681 ! (NUEVA) Sendt ea 2005
```

```
!
! ***HS2/H2S2 reactions****
!
!
HS2+H=H2S+S              1.5E8    1.55     2259 ! Zhou ea 2009
DUP
HS2+H=H2S+S              4.2E18  -1.56      472 ! Zhou ea 2009
DUP
HS2+H=H2+S2            1.0E08   1.750    -877 ! (Updated) Zhou ea 2009 (113)
DUP
HS2+H=H2+S2            2.9E16  -0.894     -56 ! (Updated) Zhou ea 2009 (113)
DUP
HS2+H+M = H2S2+M       1.0E16   0.0         0 ! est Maria
HS2+H=SH+SH              9.7E7    1.62    -1030 ! Sendt ea 2002
DUP
HS2+H=SH+SH              1.6E18  -0.983     261 !
DUP
HS2+O = S2+OH            7.5E07   1.75     2900 ! est h2s+O  **no rev
!HS2+O = S2+OH           1.0E14   0.0         0 ! (Update?) Zhou est 2009
HS2+OH = S2+H2O          2.7E12   0.0         0 ! est h2s+oh **no rev
!HS2+OH = S2+H2O         1.0E14   0.0         0 ! (Update?) Zhou est 2009
HS2+O2=S2+HO2            8.4E01   2.95     7071 ! Song ea 2016
HS2+SH=S2+H2S            6.3E3    3.05    -1105 ! Sendt ea 2002
HS2+S = S2+SH            2.0E13   0.0      7400 ! est h2s+s **no rev
!HS2+S = S2+SH           4.2E6    2.2      -600 ! (Update?) Sendt 2002
H2S2+H=HS2+H2            5.0E07   1.93    -1408 ! (Updated) Sendt 2002
H2S2+O = HS2+OH          7.5E07   1.75     2900 ! est h2s+o **no rev
!H2S2+O = HS2+OH         1.0E14   0.0         0 ! (Update?) Zhou est 2009
H2S2+OH = HS2+H2O        1.0E13   0.0         0 ! (Updated) Zhou est 2009 (antes 2.7E12)
H2S2+S = HS2+SH          2.0E13   0.0      7400 ! est h2s+s **no rev
!H2S2+S=HS2+SH                    2.9E6    2.3      1204 ! (Update?) Sendt 2002
H2S2+SH=HS2+H2S                   6.4e03   2.98    -1480 ! Sendt ea PCI2002
HS2+O2=HSO+SO            6.6E3    1.9      7071 ! Song ea 2016 (Juanma nueva Julio '17)
H2S2+H=H2S+SH            3.7E8    1.72      477 ! (NUEVA) Sendt ea 2002
H2S2+O=HSO+SH                     1.0E14   0.0         0 ! (NUEVA) Zhou est 2009
H2S2+HO2=HS2+H2O2        1.0E13   0.0         0 ! (NUEVA) Zhou est 2009
H2S2+O2=HS2+HO2                   1.0E13   0.0         0 ! (NUEVA) Zhou est 2009
H2S2+SO=HS2+HSO                   1.0E13   0.0     15000 ! (NUEVA) Zhou est 2009
```

```
H2S2+SO=HS2+HOS              1.0E13   0.0     19000 ! (NUEVA) Zhou est 2009
H2S2+HSO=HS2+HSOH 1.0E13   0.0      2000 ! (NUEVA) Zhou est 2009
H2S2+HOS=HS2+HSOH 1.0E13   0.0      2000 ! (NUEVA) Zhou est 2009
HS2+O=SH+SO              1.0E14   0.0        0 ! (NUEVA) Zhou est 2009
HS2+HO2=S2+H2O2              1.0E13   0.0          26000 ! (NUEVA) Zhou est 2009
HS2+SO=S3+OH                 1.0E13   0.0     14900 ! (NUEVA) Zhou est 2009
HS2+SO3=HS2O+SO2     1.0E13   0.0     10000 ! (NUEVA) Zhou est 2009
HS2+HSO=HS2O+SH              1.0E13   0.0      7000 ! (NUEVA) Zhou est 2009
HS2+HSO=S2+HSOH              1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HS2+HOS=S2+HSOH              1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HS2+HS2=H2S2+S2              9.6E0    3.37    -1672 ! (NUEVA) Sendt 2002
!
!
! ****** SH reactions *********
!
SH+O = H+SO              4.25E11  0.724   -1027 ! Sendt/Hay2007
SH+O=S+OH                1.8E12   0.0        0 ! zhou ea ijck2016
DUP
SH+O=S+OH                4.3E11   0.724      0 !
DUP
SH+OH=S+H2O              1.0E14   0.0           0 ! Song ea 2016
!SH+OH=S+H2O             1.7E5    2.47        -1637 ! Zhou TST 2009
SH+OH=HOS+H              1.0E13   0.0     7400 ! Zhou ea PCI 2013
SH+HO2=SO+H2O            3.2E2    2.58    -2071 ! Zhou ea 2013
SH+HO2=HSO+OH            2.5E8    1.48    -2169 ! Zhou TST 2009
S+H2O2=SH+HO2            4.1E6    2.2     12619 ! Zhou ea 2013
SH+O2=HSO+O              2.3E6    1.816   20008 ! Zhou ea 2009
SH+O2=S+HO2              4.7E6    2.02    36913 ! Zhou ea 2009
SH+O2=SO+OH              7.5E4    2.05    16384 ! Zhou ea 2009
SH+O2=SO2+H              1.5E5    2.12    11020 ! Song ea 2016
SH+O2(+M)=HSOO(+M)           8.7E14  -0.26      298 ! Goumri ea JPCA99! check A=2E14???)
          LOW /3.1E19 -0.201 20/
SH+O3=HSO+O2             5.7E12   0.0      556 ! Atk2004
SH+H2O2=HSOH+OH              9.5E3    2.8      9829 ! Zhou ea2009
SH+SH(+M)=H2S2(+M)           9E11     0.155   -1432 ! Zhou ea JPCA2009
          LOW /2.3E31 -4.94 1998/              ! Gao ea 2011
          TROE/ 1.0 254 2373 /
!SH+S+M=HS2+M         6E11     0.0        0 !
```

```
!SH+SH = S2+H2          1.0E12   0.0        0 ! **no rev
!SH+S = S2+H            3.0E13   0.0        0 ! **no rev
SH+S=S2+H           3.3E12   0.543     -29 ! (NUEVA) Zhou QRRK 2009
SH+SO=HSO+S         1.0E13   0.0     25000 ! (NUEVA) Zhou est 2009
SH+SO=HOS+S         1.0E13   0.0     30000 ! (NUEVA) Zhou est 2009
SH+HSO=S+HSOH               1.0E11   0.0     11000 ! (NUEVA) Zhou est 2009
SH+HSO=S2O+H2               1.0E14   0.0     14250 ! (NUEVA) Zhou est 2009
SH+SO=S2O+H         1.0E12   0.0      5000 ! (NUEVA) Zhou est 2009
SH+SO2=HSO+SO               1.0E14   0.0     32000 ! (NUEVA) Zhou est 2009
SH+SO2=HOS+SO               1.0E14   0.0     36000 ! (NUEVA) Zhou est 2009
SH+SO2=OH+S2O               1.0E14   0.0     32000 ! (NUEVA) Zhou est 2009
SH+SO2=HSSO2                1.0E13   0.0     33000 ! (NUEVA) Zhou est 2009
!
!
! ***** S/S2/S3... reactions ********
!
S+H+M=SH+M          6.2E16  -0.6        0 ! Sendt ea PCI2002  **no rev
S+H2 = SH+H             1.4E14   0       19300 ! Shiina+98 (9906) **no rev
S+OH = H+SO             1.5E13   0.2     -1361 ! Sendt ea PCI2007
S+HO2=SO+OH             5.7E13   0.0        0 ! Ballester/VAr IJCK2008
S+O2 = SO+O             5.4E05   2.1     -1450 ! Lu ea JCM2004
S+HO2=HOS+O             1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
S+O3=SO+O2              7.2E12   0.0        0 ! (NUEVA) Atkinson 2004
S+H2O2=HOS+OH               1.0E12   0.0        0 ! (NUEVA) Zhou est 2009
S+S(+M)=S2(+M)      1.4E10   0.0      -825 ! (Updated) Du 2008 (tenía la inversa sin ref)
   LOW  /7.2E14 0.0 -408 /
S2+H+M=HS2+M        1.2E25  -2.840    1665 ! (Updated) Sendt 2002 (tenía 1E16)
  H2S /1.1/ AR /0.88/
S2+O=SO+S           1.4E11   0.7      -231 ! (Updated) Zhou TST 2009
S2+O+M=S2O+M        1.9E21  -2.8        0 ! (NUEVA) Zhou est O+O+M 2009
S2+O2=S2O+O             1.7E4    2.54    34376 ! (NUEVA) Zhou TST 2009
S2+O2=SO+SO             2.3      2.45    30440 ! (NUEVA) Zhou TST 2009
S2+S+M=S3+M         1.9E15   0.0     -1788 ! (NUEVA) Zhou est 2009
S2+S2+M=S4+M        1.9E15   0.0     -1788 ! (NUEVA) Zhou est 2009
S3+H2O=HSSSOH       1.0E14   0.0     25000 ! (NUEVA) Zhou est 2009
S3+S2+M=S5+M        1.9E15   0.0     -1788 ! (NUEVA) Zhou est 2009
S3+S3+M=S6+M        1.9E15   0.000   -1788 ! (NUEVA) Zhou est 2009
S3+S2O=S4+SO        1.0E14   0.000   16000 ! (NUEVA) Zhou est 2009
```

```
S3+S4+M=S7+M          1.9E15   0.000   -1788 ! (NUEVA) Zhou est 2009
S4+S4+M=S8+M          1.9E15   0.000   -1788 ! (NUEVA) Zhou est 2009
!
!
!***** S2O reactions *******
!
S2O+H2=SH+HOS         1.0E13   0.0     46000 ! (NUEVA) Zhou est 2009
S2O+H+M=HS2O+M        6.4E22  -2.59      287 ! (NUEVA) Zhou est HSO+M 2009
S2O+H=OH+S2           1.0E13   0.0         0 ! (NUEVA) Zhou est 2009
S2O+O=SO+SO           9.3E11   0.0         0 ! (NUEVA) Singleton 1988
S2O+OH=S2+HO2         1.0E13   0.0     40000 ! (NUEVA) Zhou est 2009
S2O+S=SO+S2           1.0E13   0.0         0 ! (NUEVA) Zhou est 2009
S2O+SH=HSO+S2         1.0E12   0.0      5000 ! (NUEVA) Zhou est 2009
S2O+SH=HS2+SO         1.0E13   0.0      8000 ! (NUEVA) Zhou est 2009
S2O+SH=S3+OH          1.0E13   0.0     21450 ! (NUEVA) Zhou est 2009
S2O+SO2=S2+SO3        1.0E13   0.0     20000 ! (NUEVA) Zhou est 2009
S2O+HSO2=HS2O+SO2     1.0E13   0.0     32000 ! (NUEVA) Zhou est 2009
S2O+S2=S3+SO          1.0E14   0.000   18000 ! (NUEVA) Zhou est 2009 (Glarborg la tenía
suprimida)
S2O+S2O=S3+SO2        1.0E12   0.000    2600 ! (NUEVA) Zhou est 2009
!
!
!***** SOx reactions ******
!
!SO+O(+M) = SO2(+M)   3.2E13   0.0         0 ! COB85,Plach/Troe84
!    LOW/1.2E21 -1.54  0/
!    TROE/0.55 1E-30 1E30/
!    N2/1.5/ SO2/10/ H2O/10/
SO+O+M=SO2+M          4.1E22  -2.170       0 ! (NUEVA) Lu 2003
 N2/1.5/ SO2/10/ H2O/10/
SO+M = S+O+M          4.0E14   0      107000 ! Plach/Troe 1984
SO+O2=SO2+O           7.6E03   2.37     2970 ! Tsuchiya+97/Woiki+95 (9906) !
!SO+HO2=SO2+OH        3.7E3    2.42     7660 ! Est Rasmussen2007
SO+HO2=SO2+OH         1.0E12   0.0         0 ! (NUEVA) (Glarborg suprime la anterior y dice que usa
esta, barrierless pw)
SO+H+M=HSO+M          1.9E20  -1.31      662 ! (NUEVA) Rasmussen 2007 (Tengo la inversa +
antigua)
   N2/1.5/ SO2/10/ H2O/10/
!HSO+M=SO+H+M         8.43E15  0.0     58600 ! Tsuchiya1994
```

```
!    N2/1.5/ SO2/10/ H2O/10/
SO+O3=SO2+O2              2.7E12   0.0      2325 ! (NUEVA) Atkinson 2004
SO+S+M=S2O+M                       4.1E22  -2.170       0 ! (NUEVA) Song ea 2016 (est as SO+O+M)
    N2/1.5/ SO2/10/ H2O/10/
SO+SH=S2+OH               1.0E12   0.0      4320 ! (NUEVA) Zhou est 2009
SO(S)+M=SO+M              1.0E13   0.0         0 ! Est Rasmussen2007
SO(S)+O2=SO2+O            1.0E13   0.0         0 ! Est Rasmussen2007
!SO+OH=SO2+H                       1.1E17   -1.35          0 ! Alzueta 2001 (disponible la inversa de
2002)
SO2+H=SO+OH             6.7E21  -2.22    30736 ! (Updated) Blitz 2002
H+SO2(+M)=OH+SO(+M)    9.19E25  2.77    20850 ! * Blitz 2006  (La teníamos suprimida, update?)
   LOW/1.35E22 -2.30 30965/            !
   TROE/0.283 272 3995/
   N2/1.0/ SO2/10/ H2O/10/ !CO2/2.5/
H+SO+M=HOS+M             3.6E20  -1.924     -29 ! (NUEVA) Sendt 2007
 N2 /0/
H+SO+N2=HOS+N2           2.0E21  -2.093     -72 ! (NUEVA) Sendt 2007
SO2*+M = SO2+M            1.3E14   0.0      3600 ! Strickler/Ito 1985
SO2*+SO2 = SO3+SO         2.6E12   0.0      2430 ! Heicklen+1980
SO2+O(+M) = SO3(+M)   3.7E11   0.0      1689 ! (Updated) Yilmaz 2006
   LOW/2.9E27 -3.58 5206/ !
   TROE/0.43 371 7442/
   SO2/10/ H2O/10/ N2/1/ !CO2/10/
SO2+O(+N2) = SO3(+N2)             3.7E11   0.00     1689 ! Naidoo2005/Yilmaz06
   LOW/2.9E27 -3.58 5206/ !
   TROE/0.43 371 7442/
SO2+OH(+M)=HOSO2(+M)          5.7E12  -0.27        0 ! Blitz2003
   LOW/1.7E27 -4.09 0/
   TROE/1.0 1E-30 412/
   N2/1.0/ SO2/5/ H2O/5/ !CO2/2.5/
SO2+H2O=VDW1                      1.0E14   0.0         0 ! (NUEVA) Zhou est 2009
SO2+O3=SO3+O2                     1.8E12   0.0     14000 ! (NUEVA) Zhou est 2009
SO2+S=SO+SO               6.0E-16  8.21    -9600 ! Murakami2003
SO3+H = HOSO+O            2.5E05   2.92    50300 ! a
SO3+H = SO2+OH            8.4E09   1.22     3319 ! Hindiyarti2007
SO3+O = SO2+O2            2.8E04   2.57    29212 ! Hindiyarti2007
SO3+OH = SO2+HO2          4.8E04   2.46    27225 ! Hindiyarti2007
SO3+SO=SO2+SO2            7.6E3    2.37     2980 ! Glarborg2004 (Chung75+est depT)
SO3+S=SO+SO2              1.0E13   0.0         0 ! (NUEVA) Zhou est 2009
```

```
!
!
!***** HSO/HOS reactions ******
!
HSO+O2=SO+HO2          6.4E5    2.63    19013 ! Zhou ea PCI2013
DUP
HSO+O2=SO+HO2          2.9E1    3.2          14529 !
DUP
HSO+O2=HSO2+O          8.4E-7   5.1          11312 ! Zhou ea PCI2013
HSO+O2=SO2+OH          3.7E01   2.764    6575 ! zHOOU EA PCI2013
HSO+O3=SH+O2+O2        1.5E12   0.0      2230 ! ATK 2004/LEE94
HSO+O3=HSO2+O2         1.3E12   0.0      2230 !
HSO+O3=SO+OH+O2        5.0E0    3.6      7191 ! Song ea IJCK2016
HSO+H = HSOH           2.5E20  -3.14      920 ! a
HSO+H = SH+OH          4.9E19  -1.86        1560 ! a
HSO+H = S+H2O          1.6E09   1.37     -340 ! a
HSO+H = H2SO           1.8E17  -2.47       50 ! a
H2S+O=HSO+H            1.4E9    1.1      5099 ! Goumri ea95
!HSO+H = H2S+O         1.1E06   1.03    10400 !
HSO+H = SO+H2          1.0E13   0.00        0 ! * est (a 1E12)
HSO+O+M = HSO2+M       1.1E19  -1.73      -50 ! a
HSO+O = SO2+H          4.5E14  -0.40        0 ! a
HSO+O+M = HOSO+M               6.9E19  -1.61     1590 ! a
HSO+O = O+HOS          4.8E08   1.02     5340 ! a
HSO+O = OH+SO          1.4E13   0.15      300 ! a
HSO+OH = HOSHO         5.2E28  -5.44     3170 ! a
HSO+OH = HOSO+H        5.3E07   1.57     3750 ! a
HSO+OH = SO+H2O        1.7E09   1.03      470 ! a
HSOO(+M)=HSO+O(+M)             2.0E19   -1.070  28374 ! Goumri ea 99
   LOW  /9.3E34 -5.87 30957/
HSO+H=HOS+H            1.0E14   0.0      4000 ! (NUEVA) Zhou est 2009
HSO+OH=H2+SO2                  1.0E11   0.0         0 ! (NUEVA) Zhou est 2009
HSO+HO2=SO+H2O2                1.0E13   0.0         0 ! (NUEVA) Zhou est 2009
HSO+HSO=SO+HSOH                1.0E13   0.0         0 ! (NUEVA) Zhou est 2009
HSO+S2=HS2+SO                  1.0E12   0.0      3000 ! (NUEVA) Zhou est 2009
HOS+M=HSO+M            5.8E11   0.0     32722 ! (NUEVA) Sendt 2007
   N2 /0/
HOS+N2=HSO+N2          2.9E11   0.0     24601 ! (NUEVA) Sendt 2007
```

```
HOS+H=H2+SO            1.0E13  0.0       0 ! (NUEVA) Zhou est 2009
HOS+O=OH+SO            1.0E14  0.0       0 ! (NUEVA) Zhou est 2009
HOS+O=H+SO2            1.0E14  0.0       0 ! (NUEVA) Zhou est 2009
HOS+OH=SO+H2O                  1.0E13  0.0       0 ! (NUEVA) Zhou est 2009
HOS+OH=H2+SO2                  1.0E11  0.0       0 ! (NUEVA) Zhou est 2009
HOS+O2=HO2+SO                  6.4E5   2.63   19013 ! (NUEVA) Zhou est 2009
HOS+O2=SO2+OH                  3.7E1   2.76    6575 ! (NUEVA) Zhou est 2009
HOS+HO2=SO+H2O2                1.0E13  0.0       0 ! (NUEVA) Zhou est 2009
HOS+HOS=SO+HSOH                1.0E13  0.0       0 ! (NUEVA) Zhou est 2009
HOS+S2=HS2+SO                  1.0E12  0.0    1000 ! (NUEVA) Zhou est 2009
HOS+S2=S3+OH                   1.0E13  0.0   13000 ! (NUEVA) Zhou est 2009
!
!
!***** HSOH reactions ******
!
HSOH = SH+OH           2.8E39  -8.75      75200 ! a
HSOH = S+H2O           5.8E29  -5.60   54500 ! a
HSOH = H2S+O           9.8E16  -3.40      86500 ! a
HSOH+HO2=HSO+H2O2              1.0E13  0.0       0 ! (NUEVA) Zhou est 2009
HSOH+HO2=HOS+H2O2              1.0E13  0.0       0 ! (NUEVA) Zhou est 2009
HSOH+O2=HSO+HO2                1.0E13  0.0   26000 ! (NUEVA) Zhou est 2009
HSOH+O2=HOS+HO2                1.0E13  0.0   30000 ! (NUEVA) Zhou est 2009
HSOH+O=HSO+OH                  1.0E14  0.0       0 ! (NUEVA) Zhou est 2009
HSOH+O=HOS+OH                  1.0E14  0.0       0 ! (NUEVA) Zhou est 2009
HSOH+H=HSO+H2                  1.0E14  0.0       0 ! (NUEVA) Zhou est 2009
HSOH+H=HOS+H2                  1.0E14  0.0       0 ! (NUEVA) Zhou est 2009
HSOH+OH=HSO+H2O                1.0E14  0.0       0 ! (NUEVA) Zhou est 2009
HSOH+OH=HOS+H2O                1.0E14  0.0       0 ! (NUEVA) Zhou est 2009
!
!
!***** HOSO reactions ******
!
!H+SO2(+M)=HOSO(+M)     2.37E8   1.63     7339 ! Blitz06  (Glarborg la utiliza en 2016)
!   LOW/1.85E37 -6.14 11075/
!   TROE/0.283 272 3995/
!    N2/1.0/ SO2/10/ H2O/10/ !CO2/2.5/
HOSO(+M)=H+SO2(+M)      1.7E10   0.80    46933 ! Alzueta2001(Goumri1999)
   LOW/1.5E31 -4.53 49178/
```

```
   TROE/0.30 1E-30 1E30/
   N2/1.0/ SO2/10/ H2O/10/
HOSO(+M) = HSO2(+M) 1.0E09   1.03       50000 ! GOU/MAR99
   LOW/1.7E35 -5.64 55400/
   TROE/0.40 1.E-30 1.E30/
   N2/1.0/ SO2/10/ H2O/10/ !CO2/2.5/
HOSO(+M)=OH+SO(+M)     9.9E21  -2.540   75891 ! (Updated) Blitz 2002 (Tenía puesta la inversa de Goumri 1999)
   LOW /1.2E46 -9.020 52953/
   TROE/0.95 2989 1.1/
!SO+OH(+M)=HOSO(+M)          1.6E12   0.50      -400 ! (PRUEBA con la inversa de GOumri'99)
!          SO2/10/ H2O/10/ N2/1.5/
!          LOW/9.5E27 -3.48 974/
!HOSO=OH+SO             3.6E18   0.0       86746 !
HOSO+M = O+HOS+M             2.5E30  -4.8    119000 ! Glarborg 1996
HOSO+H=SO(S)+H2O             2.4E14   0.0       0 ! Marshall-Hu05
HOSO+H=SO2+H2         1.8E7    1.72    -1286 ! Marshall-Hu05
HOSO+O=SO2+OH                1.0E13   0.0       0 ! (Updated) Zhou est 2009 (Tenía puesta la inversa con valores de ref desconocida)
HOSO+OH=SO2+H2O       6.0E12   0.0       0 ! (Updated) Rasmussen est 2007 (Yo tenía est 1E12)
HOSO+HO2=SO2+H2O2     1.0E13   0.0       0 ! (NUEVA) Zhou est 2009
!HOSO+O2=HO2+SO2              9.6E1    2.35   -10130 ! (Updated) Rasmussen 2007 (La tenía suprimida, y utilizaba valor Glarborg 96)
HOSO+O2=SO2+HO2     1.0E12   0.00  500  !Alzueta01 (Glarborg1996)
HOSO+SH=SO2+H2S              1.0E13   0.0       0 ! (NUEVA) Zhou est 2009
HOSO+S=SO2+SH                1.0E13   0.0       0 ! (NUEVA) Zhou est 2009
HOSO+SO=SO2+HSO              1.0E13   0.0       0 ! (NUEVA) Zhou est 2009
HOSO+SO=SO2+HOS              1.0E13   0.0       0 ! (NUEVA) Zhou est 2009
HOSO+HSO=SO2+HSOH     1.0E13   0.0       0 ! (NUEVA) Zhou est 2009
HOSO+HOS=SO2+HSOH     1.0E13   0.0       0 ! (NUEVA) Zhou est 2009
HOSO+HS2=SO2+H2S2  1.0E13   0.0       0 ! (NUEVA) Zhou est 2009
HOSO+S2=SO2+HS2              1.0E13   0.0       0 ! (NUEVA) Zhou est 2009
!
!
!***** HSO2 reactions ******
!
H+SO2(+M)=HSO2(+M)     5.31E8   1.59     2472 ! Blitz 2006
   LOW/1.41E31 -5.19 4513/          !
   TROE/0.390 167 2191/
```

```
   N2/1.0/ SO2/10/ H2O/10/ !CO2/2.5/
!HSO2(+M)=H+SO2(+M) 2.03E11  0.9     18360 ! Goumri '99 inversa
!     LOW/5.74E1 -3.29 19095/
!     N2/1.0/ SO2/10/ H2O/10/
HSO2+H = SO2+H2         5.0E12   0.46     -262 ! Marshall/Hu2005
HSO2+O2 = HO2+SO2     1.1E3    3.20     -235 ! Est Rasmussen2007
HSO2+O=SO2+OH                  1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO2+OH=SO2+H2O                1.0E13   0.0        0 ! la tenía estimada así ya
HSO2+HO2=SO2+H2O2  1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO2+O3=SO2+OH+O2  1.0E13   0.0        0 ! (NUEVA) Song est 2016
HSO2+SH=SO2+H2S                1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO2+S=SO2+SH                  1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO2+SO=SO2+HSO                1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO2+SO=SO2+HOS                1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO2+HSO=SO2+HSOH 1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO2+HS2=SO2+H2S2   1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSO2+S2=SO2+HS2                1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HSOO=HSO2              1E17   0.0        21300 ! est present work
!HSOO=HSO2              1E13   0.0        0 ! est present work
!
!
!***** HS2O reactions ******
!
HS2O+H=S2O+H2                  1.0E12   0.0          2600 ! (NUEVA) Zhou est 2009
HS2O+H=HS2+OH                  1.0E13   0.0            0 ! (NUEVA) Zhou est 2009
HS2O+O=S2O+OH                  1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HS2O+O=SH+SO2                  1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HS2O+OH=S2O+H2O                1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HS2O+OH=HS2+HO2                1.0E13   0.0     27000 ! (NUEVA) Zhou est 2009
HS2O+HO2=S2O+H2O2  1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HS2O+S=HS2+SO                  1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HS2O+S=S2O+SH                  1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HS2O+SH=S2O+H2S                1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HS2O+HS2=S2O+H2S2   1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
!
!
!***** SSO2 reactions ******
!
```

```
SO2+S(+M)=SSO2(+M)      3.7E12   0.0      1689 ! (NUEVA) Song es 2016 (est 10 x SO2+O+M)
  LOW  /2.9E28 -3.58 5206/
  TROE /0.43 371 7442/
  N2/1/ SO2/10/ H2O/10/
!SSO2+M=S+SO2+M       1.0E15   0.0     30000 ! (NUEVA) Zhou est 2009 (glarborg la tenía suprimida)
SSO2+H=SH+SO2                  1.0E13   0.0        0 ! (NUEVA) Song est 2016
SSO2+O=SO+SO2                  1.0E13   0.0            0 ! (NUEVA) Song est 2016
SSO2+OH=HOS+SO2                1.0E13   0.0        0 ! (NUEVA) Song est 2016
SSO2+S=S2+SO2                  1.0E13   0.0        0 ! (NUEVA) Song est 2016
!
!
!***** OSSO reactions ******
!
SO+SO+M=OSSO+M                 3.2E32  -5.75        3044 ! (NUEVA) Zhou TST 2009
OSSO+H=OH+S2O                  1.0E13   0.0            0 ! (NUEVA) Zhou est 2009
OSSO+H=SO+HSO                  1.0E13   0.0            0 ! (NUEVA) Zhou est 2009
OSSO+H=SO+HOS                  1.0E13   0.0            0 ! (NUEVA) Zhou est 2009
OSSO+H=HO2+S2                  1.0E13   0.0     12570 ! (NUEVA) Zhou est 2009
OSSO+O=SO+SO2                  1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
OSSO+O=O2+S2O                  1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
OSSO+OH=HO2+S2O                1.0E13   0.0     11350 ! (NUEVA) Zhou est 2009
OSSO+OH=HOSO+SO                1.0E12   0.0            0 ! (NUEVA) Zhou est 2009
OSSO+SO=SO2+S2O                1.0E10   0.0        0 ! (NUEVA) Zhou est 2009
OSSO+S=S2O+SO                  1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
OSSO+S=S2+SO2                  1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
OSSO+SH=HSO+S2O                1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
OSSO+S2=S2O+S2O                1.0E12   0.0        0 ! (NUEVA) Zhou est 2009
!
!
!***** HOSO2/HOSHO ******
!
HOSO2+S=SH+SO3                 1.0E13   0.0        0 ! (NUEVA) Zhou est 2009
HOSO2 = HOSO+O         5.4E18  -2.34   106300 ! Glarborg 1996
HOSO2 = SO3+H          1.4E18  -2.91    54900 ! Glarborg 1996
HOSO2+H = SO2+H2O      1.0E12   0.0         0 ! Glarborg 1996
HOSO2+O = SO3+OH       5.0E12   0.0         0 ! Glarborg 1996
HOSO2+OH = SO3+H2O             1.0E12   0.0        0 ! Glarborg 1996
HOSO2+O2 = HO2+SO3             7.8E11   0.0      656 ! Atkinson 2004
```

```
HOSHO = HOSO+H        6.4E30  -5.89    73800 ! Glarborg 1996
HOSHO = SO+H2O        1.2E24  -3.59    59500 ! Glarborg 1996
HOSHO+H = HOSO+H2             1.0E12   0.0        0 ! Glarborg 1996
HOSHO+O = HOSO+OH             5.0E12   0.0        0 ! Glarborg 1996
HOSHO+OH = HOSO+H2O           1.0E12   0.0        0 ! Glarborg 1996
!
!
!***** OTHERS ******
!
H2SO = H2S+O          4.9E28  -6.66       71700 ! Glarborg 1996
HSSO2+M=SH+SO2+M  1.0E17   0.0      3000 ! (NUEVA) Zhou est 2009
HSSO2=S2O+OH                  1.0E13   0.0     33700 ! (NUEVA) Zhou est 2009
H2S2O2+H2O=H2S+VDW1           3.9E5    1.66     3740 ! (NUEVA) Sendt 2005
H2S2O2+H2O=2H2O+S2O           3.6E5    1.56    14290 ! (NUEVA) Sendt 2005
H2S2O2+SH=H2S2+HOSO           1.0E13   0.0      8000 ! (NUEVA) Sendt 2005
!
!
SO2+CO=SO+CO2    1.9E13     0    65900   ! Bacskay2005
CO+SO=CO2+S      5.10E13    0    53400   ! Bacskay2005
!
!
!
!*************Subset de Murakami et al. Bull.Chem.Soc.Jpn., 74 (2001)
!
O+CS2=CS+SO           3.6E13   0          1696 !
O+CS=CO+S             3.2E13   0          0 !
O+CS2=CO+S2           1.7E12   0          1194 !
O+CS2=COS+S           7.1E12   0          2102 !
S+CS2=CS+S2           1.0E14   0          4060 !
CS2+O2=CS+SO2                  1.0E12   0          31050 !
!
!
!Optimizadas
CS+O2=COS+O           6.1E12   0          16500 ! Murakami2001- Opt. Ea
!!!!CS+O2=COS+O                1.3E07   1.970     28124 ! Glarborg 2014 CS2
CS+O2=CO+SO           6.1E12   0          16500 ! Analogia a CS+O2=COS+O
!
!
```

```
!
CS2 + OH = COS + SH     5.79E8       0      -1174  ! Leu1982
COS + OH = CO2 + SH      2.41E10     0.0    0    ! COX1980
CS2 + OH => CS2OH       1.04E10 0           1743 ! MURRELLS 1990
CS2OH + O2 => COS + HSO2       1.57E10 0           0 !BASADA EN MURRELLS 1990, CS2OH +
O2
!
CS2 + H2O = H2S + COS 2.07E13 0           41497 ! nuestra, basada en Ling2011
COS + H2O = H2S + CO21.54E13 0           35299 ! nuestra, basada en Ling2011
!
CS2 + SO = COS + S2      6.90E-05    0     -6339   ! Wood1971
!
!
!!!!CS + S + M = CS2 + M            0.617E15            0           3000 ! analogía a CO+O+M=CO2+M
NBS
!
!!!!CO + S + M = COS + M           0.617E15            0           3000 ! analogía a CO+O+M=CO2+M
NBS
CO+SH=COS+H             2.50E10 0           15200
COS+O=CO+SO             4.7E13   0           5200
 DUP
COS+O=CO+SO             -2.0E13  0           7385
 DUP
COS+O=CO2+S             2.0E13 0            7385
COS+S=CO+S2             4.0E04 2.57         2345
COS+M=CO+S+M           2.50E+14    0.0    61400.0
!
CS+S(+M)=CS2(+M)                  1.9E26  -4.300      0 !
 LOW  / 6.2E23 -2.42 0 /                            !
! Troe, J.; Marshall, P.; Glarborg, P., in preparation (2013).
CS+SH=CS2+H                       1.2E13   0.000      0 !
! Woiki, D.; Roth, P. Int J Chem Kinet 1995, 27, 59-71.
! P Glarborg B Halaburt P Marshall J Troe M Thellefsen K Christensen, pw
!
!
!**************MECANISMO CxHy-SO2 *********************************
!
!
C2 + H2S = C2H + SH      5.36E12 0           0 ! Huang2004
```

C2 + SO2 = C2O + SO 1.40E12 0 0 ! Huang2004
C2H + M = C2 + H + M 1.74E35 -5.16 57367 ! Kruse1997
N2/1.0/ SO2/5/ H2O/5/
CO + CH3S = COS + CH3 6.62E07 1.57 6675 ! Tang2008
CH3S + H2O2 = CH3SH + HO2 1.81E11 0 0 ! Turnipseed1996
CH3S+O2 = CH2S+HO2 4.74E24 -4.70 8300 ! Zhu2006
CH3S + O2 = CH3 + SO2 9.47E25 -3.80 12300 ! Zhu2006
!CH3SH + H = CH3 + H2S 6.90E12 0 1671 ! Amano1983
!CH3SH + OH = CH3S + H2O 1.31E07 1.77 -1689 ! Masgrau2003
!CH3 + SH = CH3SH 1.00E13 0 0 ! Shum1985
CH3 + SO2 = CH3OSO 1.55E12 0.0 1291 ! Frank1999
CH3 + SO2 = CH3SO2 9.69E10 2.90 -340 ! Frank1999
CH3SO2 = CH3OSO 1.20E11 0.75 46300 ! zhu2006
CH3OSO = CH3O + SO 4.00E08 0.0 57300 ! zhu2006
CH3OSO = CH2O + HSO 2.44E06 1.82 53000 ! zhu2006
CH3O2 + SO2 = CH3O + SO3 3.01E07 0.0 0 ! ATKINSON1989
CH2S + CH3 = CH3CH2S 3.98E11 0.0 2007 ! SHUM1985
CH3SCH3 + H = CH3SH + CH3 1.80E08 1.70 2152 ! ZHANG2005
CH3CH2S = CH2CH2SH 2.00E13 0.0 32000 ! SHUM1985
CH2CH2SH = C2H4 + SH 1.58E13 0.0 11000 ! SHUM1985
CH3SCH3 + O = CH3 + CH3SO 7.83E12 0 -813 ! Baulch2004
CH3S + O2 = O + CH3SO 5.24E13 -1.50 1.69E04 ! zHU2006
CH3SCH3 + OH = CH3OH + CH3S 0.04 0 0 ! BARONE1995
CH3SCH3 = CH3 + CH3S 6.10E15 0 75800 ! MOUSAVIPOUR2002
CH4 + S = CH3 + SH 2.04E14 0.0 19900 ! TSUCHIYA1996
CH3 + H2S = CH4 +SH 3.80E11 0.0 2603 ! ARTHUR1978
C2H + C2H = C2H2 + C2 1.81E12 0 0 ! Tsang1986
!!!!!H2S+CO=COS+H2 1.0E11 0 0 ! nuestra est.
SO + C2H2 = COS + CH2 1.0E11 0 0 ! nuestra est.
SO + C2H4 = COS + CH4 1.0E11 0 0 ! nuestra est.
SO + CH2 = COS + H2 1.0E11 0 0 ! nuestra est.
SO + CH = COS + H 1.0E11 0 0 ! nuestra est.
SO + HCO = COS + OH 1.0E11 0 0 ! nuestra est.
SO + CH2O = COS + H2O 1.0E11 0 0 ! nuestra est.
SO + C2H2 = CS + CH2O 1.0E11 0 0 ! nuestra est.
SO + C2H4 = CS + CH3OH 1.0E11 0 0 ! nuestra est.
SO + CH2 = CS + H2O 1.0E11 0 0 ! nuestra est.
SO + CH = CS + OH 1.0E11 0 0 ! nuestra est.

SO2 + CH = CS + HO2 1.0E11 0 0 ! nuestra est.

SO2 + CH = COS + OH 1.0E11 0 0 ! nuestra est.

SO2 + CH2 = COS + H2O 1.0E11 0 0 ! nuestra est.

SO2 + CH2 = CS + H2O2 1.0E11 0 0 ! nuestra est.

SO2 + C2H = CS + HCOO 1.0E11 0 0 ! nuestra est.

S2 + C2H2 = CS2 + CH2 1.0E11 0 0 ! nuestra est.

S2 + CH2 = CS2 + H2 1.0E11 0 0 ! nuestra est.

S2 + CH = CS2 + H 1.0E11 0 0 ! nuestra est.

SH + C2H = CS + CH2 1.0E11 0 0 ! nuestra est.

SH + C2H2 = CS + CH3 1.0E11 0 0 ! nuestra est.

SH + C2H3 = CS + CH4 1.0E11 0 0 ! nuestra est.

H2S + C2H2 = CS + CH4 1.0E11 0 0 ! nuestra est.

CS + H2S = CS2 + H2 1.0E11 0 0 ! nuestra est.

!!!!!!!!!COS + SO = CO2 + S2 1.0E11 0 0 ! nuestra est. DIAGRAMA DE CLARK2001

!

!!mmo Jorge

CH4+OH=CH3+H2O 1E+06 2.183 2300.000

CH4+O=CH3+OH 4.39E5 2.5 6578.

CH3+O2=CH2O+OH 6.38E11 0.0 13515

CH3+O2=CH3O+O 2.7E12 0.0 25000

CH3+OH=CH2+H2O 7.8E+12 0.000 0.0

CH3O+H=CH3+OH 1.2E+9 1.010 12000.000

CH2OH+H=CH3+OH 6.600E+9 1.000 3200.000

C2H6+OH=C2H5+H2O 6.62E13 0.0 5042

C2H6+H=C2H5+H2 9.8E013 0.00 9220

C2H6+O=C2H5+OH 1.8E05 2.80 5802

C2H6+HO2=C2H5+H2O2 1.1E5 2.50 16850

C2H6+O2=C2H5+HO2 7.29E5 2.5 49160

C2H6+CH3=C2H5+CH4 5.6E10 0.00 9418

DUP

C2H6+CH3=C2H5+CH4 8.4E14 0.00 22250

DUP

C2H4+H(+M)=C2H5(+M) 3.97E9 1.28 1292

LOW/4.71E18 0.0 755.0/

H2/2/ CO/2/ CO2/3/ H2O/5/

C2H4+OH=C2H3+H2O 2.23E4 2.745 2216

C2H4+H=C2H3+H2 2.35E2 3.62 11266

CH3+NO=HCN+H2O 1.50E11 0.0 15000

CH3+NO=H2CN+OH 4.50E11 0.0 15000

CH3+NO(+M)=CH3NO(+M) 9.0E12 0.0 192 ! Rasmussen et al., 2008

LOW/2.5E16 0.0 -2841/

TROE/5.0 1.0E-30 120 1E30/

CH2+NO=HCN+OH 3.9E11 0.0 378

CH2+NO=HCNO+H 3.1E12 0.0 378

HCO+NO=CO+HNO 7.0E21 0.0 0

NH3+O=NH2+OH 2.8E2 3.29 4471

NH2+O=HNO+H 6.6E13 0.0 0

NH2+O=NH+OH 7.0E12 0.0 0

DUP

NH2+O=NH+OH 8.6E-1 4.01 1673

DUP

H2NO+O = NH2+O2 2.6E11 0.4872 29050

NH2+NO=N2+H2O 2.8E20 -2.654 1258

NH2+NO=NNH+OH 2.3E10 0.425 -814

NNH=N2+H 1.0E9 0.0 0

NNH+O=N2+OH 1.2E13 0.145 -217

NNH+O=N2O+H 1.9E14 -0.274 -22

NNH+O=NH+NO 5.2E11 0.388 -409

NNH+O2=N2+HO2 5.6E14 -0.385 13

NH+NO=N2O+H 18E14 -0.351 -244

NH+NO=N2+OH 2.7E12 -0.0721 -512

HCN+O=NCO+H 7.6E10 0.48 7810

HCN+O=NH+CO 4.0E14 -0.65 8514

HCN+O=CN+OH 4.2E10 0.40 20665

HNCO+OH=NCO+H2O 3.3E6 1.5 3597

HNCO+CN=NCO+HCN 5.0E12 0.0 0

NCO+NCO=N2+CO+CO 3.6E13 0.0 0

!HOSO(+M)=H+SO2(+M) 2.37E8 1.63 7339 ! Blitz et al., 2006

! LOW/1.85E37 -6.14 11075/

! TROE/0.283 272 3995/

! CO2/2.5/ SO2/10/ H2O/10/

!HOSO+O2=HO2+SO2 9.6E1 2.36 -10130

H+H+H2=H2+H2 0.920E+17 -0.6 0.0

H+H+CO2=H2+CO2 0.549E+21 -2.0 0.0

CH3O2+OH = CH3OH+O2 6.0E13 0.0 0

CH3O2+HO2 = CH3OOH+O2 2.5E11 0.0 -1570

```
CH3O2+H2O2 = CH3OOH+HO2   2.4E12   0.0        9940
CH3O2+CH2O = CH3OOH+HCO   2.0E12   0.0        11665
CH3O2+CH4 = CH3OOH+CH3     1.8E11   0.0        18500
CH3O2+CH3O = CH2O+CH3OOH           3.0E11   0.0        0
CH3O2+CH2OH = CH2O+CH3OOH          1.2E13   0.0        0
CH3O2+CH3OH = CH3OOH+CH2OH         1.8E12   0.0        13700
CH3O2+CH3O2 = CH3O+CH3O+O2         1.0E11   0.0        300
CH3O2+CH3O2 = CH3OH+CH2O+O2        4.0E09   0.0        -2210
CH3OOH = CH3O+OH    6.3E14   0.0        42300
CH3OOH+H = CH3O2+H2          8.8E10   0.0        1860
CH3OOH+H = CH3O+H2O          8.2E10   0.0        1860
CH3OOH+O = CH3O2+OH          1.0E12   0.0        3000
CH3OOH+OH = CH3O2+H2O        1.8E12   0.0        -378
C2H3+CH2=C3H4+H       3.0E13   0.0        0.0
C2H3+C2H=H2CCCCH+H           3.0E13   0.0        0.0
C2H3+C2H3=CH2CHCCH2+H        9.0E12   0.0        0.0
CH2HCO+CH3=C2H5+HCO          5.0E13   0.0        0.0
CH2HCO+O2=OH+OCHCHO          2.22E11 0.0        1500.
CH2HCO+M=CH3+CO+M              2.0E16    0.0     42000
  H2/2/ CO/2/ CO2/3/  H2O/5/
C2H+C2H2=C4H2+H       2.47E12 0.5        -391.
CH2(S)+M=CH2+M                 0.100E+14  0.000      0.000
   H/0.0/ H2O/0.0/ C2H2/0.0/ C6H6/0.0/ N2/0.0/ AR/0.0/
CH2(S)+C2H2=CH2+C2H2         4.0E13   0.0        0.0
NH+CO2=CO+HNO        8.2E13   0.0        34500
HNCO+M=CO+NH+M  1.1E16     0.0        86000
N2/1.0/  CO2/2.0/  AR/0.7/
HNCO+OH=NH2+CO2    1.8E06   1.5        3597
SH+SH = S2+H2 1.0E12   0.0        0.0
CH3SH(+M)=CH2SH+H(+M) 2.7E16  -0.08  98940
LOW/2.34E40  -6.33  103100/
TROE/0.773 693 5333/
CH3SH = CH4+S              1.0E13   0          73000
CH3SH + O = CH3 + HSO          1.78E10 0          0
CH3SH + O = CH3SO + H          1.07E10 0          0
CH3SH + O = CH3O + SH          1.78E10 0          0
CH3SH + OH = CH3 + H2SO        1.0E13   0          0
CH3SH + OH = CH4 + HSO         1.0E13   0          0
```

```
CH3SH + O2 = CH2SH + HO2       2.1E13   0.00       44900
CH2SH + O2 = CH2S + HO2 1.6E15          -1.0       0
DUP
CH2SH + O2 = CH2S + HO2 7.2E13          0.0        3577
DUP
CH2SH+H=CH2S+H2      4.8E13   0.00       0
CH2SH+O=CH2S+OH      6.5E13   0.00       -700
!! Modificaciones mmo 2
HCO(+M)=H+CO(+M)                4.93E+16          -0.9       19724 ! Klayton R. 2018
LOW/ 7.43E21  -2.36  19383/
     TROE/ 0.103  139. 10900. 4550/

  N2/1.5/ O2/1.5/ CO/1.5/   H2/2.0/  CH4/5.0/ CO2/3./ H2O/15./
CH3+OH=CH2(S)+H2O   4.30E+15          -0.9       1888
CH2+O2=CO2+H+H       2.1E09   0.9929   -269
CH4+O2=CH3+HO2       2.03E+05          2.7        51714
CH3+HO2=CH3O+OH      6.8E12   0.0        0.0
CH4+H=CH3+H2         4.1E03   3.156      8755
CH3+H(+M)=CH4(+M)           5.54E24     -2.17   0.  ! Golden 2008
  LOW/1.75E33  -4.76 2440.0/
  TROE/0.783  74.0 2941.0 6964.0/
 H2/2.86/ H2O/8.57/ CH4/2.86/  CO/2.14/ CO2/2.86/ C2H6/4.29/ N2/1.43/
CH3+CH3(+M)=C2H6(+M)              9.5E14  -0.538     179 !
 LOW  /1.269E39 -7.0 2762/                          !
 TROE /0.62 73 1180 1E30/                           ! Fc=0.38exp(-T/73)+0.62exp(-T/1180)
! S.J. Klippenstein, et al., Phys. Chem. Chem. Phys. 8 (2006) 1133–1147.
! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker D Troe J Tsang W
Walker RW Warnatz J JPCRD 34:757-1397 2005
!!!!!!!!!!!!!!!Gri mech 3.0
O+CH2<=>H+HCO                     8.000E+13     .000       .00
O+CH2(S)<=>H2+CO                   1.500E+13     .000       .00
O+CH2(S)<=>H+HCO                   1.500E+13     .000       .00
O+CH3OH<=>OH+CH3O                      1.300E+05    2.500    5000.00
H+2O2<=>HO2+O2                     2.080E+19   -1.240       .00
H+O2+H2O<=>HO2+H2O                     11.26E+18    -.760       .00
H+CH2(+M)<=>CH3(+M)                  6.000E+14     .000       .00
    LOW  /  1.040E+26   -2.760   1600.00/
    TROE/   .5620  91.00  5836.00  8552.00/
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
```

```
H+CH2OH<=>CH2(S)+H2O                 3.280E+13    -.090     610.00
H+CH3O(+M)<=>CH3OH(+M)               2.430E+12     .515      50.00
    LOW  /  4.660E+41   -7.440   14080.0/
    TROE/   .700  100.00  90000.0 10000.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH3O<=>H+CH2OH                    4.150E+07    1.630    1924.00
H+CH3O<=>CH2(S)+H2O                 2.620E+14    -.230    1070.00
HO2+CH2<=>OH+CH2O                   2.000E+13     .000       .00
CH2+CH2<=>H2+C2H2                    1.600E+15     .000   11944.00
CH2(S)+O2<=>CO+H2O                  1.200E+13     .000       .00
CH2(S)+H2O(+M)<=>CH3OH(+M)           4.820E+17   -1.160    1145.00
    LOW  /  1.880E+38   -6.360   5040.00/
    TROE/   .6027  208.00  3922.00  10180.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH2(S)+CO<=>CH2+CO                   9.000E+12     .000       .00
CH2(S)+CO2<=>CH2+CO2                 7.000E+12     .000       .00
HCO+H2O<=>H+CO+H2O                    1.500E+18   -1.000   17000.00
C2H+O2<=>HCO+CO                     1.000E+13     .000    -755.00
NH+H2O<=>HNO+H2                     2.000E+13     .000   13850.00
NNH+M<=>N2+H+M                      1.300E+14    -.110    4980.00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
NNH+CH3<=>CH4+N2                    2.500E+13     .000       .00
HCN+M<=>H+CN+M                      1.040E+29   -3.300  126600.00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH+N2(+M)<=>HCNN(+M)                 3.100E+12     .150       .00
   LOW  /  1.300E+25   -3.160    740.00/
    TROE/   .6670  235.00  2117.00  4536.00 /
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ 1.0/
CH2(S)+N2<=>NH+HCN                   1.000E+11     .000   65000.00
CH2+NO<=>H+HNCO                     3.100E+17   -1.380    1270.00
CH2(S)+NO<=>H+HNCO                   3.100E+17   -1.380    1270.00
CH2(S)+NO<=>H+HCNO                   3.800E+13    -.360     580.00
HCNN+O<=>CO+H+N2                    2.200E+13     .000       .00
HCNN+O<=>HCN+NO                     2.000E+12     .000       .00
HCNN+O2<=>O+HCO+N2                    1.200E+13     .000       .00
HCNN+OH<=>H+HCO+N2                    1.200E+13     .000       .00
HCNN+H<=>CH2+N2                     1.000E+14     .000       .00
HCNO+H<=>H+HNCO                      2.100E+15    -.690    2850.00
```

```
HCNO+H<=>NH2+CO                    1.700E+14   -.750   2890.00
HOCN+H<=>H+HNCO                    2.000E+07   2.000   2000.00
CH3+N<=>HCN+H2                     3.700E+12    .150    -90.00
O+CH3=>H+H2+CO                     3.370E+13    .000     .00
O+C2H4<=>H+CH2CHO                  6.700E+06   1.830    220.00
O+C2H5<=>H+CH3CHO                  1.096E+14    .000     .00
OH+CH3=>H2+CH2O                    8.000E+09    .500   -1755.00
CH+H2(+M)<=>CH3(+M)                1.970E+12    .430    -370.00
  LOW/ 4.820E+25  -2.80  590.0 /
  TROE/ .578  122.0  2535.0  9365.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH2(S)+H2O=>H2+CH2O                6.820E+10    .250    -935.00
C2H3+O2<=>O+CH2CHO                 3.030E+11    .290      11.00
O+CH3CHO<=>OH+CH2CHO               2.920E+12    .000    1808.00
O+CH3CHO=>OH+CH3+CO                2.920E+12    .000    1808.00
O2+CH3CHO=>HO2+CH3+CO              3.010E+13    .000   39150.00
H+CH3CHO<=>CH2CHO+H2               2.050E+09   1.160    2405.00
H+CH3CHO=>CH3+H2+CO                2.050E+09   1.160    2405.00
OH+CH3CHO=>CH3+H2O+CO              2.343E+10   0.730   -1113.00
HO2+CH3CHO=>CH3+H2O2+CO            3.010E+12    .000   11923.00
CH3+CH3CHO=>CH3+CH4+CO             2.720E+06   1.770    5920.00
H+CH2CO(+M)<=>CH2CHO(+M)           4.865E+11   0.422   -1755.00
   LOW/ 1.012E+42  -7.63  3854.0/
   TROE/ 0.465  201.0  1773.0  5333.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
O+CH2CHO=>H+CH2+CO2                1.500E+14    .000     .00
O2+CH2CHO=>OH+CO+CH2O              1.810E+10    .000     .00
O2+CH2CHO=>OH+2HCO                 2.350E+10    .000     .00
H+CH2CHO<=>CH3+HCO                 2.200E+13    .000     .00
H+CH2CHO<=>CH2CO+H2                1.100E+13    .000     .00
OH+CH2CHO<=>H2O+CH2CO              1.200E+13    .000     .00
OH+CH2CHO<=>HCO+CH2OH              3.010E+13    .000     .00
CH3+C2H5(+M)<=>C3H8(+M)            .9430E+13    .000     .00
    LOW/ 2.710E+74  -16.82  13065.0 /
    TROE/ .1527  291.0  2742.0  7748.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
O+C3H8<=>OH+C3H7                   1.930E+05   2.680   3716.00
H+C3H8<=>C3H7+H2                   1.320E+06   2.540   6756.00
```

```
OH+C3H8<=>C3H7+H2O                  3.160E+07    1.800    934.00
C3H7+H2O2<=>HO2+C3H8                 3.780E+02    2.720   1500.00
CH3+C3H8<=>C3H7+CH4                  0.903E+00    3.650   7154.00
CH3+C2H4(+M)<=>C3H7(+M)              2.550E+06    1.600   5700.00
    LOW/ 3.00E+63  -14.6  18170./
    TROE/ .1894  277.0  8748.0  7891.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
O+C3H7<=>C2H5+CH2O                   9.640E+13     .000       .00
H+C3H7(+M)<=>C3H8(+M)                3.613E+13     .000       .00
    LOW/ 4.420E+61  -13.545  11357.0/
    TROE/ .315  369.0  3285.0  6667.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C3H7<=>CH3+C2H5                    4.060E+06    2.190    890.00
OH+C3H7<=>C2H5+CH2OH                 2.410E+13     .000       .00
HO2+C3H7<=>O2+C3H8                   2.550E+10    0.255   -943.00
HO2+C3H7=>OH+C2H5+CH2O               2.410E+13     .000       .00
CH3+C3H7<=>2C2H5                     1.927E+13   -0.320       .00
!!!
! Klayton R. 2018
H2O+H2O=H+OH+H2O             1.01E+26          -2.4       120180
!O+O2+M=O3+M                 1.88E+21          -2.8       0
!O+O3=O2+O2             4.80E+12          0          4090
!H+O3=OH+O2             8.43E+13          0          950
!OH+O3=HO2+O2                1.14E+12          0          2000
!HO2+O3=OH+O2+O2             8.43E+09          0          1200
CO+OH=HOCO              2.00E+20          -3.5       1309
 PLOG/ 0.013158              1.7E15  -2.680     859/

 PLOG/ 0.13158               5.9E18  -3.350     887/
 PLOG/ 1.3158                2.6E20  -3.500    1309/

 PLOG/ 13.158                7.1E20  -3.320    1763/
 PLOG/ 131.58                1.1E20  -2.780    2056/
CO+H2O2=HOCO+OH              3.60E+04          2.5        28660
HOCO(+M)=CO2+H(+M)                   8.20E+11          0.4        35335
 LOW  /                  6.0E26  -3.148   37116 /                    !
 TROE / 0.39 1.0E-30 1.0E30 /                    ! Fc = 0.39
HOCO+H=CO2+H2                3.10E+17          -1.3       555
HOCO+H=CO+H2O                6.00E+15          -0.5       2125
```

HOCO+O=CO2+OH 9.00E+12 0 0
HOCO+OH=CO2+H2O 4.60E+12 0 -89
DUPLICATE
HOCO+OH=CO2+H2O 9.50E+06 2 -89
DUPLICATE
HOCO+HO2=CO2+H2O2 4.00E+13 0 0
HOCO+O2=CO2+HO2 4.00E+09 1 0
CH2O+H=H+CO+H2 5.11E+07 2.2 11524
PLOG/0.04 7.20E+08 1.903 11733 /
PLOG/1 5.11E+07 2.182 11524 /
PLOG/10 1.16E+09 1.812 13163 /
CH2O+O=H+CO+OH 2.51E+21 -1.9 22674

CH2O+O2=H+CO+HO2 1.44E+15 0 56388.3
CH2O+OH=H+CO+H2O 7.24E+10 0.9 9310
PLOG/0.04 7.03E+10 0.911 8646 /
PLOG/1 7.24E+10 0.892 9310 /
PLOG/10 8.37E+10 0.879 9843 /

CH2O+HO2=H+CO+H2O2 2.45E+14 0 30120

CH2O+CH3=H+CO+CH4 1.92E+11 0.9 24224

CH3+OH=CH3OH 6.20E+13 0 -33.3
PLOG / 0.001316 6.9E30 -6.63794 2829/
PLOG / 0.013158 1.1E32 -6.63695 3364/
PLOG / 0.131579 1.5E32 -6.36057 3954/
PLOG / 1.315789 5.6E30 -5.64842 4214/
PLOG / 13.157895 1.4E27 -4.33275 3685/
PLOG / 131.578947 1.3E22 -2.66369 2451/

CH3+OH=H2+HCOH 6.5E11 0.11155 932 !
PLOG / 0.001316 1.2E09 0.83024 -2323 /
PLOG / 0.013158 6.4E09 0.63305 -1701 /
PLOG / 0.131579 8.0E10 0.33964 -565 /
PLOG / 1.315789 6.5E11 0.11155 932 /
PLOG / 13.157895 2.1E11 0.29509 2200 /
PLOG / 131.578947 9.4E07 1.28631 2424 /

! Jasper AW Klippenstein SJ Harding LB Ruscic B JPCA 111:3932-3950 2007

! cis and trans products are combined as HCOH

! CH2+...

CH2+M=CH+H+M 5.6E15 0.000 89000 ! TIA/QI09 BAU/WAG95

! Bauerle S Klatt M Wagner HGg BBPC 99:870 1995

CH2+M=C+H2+M 5.8E12 0.500 68500 ! TIA/QI09 BAU/WAG95

! Bauerle S Klatt M Wagner HGg BBPC 99:870 1995

CH2(S)+O2=CH2+O2 3.1E13 0.000 0 ! ISC=100%

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

CH+OH=H+CO+H 1.796E+23 -2.473 19927.3

CH+O2=H+CO+O 1.975E+23 -2.473 19927.3

CH+CO2=H+CO+CO 5.268E+16 -0.723 18887.3

! **

! MeOH subset *

! **

CH3OH+HO2=CH3O+H2O2 1.5E-3 4.61 15828 !ARANDA/GLA12--REF21->SKODAV10

! Alecu, I.M.; Truhlar, D.G. J Phys Chem A 2011, 115, 14599-14611.

CH3O+HO2=CH3OH+O2 1.4E+11 0.00 0

! Mousavipour, S. H.; Homayoon, Z. J Phys Chem A 2011, 115, 3291-3300.

! HH@160506:

CH2OH+O2=CH2O+HO2 7.2E13 0.000 3736 ! RAS/GLA08c CEC05

DUPLICATE !

CH2OH+O2=CH2O+HO2 2.9E16 -1.500 0 ! RAS/GLA08c CEC05

DUPLICATE !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

CH2OH+CH3=C2H4+H2O 7.2E29 -5.0344 9245 !

PLOG/ 0.001 6.3E24 -3.7134 2798 /

PLOG/ 0.010 1.2E25 -3.7867 3001 /

PLOG/ 0.100 3.2E27 -4.4500 5345 /

PLOG/ 1.000 7.2E29 -5.0344 9245 /

PLOG/ 10.00 1.7E27 -4.1839 11152 /

PLOG/ 100.0 3.9E17 -1.3688 8978 /

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455

CH3OH+H+CO=CH2OH+CH2O 8.316E-05 5.095 14283.2

CH3OH+CH2(S)=CH2OH+CH3 3.54E-04 4.1900 3600.4

! Shi, Ran, Qin, Qi, Zhang, Comput. Theor. Chem. 1074 (2015) 73-82

CH3OH+CH2(S)=CH3O+CH3 1.36E-04 4.2600 5626.0

! Shi, Ran, Qin, Qi, Zhang, Comput. Theor. Chem. 1074 (2015) 73-82

CH3OH+H+CO=CH3O+CH2O 2.049E+06 2.065 27598.5

! ---------- CH3OOH ...

CH3OOH+H=CH2OOH+H2 5.4E10 0.000 1860 ! RAS/GLA08b SLE/WAR77 (45%)

! Slemr F Warneck P IJCK 9:267 1977

CH3OOH+O=CH2OOH+OH 1.6E13 0.000 4750 ! RAS/GLA08b CEC05

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

CH3OOH+OH=CH2OOH+H2O 7.2E11 0.000 -258 ! RAS/GLA08b CEC05 (fit to VAG/RAV89)

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

CH3O2+HCO=CH3O+H+CO2 3.0E13 0.000 0 !

! CL Rasmussen JG Jacobsen P Glarborg IJCK 40 (2008) 778-807

! est HCO+HO2=CO2+OH+H

```
CH3O2+CO=CH3O+CO2                  1.6E05   2.180   17940 !
! CL Rasmussen JG Jacobsen P Glarborg IJCK 40 (2008) 778-807
! est CO+HO2=CO2+OH
CH3O2+CH2O=CH3OOH+H+CO         2.454E+14   0.027   30133.3
CH2OOH=CH2O+OH                   2.4E12  -0.925    1567 !
 PLOG/ 0.04                       9.6E10  -0.925    1567/ ! extrapolation
 PLOG/ 1.0                       2.4E12  -0.925    1567/
 PLOG/ 10.                       2.5E13  -0.927    1579/
 PLOG/ 100.                       7.0E14  -1.064    1744/
! Ing W-C Sheng CY Bozzelli JW FPT 83:111-145 2003
! the reverse one: CH2O+OH<=>CH2OOH is disabled

! ---------- HCOH ...

HCOH=CO+H2  6.560E+13          0.000     49465
! Xiong et al., Combust. Flame 161 (2014) 885–897

HCOH=CH2O     5.150E+13          0.000     32109
! Xiong et al., Combust. Flame 161 (2014) 885–897

HCOH+H=CH2O+H                    1.0E14   0.000       0 ! #160409#
! est
!
HCOH+H=HCO+H2                    2.0E13   0.000       0 ! #160409#
! est
!
HCOH+H=H+CO+H2                    1.0E13   0.000       0 ! #160409#
! est
!
HCOH+O=CO2+2H                   3.0E13   0.000       0 ! #160409#
! est
!
HCOH+OH=HCO+H2O                   2.0E13   0.000       0 ! #160409#
! est
!
HCOH+OH=H+CO+H2O                   1.0E13   0.000       0 ! #160409#
! est
```

```
! ****************************************************************************
!    C2 subset                                                 *
! ****************************************************************************

! ------------- C2H6 ...
C2H6+CH3O2=CH3OOH+C2H5              1.9E01   3.640   17100 ! RAS/GLA08b CAR/DEA05
! Carstensen H-H Dean AM PCI 30:995-1003 2005

! ------------- C2H5 ...


C2H5+HO2=CH3CH2O+OH                 3.1E13   0.000       0 ! RAS/GLA08b LUD/TEM06
! Ludwig W Brandt B Friedrichs G Temps F JPCA 110:3330-3337 2006

          ! Miller and Klippenstein, Int. J. Chem. Kinet. 33 (2001) 654--668
! HH@160510:
C2H5+O2(+M)=CH3CH2OO(+M)            1.5E15  -1.000       0
          LOW  /3.3E31 -4.90                    0/
          TROE /1E-30 540 1E30 1E-30/
! R.X. Fernandes, K. Luther, G. Marowsky, M.P. Rissanen, R. Timonen, J. Troe, J Phys Chem A 2015, 119, 7263-7269.

C2H5+CH3O2=CH3O+CH3CH2O             5.1E12   0.000   -1410
 ! CL Rasmussen JG Jacobsen P Glarborg IJCK 40 (2008) 778-807
 ! est CH3O2+CH3=CH3O+CH3O

! ------------- C2H4 ...
C2H4(+M)=H2CC+H2(+M)                8.0E12   0.440   88800 ! GIM/GLA09  WAN01
   LOW/7.0E50 -9.31 99900/
   TROE/0.735 180 1035 5417/
   H2O/6/ AR/0.7/
! Wang H IJCK 33:698-706 2001
C2H4+OH=CH3+CH2O                    1.8E05   1.68     2061 !
 PLOG /0.01                          5.4E00   2.92    -1733/
 PLOG /0.025                         3.2E01   2.71    -1172/
 PLOG /0.1                          5.6E02   2.36     -181/
 PLOG /1.                           1.8E05   1.68     2061/
 PLOG /10.                          2.4E09   0.56     6007/
 PLOG /100.                          2.8E13  -0.50    11455/
```

```
! Senosiain JP Klippenstein SJ Miller JA JPCA 110:6960-6970 2006

C2H4+OH=CH3CHO+H                  2.4E-2   3.91     1723 !
 PLOG /0.01                       2.4E-7   5.30    -2051./
 PLOG /0.025                      8.7E-5   4.57     -618./
 PLOG /0.1                        4.0E-1   3.54     1882./
 PLOG /1.                        2.4E-2   3.91     1723./
 PLOG /10.                        8.3E08   1.01    10507./
 PLOG /100.                       6.8E09   0.81    13867./
! Senosiain JP Klippenstein SJ Miller JA JPCA 110:6960-6970 2006

C2H4+OH=CH2CHOH+H                    3.2E05   2.19     5256 !
 PLOG /0.01                       1.0E04   2.60     4121./
 PLOG /0.025                      1.1E04   2.60     4129./
 PLOG /0.1                        1.5E04   2.56     4238./
 PLOG /1.                        3.2E05   2.19     5256./
 PLOG /10.                        1.9E08   1.43     7829./
 PLOG /100.                       8.6E10   0.75    11491./
! Senosiain JP Klippenstein SJ Miller JA JPCA 110:6960-6970 2006

C2H4+OH=CH2CH2OH    5.91E+41    -10.43    4832.    ! JPCA 110 6960-6970 (2006)
 PLOG /0.01    2.76E+47    -11.64  11099./
 PLOG /0.025   6.02E+37    -9.76    1995./
 PLOG /0.1     6.02E+37    -9.65    2363./
 PLOG /1.      6.02E+37    -8.14    8043./
 PLOG /10.     6.02E+37    -7.77   10736./
 PLOG /100.    6.02E+37    -7.44   14269./
! inf    6.02E+37   -8.88     5170
! inf    4.46E+07    1.55    -1564
DUPLICATE
C2H4+OH=CH2CH2OH  1           1           1
 PLOG /0.025   4.96E+37    -8.68    5355./
 PLOG /0.1     2.56E+35    -7.79    5017./
 PLOG /1.      7.29E+31    -6.91    2855./
 PLOG /10.     3.02E+26    -4.87    2297./
 PLOG /100.    2.79E+19    -2.41    1011./
DUPLICATE
! Senosiain JP Klippenstein SJ Miller JA JPCA 110:6960-6970 2006
```

```
! HH@160503: back to the former rate, replacing the reverse reaction

! HH@160503: back to the former rate, enabled now
C2H4+HO2=cC2H4O+OH    1 1 1
  PLOG/0.01316   3.342E+04         2.311     13735.46/
  PLOG/0.98692   1.796E+06         1.809     14760.59/
  PLOG/9.86923   1.181E+09         1.006     16673.46/
  PLOG/98.69233   1.892E+15        -0.736    21411.27/
! J. Zador, S. J. Klippenstein, J. A. Miller, J. Phys. Chem. A 115 (2011) 10218–10225.

! HH@160503: back to the former rate, replacing the reverse reaction
C2H4+HO2=CH3CH2OO  1          1                    1
  PLOG/0.01316   2.603E+47         -12.450  18714.68/
  PLOG/0.98692   6.596E+47         -12.159  20887.07 /
  PLOG/9.86923   1.602E+45         -11.101  21253.55 /
  PLOG/98.69233  1.005E+41         -9.543    21399.20/
  PLOG/1000        1.124E+01          2.950    7093.14 /
! J. Zador, S. J. Klippenstein, J. A. Miller, J. Phys. Chem. A 115 (2011) 10218–10225.

! HH@160503: back to the former rate, replacing the reverse reaction
C2H4+HO2=CH2CH2OOH    1 1 1
  PLOG/0.01316              1.323E+07         -0.142    11075.88/
  PLOG/0.98692              1.438E+05         0.878     7815.54/
  PLOG/9.86923              3.377E+16         -2.209    13289.24/
  PLOG/98.69233             6.496E+26         -4.893    19947.94/
  PLOG/1000                 2.818E+04         2.487     14733.97/
! J. Zador, S. J. Klippenstein, J. A. Miller, J. Phys. Chem. A 115 (2011) 10218–10225.



C2H4+CH2(S)=C2H3+CH3          4.92E+09          1.02       600
PLOG / 0.01                   1.77E+19          -1.95      6787     /
PLOG / 0.1                    1.68E+19          -1.80      4310     /
PLOG / 1                      4.16E+24          -3.19      9759     /
PLOG / 10                     7.89E+24          -3.08      13894    /
PLOG / 100                    7.36E+29          -4.28      23849    /
DUPLICATE
C2H4+CH2(S)=C2H3+CH3          4.92E+09          1.02       600
```

PLOG / 0.01 4.30E+12 0.19 -110 /

PLOG / 0.1 2.26E+11 0.54 48 /

PLOG / 1 4.92E+09 1.02 600 /

PLOG / 10 1.47E+08 1.33 1228 /

PLOG / 100 8.11E+10 0.55 5507 /

DUPLICATE

! Ye, Georgievskii, Klippenstein, Proceed. Combust. Inst. 35 (2015) 223–230

! ---------- C2H3 ...

C2H3+HO2=CH2CHO+OH 3.0E13 0.000 0 ! RAS/GLA08b NBS86

! Tsang W Hampson RF JPCRD 15:1087 1986

C2H3+O2=CH2CHOO 4.07E+27 -4.67 5222.0

PLOG/1.00E-02 1.6E24 -5.450 9662/

PLOG/1.00E-02 1.8E-9 4.150 -4707/

PLOG/1.00E-01 3.5E56 -15.010 19160/

PLOG/1.00E-01 2.4E22 -4.520 2839/

PLOG/3.16E-01 1.3E64 -16.970 21290/

PLOG/3.16E-01 2.0E26 -5.430 2725/

PLOG/1.00E+00 3.3E61 -15.790 20150/

PLOG/1.00E+00 6.1E28 -5.890 3154/

PLOG/3.16E+00 7.3E53 -13.110 17300/

PLOG/3.16E+00 2.1E29 -5.800 3520/

PLOG/1.00E+01 4.2E48 -11.210 16000/

PLOG/1.00E+01 3.5E28 -5.370 3636/

PLOG/3.16E+01 2.3E43 -9.380 14810/

PLOG/3.16E+01 3.3E27 -4.950 3610/

PLOG/1.00E+02 3.4E39 -8.040 14360/

PLOG/1.00E+02 1.0E27 -4.720 3680/

! C.F. Goldsmith, L.B. Harding, Y. Georgievskii, J.A. Miller, S.J. Klippenstein, J Phys Chem A 2015, 119, 7766-7779 (400-2200).

C2H3+O2=CHCHO+OH 2.84E+14 -0.80 7232.0 ! ##

PLOG/1.00E-02 3.9E11 -0.110 2131/

PLOG/1.00E-02 9.9E11 -0.660 -1/

PLOG/1.00E-01 1.1E09 0.550 46/

PLOG/1.00E-01 6.9E14 -1.160 4542/

PLOG/3.16E-01 8.5E08 0.560 1/

PLOG/3.16E-01 2.8E13 -0.720 3479/
PLOG/1.00E+00 2.8E14 -1.830 5/
PLOG/1.00E+00 5.0E11 -0.140 1995/
PLOG/3.16E+00 2.6E20 -2.840 7530/
PLOG/3.16E+00 2.4E10 0.230 1573/
PLOG/1.00E+01 9.2E14 -2.260 0/
PLOG/1.00E+01 1.7E14 -0.820 4450/
PLOG/3.16E+01 6.1E25 -4.210 13050/
PLOG/3.16E+01 1.4E11 0.050 3774/
PLOG/1.00E+02 1.7E30 -5.350 18430/
PLOG/1.00E+02 3.2E11 -0.020 5338/

! C.F. Goldsmith, L.B. Harding, Y. Georgievskii, J.A. Miller, S.J. Klippenstein, J Phys Chem A 2015, 119, 7766-7779 (400-2200).

C2H3+O2=CH2CO+OH 1.17E+03 2.43 7074.0
PLOG/1.00E-02 8.7E02 2.41 6061/
PLOG/1.00E-02 1.8E-1 3.12 1331/
PLOG/1.00E-01 8.9E02 2.41 6078/
PLOG/1.00E-01 2.1E-1 3.11 1383/
PLOG/3.16E-01 9.4E02 2.40 6112/
PLOG/3.16E-01 2.7E-1 3.08 1496/
PLOG/1.00E+00 1.1E03 2.39 6180/
PLOG/1.00E+00 5.3E-1 3.01 1777/
PLOG/3.16E+00 1.1E03 2.38 6179/
PLOG/3.16E+00 1.4E00 2.90 2225/
PLOG/1.00E+01 1.4E03 2.36 6074/
PLOG/1.00E+01 4.2E-1 2.93 2052/
PLOG/3.16E+01 2.5E06 1.42 8480/
PLOG/3.16E+01 1.2E-4 4.21 2043/
PLOG/1.00E+02 1.7E10 0.36 12010/
PLOG/1.00E+02 1.3E-3 3.97 3414/

! C.F. Goldsmith, L.B. Harding, Y. Georgievskii, J.A. Miller, S.J. Klippenstein, J Phys Chem A 2015, 119, 7766-7779 (400-2200).

C2H3+O2=OCHCHO+H 3.08E+12 -0.26 3277.0
PLOG/1.00E-02 4.8E14 -1.03 912/
PLOG/1.00E-02 2.8E-4 4.04 -7019/
PLOG/1.00E-01 5.0E14 -1.04 923/
PLOG/1.00E-01 3.5E-4 4.01 -6978/

PLOG/3.16E-01 6.4E14 -1.07 983/

PLOG/3.16E-01 9.7E-4 3.89 -6768/

PLOG/1.00E+00 3.7E15 -1.29 1441/

PLOG/1.00E+00 5.0E-1 3.15 -5496/

PLOG/3.16E+00 2.4E18 -2.13 3234/

PLOG/3.16E+00 1.3E05 1.67 -2931/

PLOG/1.00E+01 1.3E15 -1.09 2393/

PLOG/1.00E+01 4.5E15 -3.08 -4836/

PLOG/3.16E+01 3.6E33 -6.50 14910/

PLOG/3.16E+01 3.8E10 0.22 941/

PLOG/1.00E+02 3.3E31 -5.76 16250/

PLOG/1.00E+02 2.8E08 0.83 858/

! C.F. Goldsmith, L.B. Harding, Y. Georgievskii, J.A. Miller, S.J. Klippenstein, J Phys Chem A 2015, 119, 7766-7779 (400-2200).

C2H3+O2=CH2O+H+CO 1.29E+16 -1.13 3791.0

PLOG/1.00E-02 6.5E36 -7.60 12640/

PLOG/1.00E-02 1.2E16 -1.28 515/

PLOG/1.00E-01 6.3E36 -7.60 12610/

PLOG/1.00E-01 1.2E16 -1.28 513/

PLOG/3.16E-01 5.1E36 -7.57 12490/

PLOG/3.16E-01 1.3E16 -1.29 521/

PLOG/1.00E+00 7.1E35 -7.32 11820/

PLOG/1.00E+00 1.6E16 -1.31 646/

PLOG/3.16E+00 3.7E36 -7.47 12460/

PLOG/3.16E+00 2.4E16 -1.36 1066/

PLOG/1.00E+01 1.3E36 -7.20 13430/

PLOG/1.00E+01 6.6E15 -1.18 1429/

PLOG/3.16E+01 8.3E20 -2.57 5578/

PLOG/3.16E+01 2.7E69 -19.23 14760/

PLOG/1.00E+02 7.1E33 -6.28 16000/

PLOG/1.00E+02 1.1E11 0.19 831/

! C.F. Goldsmith, L.B. Harding, Y. Georgievskii, J.A. Miller, S.J. Klippenstein, J Phys Chem A 2015, 119, 7766-7779 (400-2200).

C2H3+O2=CH3O+CO 3.09E+13 -0.89 3682.0

PLOG/1.00E-02 8.2E18 -2.66 3201/

PLOG/1.00E-02 1.3E09 0.18 -1717/

PLOG/1.00E-01 4.1E14 -1.32 886/

PLOG/1.00E-01 6.0E11 -2.93 -9564/

PLOG/3.16E-01 4.3E14 -1.33 901/

PLOG/3.16E-01 2.9E11 -2.93 -10120/

PLOG/1.00E+00 1.0E11 -0.33 -748/

PLOG/1.00E+00 5.8E21 -3.54 4772/

PLOG/3.16E+00 1.9E12 -3.00 -8995/

PLOG/3.16E+00 5.0E15 -1.62 1849/

PLOG/1.00E+01 1.9E24 -5.63 2/

PLOG/1.00E+01 9.3E16 -1.96 3324/

PLOG/3.16E+01 1.1E18 -2.22 5178/

PLOG/3.16E+01 1.0E72 -20.69 15860/

PLOG/1.00E+02 5.8E32 -6.45 16810/

PLOG/1.00E+02 1.1E09 0.31 1024/

! C.F. Goldsmith, L.B. Harding, Y. Georgievskii, J.A. Miller, S.J. Klippenstein, J Phys Chem A 2015, 119, 7766-7779 (400-2200).

C2H3+O2=CO2+CH3 6.16E+13 -1.05 3743.0

PLOG/1.00E-02 2.4E35 -7.76 12630/

PLOG/1.00E-02 6.3E13 -1.16 406/

PLOG/1.00E-01 1.7E35 -7.72 12520/

PLOG/1.00E-01 6.2E13 -1.16 401/

PLOG/3.16E-01 4.5E34 -7.55 12140/

PLOG/3.16E-01 6.1E13 -1.16 397/

PLOG/1.00E+00 7.3E31 -6.70 10440/

PLOG/1.00E+00 5.3E13 -1.14 447/

PLOG/3.16E+00 3.6E35 -7.75 12830/

PLOG/3.16E+00 1.5E14 -1.26 988/

PLOG/1.00E+01 2.1E35 -7.53 14050/

PLOG/1.00E+01 5.0E13 -1.11 1409/

PLOG/3.16E+01 3.8E18 -2.44 5408/

PLOG/3.16E+01 1.4E70 -20.11 15430/

PLOG/1.00E+02 1.2E32 -6.32 16190/

PLOG/1.00E+02 9.2E08 0.25 855/

! C.F. Goldsmith, L.B. Harding, Y. Georgievskii, J.A. Miller, S.J. Klippenstein, J Phys Chem A 2015, 119, 7766-7779 (400-2200).

C2H3+CH3OH=C2H4+CH3O 1.03E6 1.51 26630

! Chen et al., Int. J. Chem. Kinet. 47 (2015) 764--772

C2H3+CH3OH=C2H4+CH2OH 1.75E-2 4.02 23370

! Chen et al., Int. J. Chem. Kinet. 47 (2015) 764--772

! ---------- C2H2 ...

C2H2(+M)=H2CC(+M) 1.8E04 3.510 43300

LOW /2.5E15 -0.640 49700/

TROE / 0.5 1.E-30 1.E30 /

! Lopez et al., Experimental and Kinetic Modeling Study of C2H2 Oxidation at High Pressure, Int. J. Chem. Kinet., 2016

C2H2+OH=CHCHOH 3.5E31 -6.200 6635 !

PLOG / .01 2.9E64 -18.570 10009. /

PLOG / .01 2.6E33 -7.360 6392. /

PLOG / .025 4.7E59 -16.870 9087. /

PLOG / .025 4.4E32 -7.020 5933. /

PLOG / 0.1 1.2E28 -5.560 3724. /

PLOG / 0.1 6.4E42 -9.960 11737. /

PLOG / 1.0 1.9E44 -11.380 6299. /

PLOG / 1.0 3.5E31 -6.200 6635. / ! dominating

PLOG / 10.0 1.5E24 -4.060 3261. /

PLOG / 10.0 4.5E31 -5.920 8761. /

PLOG / 100. 6.2E20 -2.800 2831. /

PLOG / 100. 1.6E29 -4.910 9734. /

! Senosiain JP Klippenstein SJ Miller JA JPCA 109:6045-6055 2005

C2H2+HO2=CH2CHOO 7.11E+20 -3.15 15650.0

PLOG/1.000E-02 4.99E+06 -1.02 9152.0/

PLOG/1.000E-02 1.88E+26 -8.34 9249.0/

PLOG/1.000E-01 6.02E+17 -3.82 10790.0/

PLOG/1.000E-01 5.26E+129 -41.74 35930.0/

PLOG/3.160E-01 2.47E+48 -12.82 25220.0/

PLOG/3.160E-01 1.96E+18 -3.67 10480.0/

PLOG/1.000E+00 4.06E+50 -13.07 27220.0/

PLOG/1.000E+00 4.93E+21 -4.37 12220.0/

PLOG/3.160E+00 9.08E+46 -11.57 26880.0/

PLOG/3.160E+00 1.92E+22 -4.28 13080.0/

PLOG/1.000E+01 4.60E+43 -10.24 26930.0/

PLOG/1.000E+01 2.11E+21 -3.78 13380.0/

PLOG/3.160E+01 5.61E+38 -8.49 26210.0/

PLOG/3.160E+01 1.39E+20 -3.30 13410.0/

PLOG/1.000E+02 2.53E+35 -7.26 26390.0/

PLOG/1.000E+02 1.42E+19 -2.91 13420.0/

! Lopez et al., Experimental and Kinetic Modeling Study of C2H2 Oxidation at High Pressure, Int. J. Chem. Kinet., 2016

C2H2+HO2=CHCHO+OH 3.24E+09 1.05 16950.0

PLOG/1.000E-02 5.49E+09 0.91 18500.0/

PLOG/1.000E-02 2.41E+07 1.54 14690.0/

PLOG/1.000E-01 5.93E+09 0.90 18550.0/

PLOG/1.000E-01 2.48E+07 1.54 14700.0/

PLOG/3.160E-01 6.80E+09 0.88 18640.0/

PLOG/3.160E-01 2.63E+07 1.54 14730.0/

PLOG/1.000E+00 1.56E+10 0.77 19040.0/

PLOG/1.000E+00 2.50E+07 1.56 14790.0/

PLOG/3.160E+00 3.48E+09 0.99 18810.0/

PLOG/3.160E+00 1.47E+08 1.32 15090.0/

PLOG/1.000E+01 5.39E+10 0.61 20740.0/

PLOG/1.000E+01 1.61E+08 1.36 15420.0/

PLOG/3.160E+01 3.70E+08 1.23 15960.0/

PLOG/3.160E+01 1.67E+07 1.59 15910.0/

PLOG/1.000E+02 1.45E+11 0.48 17730.0/

PLOG/1.000E+02 7.21E+06 1.73 16020.0/

! CHCHO not replaced by CH2CO

! Lopez et al., Experimental and Kinetic Modeling Study of C2H2 Oxidation at High Pressure, Int. J. Chem. Kinet., 2016

C2H2+HO2=CH2CO+OH 5.16E-04 3.99 18890.0

PLOG/1.000E-02 6.25E-07 4.75 15530.0/

PLOG/1.000E-02 1.31E-14 6.58 10270.0/

PLOG/1.000E-01 6.70E-07 4.74 15550.0/

PLOG/1.000E-01 1.29E-14 6.59 10330.0/

PLOG/3.160E-01 4.18E-07 4.81 15410.0/

PLOG/3.160E-01 3.99E-14 6.36 10270.0/

PLOG/1.000E+00 5.28E-07 4.78 15460.0/

PLOG/1.000E+00 3.28E-15 6.70 10090.0/

PLOG/3.160E+00 1.04E-06 4.69 15640.0/

PLOG/3.160E+00 8.71E-21 8.30 8107.0/

PLOG/1.000E+01 4.68E-05 4.22 16780.0/

PLOG/1.000E+01 8.36E-22 8.76 8804.0/

PLOG/3.160E+01 8.99E-01 2.97 19730.0/

PLOG/3.160E+01 6.87E-14 6.67 13130.0/

PLOG/1.000E+02 3.58E+03 1.97 23010.0/

PLOG/1.000E+02 6.63E-12 6.15 14730.0/

! Lopez et al., Experimental and Kinetic Modeling Study of C2H2 Oxidation at High Pressure, Int. J. Chem. Kinet., 2016

C2H2+HO2=CH2CHO+O 1.41E+05 1.86 15460.0

PLOG/1.000E-02 5.50E+06 1.19 12880.0/

PLOG/1.000E-02 2.94E-04 4.16 7736.0/

PLOG/1.000E-01 1.16E+08 0.77 13600.0/

PLOG/1.000E-01 6.14E-03 3.81 8394.0/

PLOG/3.160E-01 1.20E+07 1.09 13050.0/

PLOG/3.160E-01 5.44E-04 4.09 8044.0/

PLOG/1.000E+00 3.02E+07 0.98 13310.0/

PLOG/1.000E+00 2.48E-04 4.19 8203.0/

PLOG/3.160E+00 1.98E+74 -16.33 109200.0/

PLOG/3.160E+00 6.57E+04 1.85 12360.0/

PLOG/1.000E+01 7.50E+14 -1.17 18350.0/

PLOG/1.000E+01 2.92E-01 3.38 10590.0/

PLOG/3.160E+01 8.63E+18 -2.27 22230.0/

PLOG/3.160E+01 1.95E+00 3.17 11740.0/

PLOG/1.000E+02 5.78E+18 -2.09 24350.0/

PLOG/1.000E+02 1.10E-01 3.52 11980.0/

! Lopez et al., Experimental and Kinetic Modeling Study of C2H2 Oxidation at High Pressure, Int. J. Chem. Kinet., 2016

C2H2+HO2=OCHCHO+H 3.94E+04 1.68 13980.0

PLOG/1.000E-02 8.51E+07 0.48 11720.0/

PLOG/1.000E-02 2.43E-06 4.43 5578.0/

PLOG/1.000E-01 7.43E+07 0.50 11690.0/

PLOG/1.000E-01 2.00E-06 4.45 5564.0/

PLOG/3.160E-01 7.91E+07 0.49 11700.0/

PLOG/3.160E-01 1.81E-06 4.46 5654.0/

PLOG/1.000E+00 2.18E+09 0.06 12470.0/

PLOG/1.000E+00 2.24E-05 4.17 6416.0/

PLOG/3.160E+00 7.00E+49 -10.18 77110.0/

PLOG/3.160E+00 7.65E+05 1.18 11340.0/

PLOG/1.000E+01 4.06E+16 -2.03 17630.0/

PLOG/1.000E+01 2.01E-02 3.38 8696.0/

PLOG/3.160E+01 9.38E+16 -2.03 19590.0/

PLOG/3.160E+01 6.06E-03 3.53 9217.0/

PLOG/1.000E+02 5.91E+21 -3.32 25030.0/

PLOG/1.000E+02 6.76E-02 3.27 10760.0/

! Lopez et al., Experimental and Kinetic Modeling Study of C2H2 Oxidation at High Pressure, Int. J. Chem. Kinet., 2016

! Replace HCO with 70% H + CO

! C2H2+HO2=CH2O+HCO 8.66E+07 0.87 14170.0

! PLOG/1.000E-02 1.30E+14 -1.17 13750.0/

! PLOG/1.000E-02 2.81E+01 2.56 7382.0/

! PLOG/1.000E-01 1.42E+01 2.64 7253.0/

! PLOG/1.000E-01 5.19E+13 -1.05 13520.0/

! PLOG/3.160E-01 8.64E-06 4.34 4525.0/

! PLOG/3.160E-01 2.30E+10 -0.00 11720.0/

! PLOG/1.000E+00 1.11E+103 -24.18 138600.0/

! PLOG/1.000E+00 2.69E+08 0.60 10850.0/

! PLOG/3.160E+00 1.74E+16 -1.75 15180.0/

! PLOG/3.160E+00 1.18E+01 2.69 8025.0/

! PLOG/1.000E+01 2.44E+36 -7.77 26970.0/

! PLOG/1.000E+01 3.28E+07 0.91 11710.0/

! PLOG/3.160E+01 5.92E+28 -5.30 25130.0/

! PLOG/3.160E+01 5.98E+04 1.70 11250.0/

! PLOG/1.000E+02 8.24E+16 -1.70 20030.0/

! PLOG/1.000E+02 1.44E-05 4.31 6829.0/

C2H2+HO2=CH2O+HCO 8.66E+07 0.87 14170.0

PLOG/1.000E-02 3.90E+13 -1.17 13750.0/

PLOG/1.000E-02 8.43E+00 2.56 7382.0/

PLOG/1.000E-01 4.26E+00 2.64 7253.0/

PLOG/1.000E-01 1.56E+13 -1.05 13520.0/

PLOG/3.160E-01 2.59E-06 4.34 4525.0/

PLOG/3.160E-01 6.90E+09 -0.00 11720.0/

PLOG/1.000E+00 3.33E+102 -24.18 138600.0/

PLOG/1.000E+00 8.07E+07 0.60 10850.0/

PLOG/3.160E+00 5.22E+15 -1.75 15180.0/

PLOG/3.160E+00 3.54E+00 2.69 8025.0/

PLOG/1.000E+01 7.32E+35 -7.77 26970.0/

PLOG/1.000E+01 9.84E+06 0.91 11710.0/

PLOG/3.160E+01 1.78E+28 -5.30 25130.0/

PLOG/3.160E+01 1.79E+04 1.70 11250.0/

PLOG/1.000E+02 2.47E+16 -1.70 20030.0/

PLOG/1.000E+02 4.32E-06 4.31 6829.0/

! Lopez et al., Experimental and Kinetic Modeling Study of C2H2 Oxidation at High Pressure, Int. J. Chem. Kinet., 2016

C2H2+HO2=CH2O+H+CO 8.66E+07 0.87 14170.0

PLOG/1.000E-02 9.10E+13 -1.17 13750.0/

PLOG/1.000E-02 1.97E+01 2.56 7382.0/

PLOG/1.000E-01 9.94E+00 2.64 7253.0/

PLOG/1.000E-01 3.63E+13 -1.05 13520.0/

PLOG/3.160E-01 6.05E-06 4.34 4525.0/

PLOG/3.160E-01 1.61E+10 -0.00 11720.0/

PLOG/1.000E+00 7.77E+102 -24.18 138600.0/

PLOG/1.000E+00 1.88E+08 0.60 10850.0/

PLOG/3.160E+00 1.22E+16 -1.75 15180.0/

PLOG/3.160E+00 8.26E+00 2.69 8025.0/

PLOG/1.000E+01 1.71E+36 -7.77 26970.0/

PLOG/1.000E+01 2.30E+07 0.91 11710.0/

PLOG/3.160E+01 4.14E+28 -5.30 25130.0/

PLOG/3.160E+01 4.19E+04 1.70 11250.0/

PLOG/1.000E+02 5.77E+16 -1.70 20030.0/

PLOG/1.000E+02 1.01E-05 4.31 6829.0/

! Lopez et al., Experimental and Kinetic Modeling Study of C2H2 Oxidation at High Pressure, Int. J. Chem. Kinet., 2016

C2H2+HO2=CO+CH3O 3.06E+05 1.07 14220.0

PLOG/1.000E-02 3.54E+11 0.00 49510.0/

PLOG/1.000E-02 2.89E+04 1.23 9903.0/

PLOG/1.000E-01 2.78E+08 0.01 11920.0/

PLOG/1.000E-01 9.67E-07 4.15 5173.0/

PLOG/3.160E-01 8.06E+07 0.18 11650.0/

PLOG/3.160E-01 1.84E-08 4.62 4517.0/

PLOG/1.000E+00 8.94E+69 -15.85 102500.0/

PLOG/1.000E+00 5.38E+05 0.86 10700.0/

PLOG/3.160E+00 5.66E+12 -1.25 14570.0/

PLOG/3.160E+00 5.37E-04 3.42 7218.0/

PLOG/1.000E+01 3.30E+23 -4.45 21210.0/

PLOG/1.000E+01 2.86E+02 1.84 10460.0/

PLOG/3.160E+01 2.43E+22 -3.96 22650.0/

PLOG/3.160E+01 8.11E+00 2.30 10560.0/

PLOG/1.000E+02 1.17E+18 -2.57 22360.0/

PLOG/1.000E+02 6.86E-04 3.42 9329.0/

! Lopez et al., Experimental and Kinetic Modeling Study of C2H2 Oxidation at High Pressure, Int. J. Chem. Kinet., 2016

C2H2+HO2=CO2+CH3 4.13E+05 0.96 14140.0

PLOG/1.000E-02 1.15E-07 4.31 4614.0/

PLOG/1.000E-02 2.01E+08 0.00 11790.0/

PLOG/1.000E-01 1.10E-07 4.32 4622.0/

PLOG/1.000E-01 2.01E+08 0.00 11780.0/

PLOG/3.160E-01 1.75E+142 -35.04 188700.0/

PLOG/3.160E-01 1.55E+05 0.95 10200.0/

PLOG/1.000E+00 3.96E+84 -19.80 119800.0/

PLOG/1.000E+00 1.38E+06 0.68 10810.0/

PLOG/3.160E+00 5.02E+13 -1.60 14980.0/

PLOG/3.160E+00 9.29E-03 3.00 7659.0/

PLOG/1.000E+01 8.56E+28 -6.15 24030.0/

PLOG/1.000E+01 1.86E+04 1.26 11230.0/

PLOG/3.160E+01 1.28E+27 -5.42 25380.0/

PLOG/3.160E+01 2.89E+02 1.79 11240.0/

PLOG/1.000E+02 1.71E+15 -1.80 20370.0/

PLOG/1.000E+02 3.90E-07 4.21 7314.0/

! Lopez et al., Experimental and Kinetic Modeling Study of C2H2 Oxidation at High Pressure, Int. J. Chem. Kinet., 2016

! C2H2+O2=HCO+HCO 6.1E12 0.000 53250 !

! DUPLICATE

! C2H2+O2=HCO+HCO 1.7E07 1.670 70960 ! triplet surface

! DUPLICATE

! ! Lopez et al., Experimental and Kinetic Modeling Study of C2H2 Oxidation at High Pressure, Int. J. Chem. Kinet., 2016

! HH@160407: including prompt dissociation of HCO (following Labbe et al., J. Phys. Chem. Lett. 2016)

```
!
!
C2H2+O2=HCO+H+CO     6.661E+33   -5.633   82336.1
    DUPLICATE
C2H2+O2=HCO+H+CO     1.069E+26   -3.525   73959.1
    DUPLICATE
!
C2H2+O2=H+CO+H+CO          1.218E+32   -4.869   93010.6
!

! ------------- H2CC ...

! H2CC=C2H2    see the reverse: C2H2(+M)=H2CC(+M)


H2CC+H=C2H2+H                    1.0E14   0.000       0 !          LAS/LAW00
! Laskin A Wang H Law CK IJCK 32:589 2000

H2CC+OH=CH2CO+H                  2.0E13   0.000       0 !          LAS/LAW00
! Laskin A Wang H Law CK IJCK 32:589 2000

H2CC+O2=CH2+CO2                  1.0E13   0.000       0 !          LAS/WAN99,JAM prd
! Laskin A Wang H Law CK IJCK 32:589 2000
! JAM est prod

! ------------- C2 ...

C2+M=C+C+M                       1.5E16   0.000  142300 !
! Kruse T Roth P JPCA 101:2138-2146 1997

C2+O=C+CO                        1.0E14   0.000       0 !
! est


! ****************************************************************************
!    EtOH (CH3CH2OH) subset                                                   *
! ****************************************************************************
```

CH3CH2OH=CH2OH+CH3 5.6E64 -14.470 107039

PLOG/0.001 1.3E51 -10.590 100869/

PLOG/0.01 5.2E59 -13.980 99850/

PLOG/0.1 1.6E66 -15.300 105331/

PLOG/1.0 5.6E64 -14.470 107039/

PLOG/10.0 1.6E58 -12.290 105708/

PLOG/100.0 1.8E47 -8.960 101002/

!R. Sivaramakrishnan, M.-C. Su, J. Michael, S. Klippenstein, L. Harding, B. Ruscic, M.-C.Su, Journal of Physical Chemistry A 114 (2010) 9425-9439.

!

CH3CH2OH=C2H5+OH 1.5E65 -14.89 112282

PLOG/0.001 8.1E46 -11.33 110991/

PLOG/0.01 1.8E56 -13.49 107178/

PLOG/0.1 4.7E63 -14.99 109561/

PLOG/1.0 1.5E65 -14.89 112282/

PLOG/10.0 2.8E61 -13.40 113016/

PLOG/100.0 6.2E51 -10.34 109879/

!R. Sivaramakrishnan, M.-C. Su, J. Michael, S. Klippenstein, L. Harding, B. Ruscic, M.-C.Su, Journal of Physical Chemistry A 114 (2010) 9425-9439.

!

CH3CH2OH=C2H4+H2O 5.2E43 -8.900 81461

PLOG/0.001 3.4E59 -14.220 83625/

PLOG/0.01 2.6E57 -13.290 85214/

PLOG/0.1 1.7E52 -11.520 84698/

PLOG/1.0 5.2E43 -8.900 81461/

PLOG/10.0 4.6E32 -5.600 76019/

PLOG/100.0 3.8E20 -2.060 69426/

!R. Sivaramakrishnan, M.-C. Su, J. Michael, S. Klippenstein, L. Harding, B. Ruscic, M.-C.Su, Journal of Physical Chemistry A 114 (2010) 9425-9439.

CH3CHOH+H=CH3CH2OH 1.2E53 -12.330 14505

PLOG/ 1.00E-02 9.9E42 -10.770 8942/

PLOG/ 1.00E-01 1.9E55 -13.560 14306/

PLOG/ 1.00E+00 1.2E53 -12.330 14505/

PLOG/ 1.00E+01 1.7E50 -11.040 15896/

PLOG/ 1.00E+02 1.6E40 -7.820 12916/

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455; personal communication 650-2000 K fit

CH3CH2O+H(+M)=CH3CH2OH(+M) 3.1E11 0.894 13 !

LOW / 3.8E51 -15.550 11101 /

! Xu et al., J. Phys. Chem. A 115 (2011) 3509–3522.

CH3CH2OH+H=CH3CHOH+H2 8.8E03 2.680 2913 !

!R. Sivaramakrishnan, M.-C. Su, J. Michael, S. Klippenstein, L. Harding, B. Ruscic, M.-C.Su, Journal of Physical Chemistry A 114 (2010) 9425-9439.

!

CH3CH2OH+H=CH2CH2OH+H2 5.3E03 2.810 7491 !

!R. Sivaramakrishnan, M.-C. Su, J. Michael, S. Klippenstein, L. Harding, B. Ruscic, M.-C.Su, Journal of Physical Chemistry A 114 (2010) 9425-9439.

!

CH3CH2OH+H=CH3CH2O+H2 9.5E02 3.140 8696 !

!R. Sivaramakrishnan, M.-C. Su, J. Michael, S. Klippenstein, L. Harding, B. Ruscic, M.-C.Su, Journal of Physical Chemistry A 114 (2010) 9425-9439.

CH3CH2OH+O=CH2CH2OH+OH 9.7E02 3.230 4660

! Wu CW Lee Yuan P Xu S Lin MC J Phys Chem A 111 (2007) 6693-6703

!

CH3CH2OH+O=CH3CHOH+OH 1.5E05 2.470 876

! Wu CW Lee Yuan P Xu S Lin MC J Phys Chem A 111 (2007) 6693-6703

!

CH3CH2OH+O=CH3CH2O+OH 1.5E-3 4.700 1730

! Wu CW Lee Yuan P Xu S Lin MC J Phys Chem A 111 (2007) 6693-6703

CH3CH2OH+OH=CH3CHOH+H2O 4.5E02 3.110 -2666 !

! Our fitting to J. Zheng and D. G. Truhlar, Faraday Discuss, 157 (2012) 59–88.

!

CH3CH2OH+OH=CH2CH2OH+H2O 9.4E03 2.670 -1004 !

! Our fitting to J. Zheng and D. G. Truhlar, Faraday Discuss, 157 (2012) 59–88.

!

CH3CH2OH+OH=CH3CH2O+H2O 2.4E03 2.820 -691 !

DUPLICATE

CH3CH2OH+OH=CH3CH2O+H2O 7.9E07 1.180 -303 !

DUPLICATE

! Our fitting to J. Zheng and D. G. Truhlar, Faraday Discuss, 157 (2012) 59–88.

CH3CH2OH+HO2=CH3CHOH+H2O2 8.2E03 2.550 10750 !

! Marinov NM IJCK 31:183 1999

!

```
CH3CH2OH+HO2=CH2CH2OH+H2O2          1.2E04   2.550   15750 !
! Marinov NM IJCK 31:183 1999
!
CH3CH2OH+HO2=CH3CH2O+H2O2           2.5E12   0.000   24000 !
! Marinov NM IJCK 31:183 1999

CH3CH2OH+CH3=CH3CHOH+CH4            2.0E01   3.370    7630 !
! Xu et al., J. Chem. Phys. 120 (2004).
!
CH3CH2OH+CH3=CH2CH2OH+CH4           2.0E00   3.570    7717 !
! Xu et al., J. Chem. Phys. 120 (2004).
!
CH3CH2OH+CH3=CH3CH2O+CH4            3.3E02   3.300   12283 !
! Xu et al., J. Chem. Phys. 120 (2004).



! ---------- CH3CHOH ...

CH3CHOH(+M)=CH3CHO+H(+M)            6.2E09   1.310   33778 !
 LOW  /                      1.8E16   0.000   20782 /
 TROE /0.187 65.2 2568 41226 /
! E.E. Dames,  Int. J. Chem. Kinet. 46 (2014) 176–188.
!
CH3CHOH(+M)=CH2CHOH+H (+M)          6.4E09   1.330   35974 !
 LOW  /                      8.2E14   0.000   21517 /
 TROE / 0.473 10 2218 2615 /
! E.E. Dames,  Int. J. Chem. Kinet. 46 (2014) 176–188.
!
CH3CHOH(+M)=CH3+CH2O(+M)            2.2E09   1.180   33987 !
 LOW  /                      5.9E15   0.000   21333 /
 TROE / 0.124  1  1729  50000       /
! E.E. Dames,  Int. J. Chem. Kinet. 46 (2014) 176–188.

CH3CHOH+H=CH2CHOH+H2                3.1E12   0.2728   -334 !
! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455
!
CH3CHOH+H=C2H4+H2O                  1.8E17  -1.216     386
```

PLOG/ 0.001 1.2E17 -1.166 284 /

PLOG/ 0.010 1.2E17 -1.162 266 /

PLOG/ 0.100 1.8E17 -1.216 386 /

PLOG/ 1.000 2.6E20 -2.079 3148 /

PLOG/ 10.00 9.3E23 -2.996 7954 /

PLOG/ 100.0 1.6E20 -1.812 9448 /

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455

!

CH3CHOH+H=CH3+CH2OH 2.3E20 -1.795 5893 !

PLOG/ 0.001 1.4E17 -0.912 3081 /

PLOG/ 0.010 1.5E17 -0.923 3116 /

PLOG/ 0.100 4.5E17 -1.052 3509 /

PLOG/ 1.000 2.3E20 -1.795 5893 /

PLOG/ 10.00 5.0E24 -2.949 10754 /

PLOG/ 100.0 4.0E23 -2.527 13637 /

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455

!

CH3CHOH+H=C2H5+OH 1.6E16 -0.697 6677 !

PLOG/ 0.001 4.0E13 0.021 4442 /

PLOG/ 0.010 4.4E13 0.010 4476 /

PLOG/ 0.100 1.1E14 -0.095 4790 /

PLOG/ 1.000 1.6E16 -0.697 6677 /

PLOG/ 10.00 6.8E20 -1.943 11331 /

PLOG/ 100.0 6.3E21 -2.106 15269 /

! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455

CH3CHOH+O=CH3CHO+OH 1.0E14 0.000 0 !

! Marinov NM IJCK 31:183 1999

!

CH3CHOH+OH=CH3CHO+H2O 5.0E12 0.000 0 !

! Marinov NM IJCK 31:183 1999

!

CH3CHOH+HO2=CH3CHO+OH+OH 4.0E13 0.000 0 !

! Marinov NM IJCK 31:183 1999

CH3CHOH+O2=CH3CHO+HO2 5.3E17 -1.638 839

PLOG/ 0.001 5.3E17 -1.637 838/

PLOG/ 0.01 5.3E17 -1.637 838/

```
 PLOG/ 0.1                    5.3E17  -1.637     838/
 PLOG/ 1                     5.3E17  -1.638     839/
 PLOG/ 10                     1.5E18  -1.771    1120/
 PLOG/ 100                    3.8E20  -2.429    3090/
! da Silva et al., J. Phys. Chem. A 113 (2009) 8923–8933

CH3CHOH+O2=CH2CHOH+HO2           7.6E02   2.450    -296
 PLOG/ 0.001                  5.1E02   2.495    -414/
 PLOG/ 0.01                   5.1E02   2.496    -414/
 PLOG/ 0.1                    5.3E02   2.490    -402/
 PLOG/ 1                     7.6E02   2.450    -296/
 PLOG/ 10                     8.9E03   2.146     470/
 PLOG/ 100                    4.4E05   1.699    2330/
! da Silva et al., J. Phys. Chem. A 113 (2009) 8923–8933



! ---------- CH2CH2OH ...

CH2CH2OH=CH2CHOH+H               3.3E28  -5.260   35583
 PLOG/ 0.0013                  2.7E15  -1.920   29383/
 PLOG/ 1                     3.3E28  -5.260   35583/
 PLOG/ 100                    2.7E27  -4.440   37205/
! Xu, Z. F.; Xu, K.; Lin, M. C. ChemPhysChem 2009, 10, 972-982

! CH3CH2O=CH2CH2OH                2.8E-29 11.900    4450 !
! Y. Zhang, S. Zhang, Q.S. Li, Chem. Phys. 308 (2005) 109–116 (kinf).
! Omitted following E.E. Dames,  Int. J. Chem. Kinet. 46 (2014) 176–188.

CH2CH2OH+H=C2H4+H2O              2.6E22  -2.599    5235 !
 PLOG/   0.001                1.7E17  -1.184     335 /
 PLOG/   0.010                1.6E17  -1.176     299 /
 PLOG/   0.100                1.7E18  -1.461    1107 /
 PLOG/   1.000                2.6E22  -2.599    5235 /
 PLOG/   10.00                6.5E23  -2.883    9307 /
 PLOG/   100.0                3.6E16  -0.716    8767 /
! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455
!
CH2CH2OH+H=CH3+CH2OH             1.9E22  -2.300    7693
```

```
 PLOG/   0.001                  1.5E17  -0.903    3024 /
 PLOG/   0.010                  1.9E17  -0.935    3120 /
 PLOG/   0.100                  2.5E18  -1.243    4062 /
 PLOG/   1.000                  1.9E22  -2.300    7693 /
 PLOG/   10.00                  2.8E25  -3.100   12454 /
 PLOG/   100.0                  7.5E20  -1.693   13429 /
! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455
!
CH2CH2OH+H=C2H5+OH                9.2E17  -1.15762  8193
 PLOG/   0.001                  3.6E13   0.05139  4302 /
 PLOG/   0.01                   4.6E13   0.02101  4392 /
 PLOG/   0.1                    3.4E14  -0.21686  5113 /
 PLOG/   1                      9.2E17  -1.15762  8193 /
 PLOG/   10                     1.6E22  -2.27331 13261 /
 PLOG/   100                    8.1E19  -1.50969 15534 /
! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455

CH2CH2OH+H(+M)=CH3CH2OH(+M)         5.2E17  -0.990    1580 !
 LOW  /                        2.0E41  -7.080    6685/                        !
 TROE /0.8422 125 2219 6882/                          !
! est c2h5+h+m

CH2CH2OH+O=CH2O+CH2OH              4.0E13   0.000       0 !
! est C2H5+O

! CH2CH2OH+OH=CH2CHOH+H2O            2.4E13   0.000       0 !
! est C2H5+OH
CH2CH2OH+OH=CH2CHOH+H2O    4.6961E+18   -1.5805   7999.2
    PLOG/   0.001   1.2926E+19   -1.9600   272.7   /
    PLOG/   0.010   1.2184E+19   -1.9533   238.8   /
    PLOG/   0.100   4.1052E+19   -2.1007   625.4   /
    PLOG/   1.000   7.9406E+22   -2.9892   3862.6   /
    PLOG/   10.000   2.7926E+24   -3.3287   7748.8   /
    PLOG/   100.000   4.6961E+18   -1.5805   7999.2   /
! est C2H5+OH
CH2CH2OH+HO2=CH3CH2OH+O2           1.0E12   0.000       0 !
! est C2H5+HO2
```

CH2CH2OH+HO2=>CH2OH+CH2O+OH 3.0E13 0.000 0 !

CH2CH2OH+O2=CH2CHOH+HO2 3.6E13 -0.880 3074.0

PLOG/ 1.30E-02 1.3E53 -11.880 35927.0/

PLOG/ 1.30E-02 2.3E10 -0.150 -791.0/

PLOG/ 1.00E-01 5.0E12 -0.790 877.0/

PLOG/ 1.00E-01 2.8E61 -14.170 43492.0/

PLOG/ 1.00E+00 3.6E13 -0.880 3074.0/

PLOG/ 1.00E+00 6.0E03 -10.000 199.0/

PLOG/ 1.00E+01 4.4E20 -2.850 8516.0/

PLOG/ 1.00E+01 6.0E03 -10.000 199.0/

PLOG/ 1.00E+02 1.9E30 -5.510 16616.0/

PLOG/ 1.00E+02 6.0E03 -10.000 199.0/

! Zador J Fernandes RX Georgievskii Y Meloni G Taatjes CA Miller JA Proc Combust Inst 2009 32 271-277

! HH@160510:

CH2CH2OH+O2=HOCH2CH2OO 6.4E38 -8.770 5859 ! 1 atm

PLOG/ 1.30E-02 1.5E44 -11.150 5523.0/

PLOG/ 1.00E-01 4.9E42 -10.340 5913.0/

PLOG/ 1.00E+00 6.4E38 -8.770 5859.0/

PLOG/ 1.00E+01 5.6E32 -6.580 5046.0/

PLOG/ 1.00E+02 4.2E26 -4.460 3940.0/

! Zador J Fernandes RX Georgievskii Y Meloni G Taatjes CA Miller JA Proc Combust Inst 2009 32 271-277

CH2CH2OH+O2=CH2O+CH2O+OH 4.4E24 -4.360 4396 ! 1 atm

PLOG/ 1.30E-02 5.6E22 -3.950 1210.0/

PLOG/ 1.00E-01 1.4E24 -4.310 2664.0/

PLOG/ 1.00E+00 4.4E24 -4.360 4396.0/

PLOG/ 1.00E+01 3.0E25 -4.500 6763.0/

PLOG/ 1.00E+02 1.2E29 -5.440 11323.0/

! Zador J Fernandes RX Georgievskii Y Meloni G Taatjes CA Miller JA Proc Combust Inst 2009 32 271-277

! ---------- CH3CH2O ...

CH3CHO+H=CH3CH2O 4.6E07 1.710 7090

! Sivaramakrishnan R Michael JV Klippenstein SJ, J. Phys. Chem. A 114 (2010) 755–764.

```
CH3CH2O+H(+M)=CH2OH+CH3(+M)         2.6E18  -1.050    5128
 LOW /                        3.0E11   0.893      17 /
! Z.F. Xu, K. Xu, M.C. Lin, J. Phys. Chem. A 115 (2011) 3509–3522.

CH3CH2O+H=CH3CHO+H2                 7.5E09   1.150     673
! Xu et al., J. Phys. Chem. A 115 (2011) 3509–3522.

CH3CH2O+OH=CH3CHO+H2O               3.0E13   0.000       0
! est

CH3CH2O+O2=CH3CHO+HO2               1.5E10   0.000     645
! Fittschen, C.; Frenzel, A.; Imrik, K.; Devolder, P. Int J Chem Kinet 1999, 31, 860–866.

! ---------- CH3CHO ...

CH3CHO=CH2CO+H2                     8.5E44  -9.770   90905
 PLOG/  5.0E-2                   4.0E44 -10.070   87428/
 PLOG/  1.0E-01                  7.4E44 -10.050   88422/
 PLOG/  1.0E+00                  8.5E44  -9.770   90905/
 PLOG/  1.0E+01                  2.2E45  -9.550   94879/
! Sivaramakrishnan, R.; Michael, J.V.; Klippenstein, S.J. J Phys Chem A 114, 755-764 (2010).
! R. Sivaramakrishnan, J.V. Michael, L.B. Harding, S.J. Klippenstein, J Phys Chem A 2015, 119, 7724-
7733.
!
CH3CHO=CH4+CO                       1.9E45  -9.430   89415
 PLOG/  5.00E-02                 5.1E45  -9.850   89018/
 PLOG/  1.00E-01                 1.4E45  -9.650   87925/
 PLOG/  1.00E+00                 1.9E45  -9.430   89415/
 PLOG/  1.00E+01                 1.6E45  -9.100   92793/
! Sivaramakrishnan, R.; Michael, J.V.; Klippenstein, S.J. J Phys Chem A 114, 755-764 (2010).
! R. Sivaramakrishnan, J.V. Michael, L.B. Harding, S.J. Klippenstein, J Phys Chem A 2015, 119, 7724-
7733.

CH3CHO=CH2CHOH                      1.1E46  -9.760   81964
 PLOG/  5.00E-02                 7.3E45 -10.040   78785/
 PLOG/  1.00E-01                 2.9E45  -9.860   78884/
 PLOG/  1.00E+00                 1.1E46  -9.760   81964/
 PLOG/  1.00E+01                 2.8E45  -9.350   84645/
```

! R. Sivaramakrishnan, J.V. Michael, L.B. Harding, S.J. Klippenstein, J Phys Chem A 2015, 119, 7724-7733.

CH3CHO+H=CH3CO+H2 1.3E05 2.580 1219

! R Sivaramakrishnan JV Michael SJ Klippenstein, J. Phys. Chem. A 114 (2010) 755–764.

CH3CHO+O=CH3CO+OH 5.8E12 0.000 1808

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

CH3CHO+OH=CH3CO+H2O 2.8E12 0.000 -709

! S. Wang, D.F. Davidson, R.K. Hanson, Proc. Combust. Inst. 35 (2015) 473-480.

!

CH3CHO+OH=CH2CHO+H2O 8.5E13 0.000 5313

! S. Wang, D.F. Davidson, R.K. Hanson, Proc. Combust. Inst. 35 (2015) 473-480.

CH3CHO+HO2=CH3CO+H2O2 1.7E13 0.000 16293

! M Altarawneh AH Al-Muhtaseb BZ Dlugogorski EM Kennedy JC Mackie J Comput Chem 32: 1725–1733, 2011

!

CH3CHO+HO2=CH2CHO+H2O2 1.1E13 0.000 23248

! M Altarawneh AH Al-Muhtaseb BZ Dlugogorski EM Kennedy JC Mackie J Comput Chem 32: 1725–1733, 2011

CH3CHO+O2=CH3CO+HO2 1.2E05 2.500 37554

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

CH3CHO+O2=CH2CHO+HO2 1.5E07 1.900 49548

! est 1/2 of c2h6+o2

CH3CHO+CH3=CH3CO+CH4 3.5E-8 6.210 1629 !

! Baulch DL Bowman CT Cobos CJ Cox RA Just Th Kerr JA Pilling MJ Stocker D Troe J Tsang W Walker RW Warnatz J JPCRD 34:757-1397 2005

CH3CHO+CH3=CH2CHO+CH4 1.8E-1 3.440 10384 !

! est 1/2 of c2h6+ch3

CH3CHO+CH3O=CH3CO+CH3OH 1.0E11 0.000 2981 !

! est ch2o+ch3o

```
CH3CHO+CH3O=CH2CHO+CH3OH            1.2E11   0.000    7100 !
! est 1/2 of c2h6+ch3o

CH3CHO+CH3O2=CH3CO+CH3OOH           1.7E13   0.000   16293 !
! est ch3hco+ho2

CH3CHO+CH3O2=CH2CHO+CH3OOH          1.1E13   0.000   23248 !
! est ch3hco+ho2

! ------------ cC2H4O ...

cC2H4O=CH2CHO+H                     1.8E13   0.200   71780 !
! A. Joshi, X. You, T.A. Barckholtz, H. Wang, J. Phys. Chem. A 109 (2005) 8016-8027
!
cC2H4O=CH3+HCO                      5.6E13   0.400   61880 !
! A. Joshi, X. You, T.A. Barckholtz, H. Wang, J. Phys. Chem. A 109 (2005) 8016-8027
!
cC2H4O=CH3CO+H                      2.4E13   0.250   65310 !
! A. Joshi, X. You, T.A. Barckholtz, H. Wang, J. Phys. Chem. A 109 (2005) 8016-8027
!
cC2H4O=CH2CO+H2                     3.6E12  -0.200   63030 !
! A. Joshi, X. You, T.A. Barckholtz, H. Wang, J. Phys. Chem. A 109 (2005) 8016-8027
!
cC2H4O=CH3CHO                       3.2E12  -0.750   46424 !
! A. Joshi, X. You, T.A. Barckholtz, H. Wang, J. Phys. Chem. A 109 (2005) 8016-8027
!
cC2H4O=C2H2+H2O                     7.6E12   0.060   69530 !
! A. Joshi, X. You, T.A. Barckholtz, H. Wang, J. Phys. Chem. A 109 (2005) 8016-8027
!
cC2H4O+H=CH3CHO+H                   5.6E13   0.000   10950 ! # commented out previously?
! A. Joshi, X. You, T.A. Barckholtz, H. Wang, J. Phys. Chem. A 109 (2005) 8016-8027
!
cC2H4O+H=cC2H3O+H2                  2.0E13   0.000    8310 !
! A. Lifshitz, H. Ben-Hamou, J. Phys. Chem. 87 (1983) 1782
!
cC2H4O+H=C2H3+H2O                   5.0E09   0.000    5000 !
! A. Lifshitz, H. Ben-Hamou, J. Phys. Chem. 87 (1983) 1782
!
```

cC2H4O+H=C2H4+OH 9.5E10 0.000 5000 !

! A. Lifshitz, H. Ben-Hamou, J. Phys. Chem. 87 (1983) 1782

!

cC2H4O+O=cC2H3O+OH 1.9E12 0.000 5250 !

! D.J. Bogan, C.W. Hand, J. Phys. Chem. 82 (1978) 2067

!

cC2H4O+OH=cC2H3O+H2O 1.8E13 0.000 3610 !

! R.R. Baldwin, A. Keen, R.W. Walker, J. Chem. Soc. Faraday Trans. 80 (1984) 435

!

cC2H4O+HO2=cC2H3O+H2O2 4.0E12 0.000 17000 !

! P. Dagaut, D. Voisin, M. Cathonnet, M. McGuinness, J.M. Simmie, Combust. Flame 106 (1996) 62-68.

!

cC2H4O+O2=cC2H3O+HO2 4.0E13 0.000 61500 !

! P. Dagaut, D. Voisin, M. Cathonnet, M. McGuinness, J.M. Simmie, Combust. Flame 106 (1996) 62-68.

!

cC2H4O+CH3=cC2H3O+CH4 1.1E12 0.000 11830 !

! R.R. Baldwin, A. Keen, R.W. Walker, J. Chem. Soc. Faraday Trans. 80 (1984) 435

! ---------- CH2CHOH ...

!CH2CHOH(+M)=CH3CHO(+M) 9.7E23 -3.290 59994 !

! LOW/ 2.9E43 -8.120 52204/

! TROE/ 0.5 863 320 100000/

! E.E. Dames, Int. J. Chem. Kinet. 46 (2014) 176–188.

! is a duplicate of CH3CHO=CH2CHOH

CH2CHOH+H=CH2CHO+H2 1.5E03 3.077 7230 !

! H-B Rao X-Y Zeng H He Z-R Li J Phys Chem A 2011, 115, 1602-1608

CH2CHOH+H=CHCHOH+H2 2.5E07 2.030 15180 !

! H-B Rao X-Y Zeng H He Z-R Li J Phys Chem A 2011, 115, 1602-1608

!

!CH2CHOH+O=CH2OH+HCO 3.9E12 0.000 1494 !

! DUPLICATE

!CH2CHOH+O=CH2OH+HCO 6.2E13 0.000 6855 !

! DUPLICATE

! est C2H4+O

```
! HH@160407: including prompt dissociation of HCO (following Labbe et al., J. Phys. Chem. Lett. 2016)
CH2CHOH+O=CH2OH+HCO              3.9E12   0.000    1494
   DUPLICATE
CH2CHOH+O=CH2OH+HCO          -2.335E+22   -2.473   21421.3
   DUPLICATE
CH2CHOH+O=CH2OH+HCO              6.2E13   0.000    6855
   DUPLICATE
CH2CHOH+O=CH2OH+HCO          -3.711E+23   -2.473   26782.3
   DUPLICATE
CH2CHOH+O=CH2OH+H+CO          3.711E+23   -2.473   26782.3
   DUPLICATE
CH2CHOH+O=CH2OH+H+CO          2.335E+22   -2.473   21421.3
   DUPLICATE


CH2CHOH+O=CH2CHO+OH              1.6E07   2.000    4400
! est CH3CH2OH+O=CH3CH2O+OH
!
CH2CHOH+OH=CHCHOH+H2O            1.3E-1   4.200    -860
! est C2H4+OH

      !CH2CHOH+OH=CH2CHO+H2O             7.5E11   0.300    1600
      ! est CH3CH2OH+OH=CH3CH2O+H2O
CH2CHOH+OH=CH2CHO+H2O                                  2.372E+03        2.82     -691.48
      DUPLICATE
CH2CHOH+OH=CH2CHO+H2O                                  7.905E+07        1.18     -303.17
      DUPLICATE
! est CH3CH2OH+OH=CH3CH2O+H2O

CH2CHOH+HO2=CH2CHO+H2O2          1.6E12   0.000    16293
! M Altarawneh AH Al-Muhtaseb BZ Dlugogorski EM Kennedy JC Mackie J Comput Chem 32: 1725–1733, 2011

CH2CHOH+HO2=CH3CHO+HO2           1.5E05   1.670    6810 !
! G. da Silva, J.W. Bozzelli, Chem. Phys. Lett. 483 (2009) 25–29 (1 atm) # check SUP
```

```
! CH2CHOH+HO2=CH3CHOH+O2                          4.11E6   1.62       15440  !---- see the
reverse rate!

        !CH2CHOH+O2=>CH2O+HCO+OH            3.5E07   1.800   39000 !
        ! est C2H4+O2
! HH@160407: including prompt dissociation of HCO (following Labbe et al., J. Phys. Chem. Lett.
2016)
CH2CHOH+O2=>CH2O+HCO+OH            3.5E07   1.800   39000 ! GIM/GLA09 C2H4+O2
   DUPLICATE
CH2CHOH+O2=>CH2O+HCO+OH         -2.095E+17   -0.673   58927.3
   DUPLICATE
CH2CHOH+O2=>CH2O+H+CO+OH         2.095E+17   -0.673   58927.3
! ------------- CHCHOH ...

CHCHOH=HCCOH+H                   1.1E31  -6.153   51383 !
 PLOG   /0.04                    4.4E29  -6.153   51383. / ! extrapolation
 PLOG   /1.0                     1.1E31  -6.153   51383. /
 PLOG   /10.                     1.5E32  -6.168   52239. /
 PLOG   /100.                    5.5E29  -5.057   52377. /
! Ing W-C Sheng CY Bozzelli JW FPT 83:111-145 2003

CHCHOH+H=CH2CHO+H                5.0E13   0.000       0 !
! Glarborg P Alzueta MU Dam-Johansen K Miller JA CF 115:1 1998
! JAM est

CHCHOH+H=HCCOH+H2                4.5E13   0.000       0 !
! est C2H3+H

CHCHOH+O=OCHCHO+H                5.0E13   0.000       0 !
CHCHOH+OH=HCCOH+H2O              2.0E13   0.000       0 !
CHCHOH+O2=OCHCHO+OH              1.8E12   0.000       -187 !
CHCHOH+O2=HOCHO+HCO                2.848E+14   -0.586   1237.3
CHCHOH+O2=HOCHO+H+CO  1.112E+22   -2.498   20265.6
CHCHOH+CH2O=CH2CHOH+HCO   1.549E+11   0.413   8163.9
DUPLICATE
CHCHOH+CH2O=CH2CHOH+HCO    5.117E+13   -0.005   14641.6
DUPLICATE
!--- Average (max) fitting error: 0.1% (0.6%) over T of 500--2500 [K]
!--- max error occurs at T of   500.000
```

CHCHOH+CH2O=CH2CHOH+H+CO 3.232E+13 0.337 25787.3

CHCHOH+HCO=CH2CHOH+CO 9.0E13 0.000 0 !
! est c2h3+hco

CHCHOH+CH3=HCCOH+CH4 2.1E13 0.000 0 !
! est c2h3+ch3

! ---------- cC2H3O ...
cC2H3O=CH2CHO 8.7E31 -6.900 14994 !
! Joshi A You X Barckholtz TA Wang H JPCA 109:8016-8027 2005
! cC2H3O=CH2CHO 9.23E+49 -12.43 24270
! Wang and Bozzeli, ChemPhysChem 2016, (DOI : 10.1002/cphc.201600152)

cC2H3O=CH2CO+H 5.0E13 0.000 14863 !
! Joshi A You X Barckholtz TA Wang H JPCA 109:8016-8027 2005

! cC2H3O=CH2CO+H 3.64E+14 -0.26 17920
! Wang and Bozzeli, ChemPhysChem 2016, (DOI : 10.1002/cphc.201600152)

cC2H3O=CH3+CO 7.1E12 0.000 14280 !
! Joshi A You X Barckholtz TA Wang H JPCA 109:8016-8027 2005

! cC2H3O=CH3+CO 4.60E+18 -1.74 18150
! Wang and Bozzeli, ChemPhysChem 2016, (DOI : 10.1002/cphc.201600152)

! cC2H3O=CH3CO 7.59E-01 -2.42 15860
! Wang and Bozzeli, ChemPhysChem 2016, (DOI : 10.1002/cphc.201600152)

! ---------- CH3CO ...
CH3CO=CH3+CO 6.5E18 -2.520 16436 !
PLOG /0.01 6.9E14 -1.970 14585./
PLOG /0.025 2.4E15 -2.000 14805./
PLOG /0.1 2.0E16 -2.090 15197./

PLOG /1. 6.5E18 -2.520 16436./

PLOG /10. 8.2E19 -2.550 17263./

PLOG /100. 1.3E20 -2.320 18012./

! Senosiain JP Klippenstein SJ Miller JA JPCA 110:5772-5781 2006

CH2CO+H=CH3CO 2.3E08 1.610 2627 ! (kinf)

! Senosiain JP Klippenstein SJ Miller JA JPCA 110:5772-5781 2006

! CH3CO=CH3+CO 5.25E+28 -5.76 19480

! CH3CO=CH2CO+H 3.58E+07 -4.34 46260

! Wang and Bozzeli, ChemPhysChem 2016, (DOI : 10.1002/cphc.201600152)

! CH3CO+H=CH3+HCO 2.1E13 0.000 0 !

! Bartels M Edelbuttal J Hoyermann K PCI 23:131 1991

! Ohmori K Miyoshi A Matsui H Washida N JPC 94:3253 1990

! HH@160407: including prompt dissociation of HCO (following Labbe et al., J. Phys. Chem. Lett. 2016)

CH3CO+H=CH3+H+CO 1.257E+23 -2.473 19927.3

CH3CO+O2=CH3C(O)OO 2.8E34 -7.210 6060 ! ¤

PLOG /0.1 3.6E31 -4.769 2188 /

PLOG /1.0 2.8E34 -7.210 6060 /

PLOG /10 4.9E31 -6.087 6541 /

! J.W. Allen, C.F. Goldsmith, W.H. Green, PhysChemChemPhys 2012, 14, 1131-1155.

! fitted from figure

CH3CO+O2=CH2CO+HO2 3.6E10 0.544 3721 ! ¤

PLOG /0.1 1.3E08 1.986 228 /

PLOG /1.0 3.6E10 0.544 3721 /

PLOG /10 7.7E13 -0.335 7510 /

! J.W. Allen, C.F. Goldsmith, W.H. Green, PhysChemChemPhys 2012, 14, 1131-1155.

! fitted from figure

CH3CO+O2=CH2O+CO+OH 4.9E23 -3.712 5895 ! ¤

PLOG /0.1 5.1E22 -3.524 3255 /

PLOG /1.0 4.9E23 -3.712 5895 /

PLOG /10 4.8E22 -3.303 8598 /

! J.W. Allen, C.F. Goldsmith, W.H. Green, PhysChemChemPhys 2012, 14, 1131-1155.

! fitted from figure

CH3CO+CH3=C2H6+CO 3.3E13 0.000 0 !
! Adachi H Basco N James DGL IJCK 13:1251-1276 1981

CH3CO+CH3=CH2CO+CH4 5.3E13 0.000 0 !
! Adachi H Basco N James DGL IJCK 13:1251-1276 1981

CH3CO+CH3O2=CH3+CO2+CH3O 2.4E13 0.000 0 !
! Tsang W Hampson RF JPCRD 15:1087 1986

! ---------- CH2CHO ...

CH2CHO=CH2CO+H 1.3E34 -6.570 49454 !
PLOG / 0.01 2.4E25 -4.800 43424./
PLOG / 0.1 2.4E30 -5.860 46114./
PLOG / 1.0 1.3E34 -6.570 49454./
PLOG / 10. 3.5E36 -6.920 52979./
PLOG / 100. 1.2E36 -6.480 55191./
! Senosiain JP Klippenstein SJ Miller JA JPCA 110:5772-5781 2006

! CH2CHO=CH2CO+H 9.30E+30 -5.71 49270
! Wang and Bozzeli, ChemPhysChem 2016, (DOI : 10.1002/cphc.201600152)

CH2CHO=CH3+CO 6.5E34 -6.870 47191 !
PLOG /0.01 1.2E30 -6.070 41332./
PLOG /0.025 1.5E31 -6.270 42478./
PLOG /0.1 6.4E32 -6.570 44282./
PLOG /1. 6.5E34 -6.870 47191./
PLOG /10. 2.2E35 -6.760 49548./
PLOG /100. 2.2E33 -5.970 50448./
! Senosiain JP Klippenstein SJ Miller JA JPCA 110:5772-5781 2006

```
!CH2CHO=CH3CO                6.05E+29          -5.49      46140
! Wang and Bozzeli, ChemPhysChem 2016,  (DOI : 10.1002/cphc.201600152)


!CH2CHO+H=CH3+HCO              1.9E22  -2.300    7693
!PLOG/   0.001                 1.5E17  -0.903    3024 /
!PLOG/   0.010                 1.9E17  -0.935    3120 /
!PLOG/   0.100                 2.5E18  -1.243    4062 /
!PLOG/   1.000                 1.9E22  -2.300    7693 /
!PLOG/   10.00                 2.8E25  -3.100   12454 /
!PLOG/   100.0                 7.5E20  -1.693   13429 /
!! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455
! HH@160407: including prompt dissociation of HCO (following Labbe et al., J. Phys. Chem. Lett. 2016)

CH2CHO+H=CH3+H+CO     1.137E+32   -4.773   27620.3
   PLOG/     1.000E-02   1.137E+27   -3.408   23047.3 /
   PLOG/     1.000E-01   1.496E+28   -3.716   23989.3 /
   PLOG/     1.000E+00   1.137E+32   -4.773   27620.3 /
   PLOG/     1.000E+01   1.676E+35   -5.573   32381.3 /
   PLOG/     1.000E+02   4.489E+30   -4.166   33356.3 /

CH2CHO+H=CH3CO+H              9.2E17  -1.15762  8193
 PLOG/   0.001                3.6E13   0.05139  4301 /
 PLOG/   0.01                 4.6E13   0.02101  4392 /
 PLOG/   0.1                  3.4E14  -0.21686  5113 /
 PLOG/   1                    9.2E17  -1.15762  8193 /
 PLOG/   10                   1.6E22  -2.27331 13261 /
 PLOG/   100                  8.1E19  -1.50969 15534 /
! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455


!CH2CHO+O = CH2O+HCO           5.0E13   0.000      0 !
! Labbe NJ Sivaramakrishnan R Klippenstein SJ, Proc. Combust. Inst. 35 (2015) 447-455
! HH@160407: including prompt dissociation of HCO (following Labbe et al., J. Phys. Chem. Lett. 2016)
CH2CHO+O=CH2O+HCO                                          5.0E13   0.000      0
   DUPLICATE
CH2CHO+O=CH2O+HCO       -2.993E+23   -2.473   19927.3
```

DUPLICATE

CH2CHO+O=CH2O+H+CO 2.993E+23 -2.473 19927.3

CH2CHO+OH=CH2OH+H+CO 5.986E+22 -2.473 19927.3

CH2CHO+HO2=CH2O+HCO+OH 3.1E13 0.000 0 ! ##151210##

!CH2CHO+CH3=C2H5+CO+H 4.9E14 -0.500 0 ! ##151209## see C2H5+HCO

! Marinov NM Pitz WJ Westbrook CK Castaldi MJ Senkan SM CST 116:211 1996

! ommited, a duplicate of C2H5+H+CO=CH3+CH2CHO

!CH2CHO+CH2=C2H4+HCO 5.0E13 0.000 0 !

! JAM est

! HH@160407: including prompt dissociation of HCO (following Labbe et al., J. Phys. Chem. Lett. 2016)

CH2CHO+CH2=C2H4+HCO 5.0E13 0.000 0 ! GLA/MIL98 JAM est

DUPLICATE

CH2CHO+CH2=C2H4+HCO -2.993E+23 -2.473 19927.3

DUPLICATE

CH2CHO+CH2=C2H4+H+CO 2.993E+23 -2.473 19927.3

!CH2CHO+CH=C2H3+HCO 1.0E14 0.000 0 !

! JAM est

! HH@160407: including prompt dissociation of HCO (following Labbe et al., J. Phys. Chem. Lett. 2016)

CH2CHO+CH=C2H3+HCO 1.0E14 0.000 0 ! GLA/MIL98 JAM est

DUPLICATE

CH2CHO+CH=C2H3+HCO -5.986E+23 -2.473 19927.3

DUPLICATE

CH2CHO+CH=C2H3+H+CO 5.986E+23 -2.473 19927.3

CHCHO+H=CH2CO+H 1.0E14 0.000 0 !

! est

CHCHO+O2=CO2+H+HCO 2.1E09 0.9929 -269 !

! est as CH2+O2

CHCHO+O2=OCHCHO+O 1.3E06 2.4202 1604 ! #

! est as CH2+O2

! ---------- HCCOH ...

! ---------- HCCO ...

HCCO+OH=HCOH+CO 1.0 0.0 0.0

PLOG / 1 3.032E+16 -0.935 659.4 /

PLOG / 1 8.694E+19 -1.792 5994.3 /

PLOG / 10 1.143E+18 -1.392 1395.1 /

PLOG / 10 3.490E+22 -2.475 9162.6 /

PLOG / 100 3.224E+18 -1.523 1626.7 /

PLOG / 100 1.261E+24 -2.902 10522.1 /

!Average (max) fitting error: 0.7-0.9% (3.2-3.8%) over T of 250--3000 [K]

DUPLICATE

HCCO+OH=HCOH+CO 2.873E+12 0.370 -24

! Xiong et al., Combust. Flame 161 (2014) 885–897

!assuming 3-HCOH=1-HCOH=HCOH

DUPLICATE

HCCO+OH=CH2O+CO 1.0 0.0 0.0

PLOG / 1 1.187E+21 -2.459 2527.6 /

! PLOG / 10 2.1E08 0.030 97/

! PLOG / 10 -1.6E16 -0.720 4883/

! HH@160426 removed as producing negative rate constant!

PLOG / 100 1.100E+08 0.110 52.0 /

HCCO+OH=OCHCO+H 1.0 0.0 0.0

PLOG / 0.01 2.632E+08 1.410 845 /

PLOG / 0.1 2.632E+08 1.410 845 /

PLOG / 1 2.638E+08 1.410 849 /

PLOG / 10 2.963E+08 1.400 917 /

PLOG / 100 8.190E+08 1.280 1531 /

! Xiong et al., Combust. Flame 161 (2014) 885–897

HCCO+OH=CO2+CH2 1.0 0.0 0.0

! PLOG / 0.01 3.366E+14 -1.400 1240 /

! PLOG / 0.01 -3.258E+17 -2.220 3684 /

```
   ! HH@160426 removed as producing negative rate constant!
PLOG / 0.1        1.698E+15        -1.190    -521 /
PLOG / 0.1        -7.407E+17       -1.920    1686 /
         !        PLOG / 1         9.334E+15        -0.970    -309 /
         !        PLOG / 1         -5.348E+18       -1.740    2024 /
! re-fitting HH@160426:
PLOG/  1.00    7.292E+27   -5.023   2468.0   /
PLOG/  1.00    1.116E+21   -2.280   16960.4 /
!--- Average (max) fitting error: 0.6% (3.2%) over T of 400--3000 [K]
PLOG / 10         5.974E+15        -0.640    363       /
PLOG / 10         -2.577E+19       -1.640    3539 /
         !        PLOG / 100       1.006E+14        0.060     447       /
         !        PLOG / 100       -5.631E+19       -1.510    5657 /
   ! HH@160426 removed as producing negative rate constant!

! Xiong et al., Combust. Flame 161 (2014) 885–897
! ASSUMING 3-CHCOOH = 1-CHCOOH ==fast==> CO2+CH2
DUPLICATE

HCCO+OH=CO2+CH2              1.0              0.0              0.0
PLOG / 0.01       1.018E+19        -2.080    44         /
PLOG / 0.1        1.397E+19        -2.120    88         /
PLOG / 1          7.106E+19        -2.300    824        /
PLOG / 10         1.789E+20        -2.340    2421  /
         !        PLOG / 100       8.190E+02        2.870     -3          /
         !        PLOG / 100       -2.276E+24       -2.700    20416 /
   ! HH@160426 removed as producing negative rate constant!
! Xiong et al., Combust. Flame 161 (2014) 885–897
! ASSUMING 3-CHCOOH = 1-CHCOOH ==fast==> CO2+CH2
DUPLICATE

         ! HCCO+O2=HCO+CO+O                2.2E02   2.690    3540 !
         ! Klippenstein SJ Miller JA Harding LB PCI 29:1209-1217 2002
! HH@160407: including prompt dissociation of HCO (following Labbe et al., J. Phys. Chem. Lett.
2016)
HCCO+O2=HCO+CO+O                2.2E02   2.690    3540
   DUPLICATE
HCCO+O2=HCO+CO+O        -1.317E+12   0.217   23467.3
   DUPLICATE
```

```
HCCO+O2=H+CO+CO+O          1.317E+12   0.217   23467.3



! ------------- C2O ...
C2O+M=C+CO+M                        2.0E15   0.000   44200 !
! Fridriechs, G.; Wagner, H.Gg. Z. Phys. Chem. 203, 1-14, 1998.
!
!
C2O+O2=CO+CO2                       1.0E13   0.000    2600 !
! Becker KH Konig R Meuser R Wiesen P Bayes KD J Photochem Photobiol A 64:1-14 1992
! Williamson DG Bayes KD JACS 89:3390 1967
!
C2O+C=CO+C2                         1.0E14   0.000       0 !
! Fridriechs, G.; Wagner, H.Gg. Z. Phys. Chem. 203, 1-14, 1998.
! ------------- CH3CH2OOH ...
CH3CH2OOH=CH3CH2O+OH   1  1  1
  PLOG/ 0.1   6.05E58   -14.05   54131 /
  PLOG/ 1.0   9.26E52   -11.91   53378 /
  PLOG/ 100   1.38E33   -5.27    48696 /
! (300-1000 K) from D. Chen et al., J. Phys. Chem. A 115 (2011) 602–611.

CH3CH2OOH+H=CH3CHOOH+H2             6.5E10   0.000    1860
! est CH3OOH+H

CH3CH2OOH+H=CH3CH2OO+H2             4.3E10   0.000    1860
! est CH3OOH+H

CH3CH2OOH+H=CH3CH2O+H2O             1.2E10   0.000    1860
! est CH3OOH+H

CH3CH2OOH+O=CH3CHOOH+OH             1.6E13   0.000    4750
! est  CH3OOH+O

CH3CH2OOH+O=CH3CH2OO+OH             8.7E12   0.000    4750
! est CH3OOH+O

CH3CH2OOH+OH=CH3CHOOH+H2O           7.2E11   0.000    -258
```

```
! est CH3OOH+OH

CH3CH2OOH+OH=CH3CH2OO+H2O          1.1E12   0.000    -437
! est CH3OOH+OH

CH3CH2OOH+HO2=CH3CH2OO+H2O2        4.1E04   2.500   10206
! est CH2O+HO2

CH3CHOOH=CH3CHO+OH                 3.50E12  -0.947     979
   PLOG/1.0                         3.50E12  -0.947     979/
   PLOG/10.0                           3.50E13  -0.947     980/
   PLOG/100.0                          5.75E14  -1.012    1068/
! RAS/GLA08b ING/BOZ03
! ---------- CH3CH2OO ...
CH3CH2OO=CH2CH2OOH                  1          1          1
PLOG/ 0.001              4.29E+08          -0.97      22110 /
PLOG/ 0.003              2.77E+07          -0.52      21990 /
PLOG/ 0.01               3.51E+05          0.16       21700 /
PLOG/ 0.03               1.58E+03          0.99       21290 /
PLOG/ 0.1                6.51E-01          2.17       20650 /
PLOG/ 0.3                4.30E+02          1.31       21600 /
PLOG/ 1                        7.32E-03          2.96       20660 /
PLOG/ 3                        3.79E-08          4.77       19590 /
PLOG/ 10                 7.38E-08          4.78       20030 /
PLOG/ 30                 8.17E-08          4.87       20420 /
PLOG/ 100                2.27E-14          7.09       18990 /
CH3CH2OO+H=CH3CH2O+OH               9.6E13   0.000       0
! est CH3OO+H

CH3CH2OO+O=CH3CH2O+O2               2.850E+10  1.0 -724
! est CH3OO+O

CH3CH2OO+OH=CH3CH2OH+O2                                                1.7E14   0
0
! est CH3OO+OH

CH3CH2OO+HO2=CH3CH2OOH+O2           4.5E11   0.000   -1391
! RAS/GLA08b TYN/WAL01
```

```
CH3CH2OO+CO=CH3CH2O+CO2            1.6E05   2.180   17940
! est CH3OO+CO

CH3CH2OO+CH3=CH3CH2O+CH3O          5.1E12   0.000   -1411
! est CH3OO+CH3

CH3CH2OO+CH4=CH3CH2OOH+CH3         4.7E04   2.500   21000
! est CH4+HO2

CH3CH2OO+CH3OH=CH3CH2OOH+CH2OH      4.0E13   0.000   19400
CH3CH2OO+CH2O=CH3CH2OOH+HCO         4.1E04   2.500   10206
   DUPLICATE
CH3CH2OO+CH2O=CH3CH2OOH+HCO         -2.454E+14   0.027   30133.3
   DUPLICATE
CH3CH2OO+CH2O=CH3CH2OOH+H+CO         2.454E+14   0.027   30133.3

CH3CH2OO+C2H5=CH3CH2O+CH3CH2O       5.1E12   0.000   -1411
! est CH3OO+CH3

CH3CH2OO+C2H6=CH3CH2OOH+C2H5        8.6E00   3.760   17200
! RAS/GLA08b CAR/DEA05

CH3CH2OO+CH3CHO=CH3CH2OOH+CH3CO     2.4E19  -2.200   14030
! est CH3CHO+HO2

CH3CH2OO+CH3CHO=CH3CH2OOH+CH2CHO    2.3E11   0.400   14864
! est CH3CHO+HO2

CH3CH2OO+CH3CH2OO=CH3CH2O+CH3CH2O+O2 2.9E11  -0.270     408
! RAS/GLA08b FEN/LIG93

CH3CH2OO+CH3CH2OO=CH3CHO+CH3CH2OH+O2 4.3E09   0.000    -850
! RAS/GLA08b FEN/LIG93

! ---------- CH2CH2OOH ...
CH2CH2OOH=cC2H4O+OH    1 1 1
  PLOG/0.01316              3.342E+27          -6.117    15373.90/
  PLOG/0.98692              4.361E+28          -5.830    17202.08/
```

```
 PLOG/9.86923              2.689E+32         -6.633    20310.67/
 PLOG/98.69233             7.544E+35         -7.331    23906.80/
 PLOG/1000   6.672E+10 0.637     15974.18/
! J. Zador, S. J. Klippenstein, J. A. Miller, J. Phys. Chem. A 115 (2011) 10218–10225.
! ---------- CH2CHOOH ...
CH2CHOOH=CH2CHO+OH               2.0E35       -6.700   47450
          PLOG/1.00                                2.0E35   -6.700   47450/
          PLOG/10.0                                                  1.12E28   -4.15    46190/
          PLOG/50.0                          2.8E26            -3.500   46340/
          PLOG/100.0                      2.22E17       -0.42    44622/
          ! est CH3OOH
CH2CHOOH+H=CH2CHOO+H2            4.3E10   0.000    1860
! est CH3OOH+H

CH2CHOOH+H=CH2CHO+H2O            1.2E10   0.000    1860
! est CH3OOH+H

CH2CHOOH+O=CH2CHOO+OH            8.7E12   0.000    4750
! est CH3OOH+O

CH2CHOOH+OH=CH2CHOO+H2O          1.1E12   0.000    -437
! est CH3OOH+OH

CH2CHOOH+HO2=CH2CHOO+H2O2        4.1E04   2.500   10206
! est CH2O+HO2
! ---------- CH2CHOO ...
CH2CHOO=CHCHO+OH           5.89E+36      -7.10    51440.0
 PLOG/1.000E-02    3.64E+49     -12.13    67420.0/
 PLOG/1.000E-02    1.17E+56     -14.81    60700.0/
 PLOG/1.000E-01    1.44E+36      -9.92    41220.0/
 PLOG/1.000E-01    2.32E+40      -9.39    50420.0/
 PLOG/3.160E-01    4.18E+40     -10.53    43670.0/
 PLOG/3.160E-01    1.61E+43      -9.99    50290.0/
 PLOG/1.000E+00    3.79E+46     -10.72    51900.0/
 PLOG/1.000E+00    2.33E+124     -36.77    70100.0/
 PLOG/3.160E+00    1.60E+49     -11.24    54150.0/
 PLOG/3.160E+00    1.88E+103     -29.49    65410.0/
 PLOG/1.000E+01    2.38E+51     -11.64    56980.0/
```

PLOG/1.000E+01 5.96E+86 -23.81 62170.0/
PLOG/3.160E+01 2.00E+54 -12.22 61840.0/
PLOG/3.160E+01 1.51E+57 -13.94 55390.0/
PLOG/1.000E+02 9.54E+195 -52.27 163500.0/
PLOG/1.000E+02 1.79E+34 -6.40 50000.0/
! Goldsmith et al., 2015, J. Phys. Chem. A 2015, 119, 7766-7779 (DOI: 10.1021/acs.jpca.5b01088)
CH2CHOO=CH2CHO+O 1.22E+29 -4.71 42340.0
PLOG/1.000E-02 2.70E+180 -48.19 169300.0/
PLOG/1.000E-02 1.47E+30 -6.64 41110.0/
PLOG/1.000E-01 3.90E+38 -8.69 42770.0/
PLOG/1.000E-01 9.65E-12 5.96 22890.0/
PLOG/3.160E-01 4.57E+47 -11.21 47050.0/
PLOG/3.160E-01 3.95E+22 -3.71 36270.0/
PLOG/1.000E+00 7.62E+81 -21.28 65080.0/
PLOG/1.000E+00 2.39E+33 -6.62 41280.0/
PLOG/3.160E+00 1.86E+68 -16.83 60680.0/
PLOG/3.160E+00 6.37E+31 -5.96 41260.0/
PLOG/1.000E+01 2.02E+55 -12.69 55840.0/
PLOG/1.000E+01 2.13E+29 -5.10 40710.0/
PLOG/3.160E+01 1.11E+53 -11.79 56690.0/
PLOG/3.160E+01 4.66E+27 -4.50 40530.0/
PLOG/1.000E+02 4.30E+48 -10.31 56090.0/
PLOG/1.000E+02 5.99E+25 -3.85 40120.0/
! Goldsmith et al., 2015, J. Phys. Chem. A 2015, 119, 7766-7779 (DOI: 10.1021/acs.jpca.5b01088)
CH2CHOO=OCHCHO+H 4.72E+20 -2.69 32320.0
PLOG/1.000E-02 6.41E+80 -22.20 51750.0/
PLOG/1.000E-02 1.19E+28 -6.01 28740.0/
PLOG/1.000E-01 3.31E+65 -17.01 48090.0/
PLOG/1.000E-01 1.40E+25 -4.80 28940.0/
PLOG/3.160E-01 5.98E+51 -12.62 43000.0/
PLOG/3.160E-01 2.91E+20 -3.29 27550.0/
PLOG/1.000E+00 1.48E+44 -10.12 40790.0/
PLOG/1.000E+00 1.58E+19 -2.82 27620.0/
PLOG/3.160E+00 1.26E+59 -14.33 51390.0/
PLOG/3.160E+00 1.93E+22 -3.54 29980.0/
PLOG/1.000E+01 4.93E+26 -4.67 34320.0/
PLOG/1.000E+01 7.51E+29 -5.75 34490.0/
PLOG/3.160E+01 2.06E+33 -6.38 39520.0/

PLOG/3.160E+01 7.14E+61 -16.16 43280.0/
PLOG/1.000E+02 1.30E+32 -5.92 40660.0/
PLOG/1.000E+02 1.14E+19 -2.56 29670.0/
! Goldsmith et al., 2015, J. Phys. Chem. A 2015, 119, 7766-7779 (DOI: 10.1021/acs.jpca.5b01088)
CH2CHOO=CH2CO+OH 1.55E+24 -3.87 49850.0
PLOG/1.000E-02 1.15E+47 -12.28 75330.0/
PLOG/1.000E-02 2.31E+02 -0.73 25710.0/
PLOG/1.000E-01 8.43E+09 -2.06 33720.0/
PLOG/1.000E-01 1.83E-23 7.84 20190.0/
PLOG/3.160E-01 6.06E+04 0.17 34220.0/
PLOG/3.160E-01 3.82E+63 -20.44 43420.0/
PLOG/1.000E+00 1.51E+19 -3.61 43060.0/
PLOG/1.000E+00 3.18E+27 -7.76 37230.0/
PLOG/3.160E+00 2.13E+33 -7.39 51610.0/
PLOG/3.160E+00 2.32E-05 3.47 31560.0/
PLOG/1.000E+01 4.44E+36 -7.99 54680.0/
PLOG/1.000E+01 1.06E-01 2.64 34160.0/
PLOG/3.160E+01 1.19E+37 -7.80 56460.0/
PLOG/3.160E+01 5.62E+02 1.70 36450.0/
PLOG/1.000E+02 9.08E+35 -7.21 57550.0/
PLOG/1.000E+02 1.11E+07 0.52 38670.0/
! Goldsmith et al., 2015, J. Phys. Chem. A 2015, 119, 7766-7779 (DOI: 10.1021/acs.jpca.5b01088)
CH2CHOO=CH2O+HCO 1.19E+20 -2.29 30170.0
PLOG/1.000E-02 1.66E+174 -55.52 60320.0/
PLOG/1.000E-02 2.27E+35 -7.97 31280.0/
PLOG/1.000E-01 9.03E+66 -17.25 48120.0/
PLOG/1.000E-01 2.08E+26 -4.96 28780.0/
PLOG/3.160E-01 1.82E+43 -9.87 37960.0/
PLOG/3.160E-01 1.45E+20 -3.08 26630.0/
PLOG/1.000E+00 8.64E+33 -6.88 34370.0/
PLOG/1.000E+00 1.06E+130 -39.38 54700.0/
PLOG/3.160E+00 7.29E+171 -43.53 191900.0/
PLOG/3.160E+00 2.35E+34 -6.87 35700.0/
PLOG/1.000E+01 1.03E+32 -6.06 35500.0/
PLOG/1.000E+01 2.18E+175 -53.78 68500.0/
PLOG/3.160E+01 1.85E+34 -6.57 38510.0/
PLOG/3.160E+01 1.07E+185 -54.22 88990.0/
PLOG/1.000E+02 5.70E+29 -5.19 36800.0/

PLOG/1.000E+02 4.68E+02 1.81 18100.0/

! Goldsmith et al., 2015, J. Phys. Chem. A 2015, 119, 7766-7779 (DOI: 10.1021/acs.jpca.5b01088)

CH2CHOO=CH2O+H+CO 1.19E+20 -2.29 30170.0

PLOG/1.000E-02 3.88E+174 -55.52 60320.0/

PLOG/1.000E-02 5.29E+35 -7.97 31280.0/

PLOG/1.000E-01 2.11E+67 -17.25 48120.0/

PLOG/1.000E-01 4.85E+26 -4.96 28780.0/

PLOG/3.160E-01 4.26E+43 -9.87 37960.0/

PLOG/3.160E-01 3.37E+20 -3.08 26630.0/

PLOG/1.000E+00 2.02E+34 -6.88 34370.0/

PLOG/1.000E+00 2.46E+130 -39.38 54700.0/

PLOG/3.160E+00 1.70E+172 -43.53 191900.0/

PLOG/3.160E+00 5.49E+34 -6.87 35700.0/

PLOG/1.000E+01 2.40E+32 -6.06 35500.0/

PLOG/1.000E+01 5.09E+175 -53.78 68500.0/

PLOG/3.160E+01 4.32E+34 -6.57 38510.0/

PLOG/3.160E+01 2.49E+185 -54.22 88990.0/

PLOG/1.000E+02 1.33E+30 -5.19 36800.0/

PLOG/1.000E+02 1.09E+03 1.81 18100.0/

! Goldsmith et al., 2015, J. Phys. Chem. A 2015, 119, 7766-7779 (DOI: 10.1021/acs.jpca.5b01088)

CH2CHOO=CO+CH3O 1.16E-01 3.16 18420.0

PLOG/1.000E-02 5.20E+33 -7.92 31320.0/

PLOG/1.000E-02 2.31E+129 -41.86 45850.0/

PLOG/1.000E-01 1.26E+98 -27.09 64060.0/

PLOG/1.000E-01 2.42E+28 -5.99 30540.0/

PLOG/3.160E-01 1.80E+33 -7.27 33760.0/

PLOG/3.160E-01 8.69E-50 16.63 -3900.0/

PLOG/1.000E+00 3.83E+33 -7.20 35100.0/

PLOG/1.000E+00 1.19E-39 13.61 -1317.0/

PLOG/3.160E+00 1.28E+79 -19.61 74870.0/

PLOG/3.160E+00 8.80E+86 -23.08 61010.0/

PLOG/1.000E+01 4.07E+32 -6.62 37210.0/

PLOG/1.000E+01 1.27E+03 1.44 18660.0/

PLOG/3.160E+01 6.86E+44 -10.04 47030.0/

PLOG/3.160E+01 1.97E+17 -2.23 28590.0/

PLOG/1.000E+02 -1.07E+04 1.33 15620.0/

PLOG/1.000E+02 1.16E-07 4.81 12010.0/

! Goldsmith et al., 2015, J. Phys. Chem. A 2015, 119, 7766-7779 (DOI: 10.1021/acs.jpca.5b01088)

CH2CHOO=CO2+CH3 6.03E-03 3.46 17420.0
PLOG/1.000E-02 5.09E+33 -7.95 31290.0/
PLOG/1.000E-02 4.20E+122 -39.75 43640.0/
PLOG/1.000E-01 1.21E+118 -33.13 73790.0/
PLOG/1.000E-01 1.96E+29 -6.29 30920.0/
PLOG/3.160E-01 8.56E+32 -7.21 33550.0/
PLOG/3.160E-01 5.10E-66 21.37 -11110.0/
PLOG/1.000E+00 3.27E+33 -7.22 34990.0/
PLOG/1.000E+00 1.76E-47 15.85 -5283.0/
PLOG/3.160E+00 3.49E-79 25.01 -21020.0/
PLOG/3.160E+00 3.82E+32 -6.80 35690.0/
PLOG/1.000E+01 8.16E+32 -6.76 37270.0/
PLOG/1.000E+01 4.62E+00 2.10 17170.0/
PLOG/3.160E+01 7.01E+37 -8.06 42200.0/
PLOG/3.160E+01 3.49E+14 -1.58 26470.0/
PLOG/1.000E+02 -2.51E+03 1.41 14420.0/
PLOG/1.000E+02 4.05E-09 5.14 10480.0/
! Goldsmith et al., 2015, J. Phys. Chem. A 2015, 119, 7766-7779 (DOI: 10.1021/acs.jpca.5b01088)

CH2CHOO+H=CH2CHO+OH 9.6E13 0.000 0 !
! est CH3OO+H=CH3O+OH

CH2CHOO+O=CH2CHO+O2 1.6E13 0.000 -145 !
! est CH3OO+O=CH3O+O2

CH2CHOO+OH=CH2CHOH+O2 2.0E15 -0.600 0 !
! est CH3OO+OH=CH3OH+O2

CH2CHOO+OH=CH2CHO+HO2 4.0E11 0.600 0 !
! est H3OO+OH=CH3O+HO2

CH2CHOO+HO2=CH2CHOOH+O2 4.5E11 0.000 -1391 !
! est CH3CH2OO+HO2

```
CH2CHOO+CO=CH2CHO+CO2              1.6E05   2.180   17940 !
! est CH3OO+CO=CH3O+CO2


CH2CHOO+CH3=CH2CHO+CH3O            5.1E12   0.000   -1411 !
! est CH3OO+CH3=CH3O+CH3O

CH2CHOO+CH4=CH2CHOOH+CH3           4.7E04   2.500   21000 !
! est CH4+HO2=CH3+H2O2

CH2CHOO+CH3OH=CH2CHOOH+CH2OH       4.0E13   0.000   19400 !
! est CH3OO+CH3OH=CH3OOH+CH2OH

        ! CH2CHOO+CH2O=CH2CHOOH+HCO          4.1E04   2.500   10206
        ! est CH3OO+CH2O
        ! HH@160407: including prompt dissociation of HCO (following Labbe et al., J. Phys. Chem. Lett. 2016)
CH2CHOO+CH2O=CH2CHOOH+HCO          4.1E04   2.500   10206 ! GIM/GLA09 CH3OO+CH2O
   DUPLICATE
CH2CHOO+CH2O=CH2CHOOH+HCO         -2.454E+14   0.027   30133.3
   DUPLICATE
CH2CHOO+CH2O=CH2CHOOH+H+CO         2.454E+14   0.027   30133.3

CH2CHOO+C2H6=CH2CHOOH+C2H5         8.6E00   3.760   17200
! est CH3CH2OO+C2H6


! ---------- OCHCHO ...

OCHCHO=CH2O+CO                  8.0E55  -12.600  76713 !1.0 bar, 800 K < T < 2500 K
 PLOG/ 0.009869                 4.2E53  -12.500  70845/
 PLOG/ 0.04935                  5.1E54  -12.600  73012/
 PLOG/ 0.09869                  1.0E55  -12.600  73877/
 PLOG/ 0.4935                   4.5E55  -12.600  75869/
 PLOG/ 0.9869                   8.0E55  -12.600  76713/
 PLOG/ 4.935                    1.1E56  -12.200  77643/
 PLOG/ 9.869                    5.5E56  -12.600  79964/
```

! Friedrichs G. Colberg M. Dammeier J. Bentz T. Olzmann M. Phys. Chem. Chem. Phys. 10 (2008) 6520-6533.

!

OCHCHO=HCOH+CO 2.6E57 -13.200 79754 ! 1.0 bar, 800 K < T < 2500 K

PLOG/ 0.009869 8.4E52 -12.600 72393/

PLOG/ 0.04935 8.3E54 -12.900 75113/

PLOG/ 0.09869 4.4E55 -13.000 76257/

PLOG/ 0.4935 1.3E57 -13.200 78851/

PLOG/ 0.9869 2.6E57 -13.200 79754/

PLOG/ 4.935 1.0E57 -12.900 81161/

PLOG/ 9.869 5.7E59 -13.300 83539/

! Friedrichs G. Colberg M. Dammeier J. Bentz T. Olzmann M. Phys. Chem. Chem. Phys. 10 (2008) 6520-6533.

!

OCHCHO=CO+CO+H2 6.1E57 -13.100 80147 ! 1.0 bar, 800 K < T < 2500 K

PLOG/ 0.009869 6.0E51 -12.100 71854/

PLOG/ 0.04935 1.4E54 -12.500 74751/

PLOG/ 0.09869 1.8E55 -12.700 76137/

PLOG/ 0.4935 1.3E57 -13.000 78972/

PLOG/ 0.9869 6.1E57 -13.100 80147/

PLOG/ 4.935 5.8E57 -12.900 81871/

PLOG/ 9.869 3.4E59 -13.300 84294/

! Friedrichs G. Colberg M. Dammeier J. Bentz T. Olzmann M. Phys. Chem. Chem. Phys. 10 (2008) 6520-6533.

!

OCHCHO=HCO+HCO 1.9E57 -12.800 84321 ! 1.0 bar, 800 K < T < 2500 K

PLOG/ 0.009869 1.0E42 -9.700 73534/

PLOG/ 0.04935 6.0E48 -11.100 77462/

PLOG/ 0.09869 1.7E51 -11.600 79111/

PLOG/ 0.4935 5.3E55 -12.500 82774/

PLOG/ 0.9869 1.9E57 -12.800 84321/

PLOG/ 4.935 2.2E59 -13.100 87258/

PLOG/ 9.869 3.0E60 -13.300 88993/

! Friedrichs G. Colberg M. Dammeier J. Bentz T. Olzmann M. Phys. Chem. Chem. Phys. 10 (2008) 6520-6533.

! OCHCHO+H=CH2O+HCO 5.4E13 0.000 4300 !

! Colberg, M., Friedrichs, G. J. Phys. Chem. A 110 (2006) 160-170.

! HH@160407: including prompt dissociation of HCO (following Labbe et al., J. Phys. Chem. Lett. 2016)

OCHCHO+H=CH2O+H+CO 3.232E+23 -2.473 24227.3

OCHCHO+O=OCHCO+OH 4.2E11 0.570 2760 !

! est CH2O+O

!

OCHCHO+OH=OCHCO+H2O 4.0E06 2.000 -1630 !

! Feierabend, K.J., Zhu, L., Talukdar, R.K., Burkholder, J.B. J. Phys. Chem. A 112 (2008) 73-82.

!

!OCHCHO+HO2=>HOCH(OO)CHO 1.3E31 -7.532 1440 !

!HOCH(OO)CHO => OCHCHO+HO2 1.9E29 -5.781 15790 !

!HOCH(OO)CHO => HOCHO+CO+OH 1.6E10 0.051 15190 !

! da Silva, G. J. Phys. Chem. A 115 (2011) 191-197.

OCHCHO+HO2=HOCHO+CO+OH 3.3E-4 3.995 300 !

! da Silva, G. J. Phys. Chem. A 115 (2011) 191-197.

OCHCHO+HO2=OCHCO+H2O2 4.1E04 2.500 10206 !

! est CH2O+HO2

OCHCHO+O2=OCHCO+HO2 2.4E05 2.500 36461 !

! est CH2O+O2

! OCHCO=HCO+CO 4.1E14 0.000 8765 ! 1.0 atm

! PLOG/ 0.01 3.8E12 0.000 8610/

! PLOG/ 0.1 3.8E13 0.000 8665/

! PLOG/ 1.0 4.1E14 0.000 8765/

! ! kinf 1.1E14 0.133 10140 !

! ! da Silva, G. Phys. Chem. Chem. Phys. 12 (2010) 6698-6705.

! HH@160407: including prompt dissociation of HCO (following Labbe et al., J. Phys. Chem. Lett. 2016)

OCHCO=HCO+CO 4.100E+14 0.000 8765.0

PLOG/ 1.000E-02 3.800E+12 0.000 8610.0 /

PLOG/ 1.000E-02 -7.988E+21 -2.359 27419.6 /

PLOG/ 1.000E-01 3.800E+13 0.000 8665.0 /

PLOG/ 1.000E-01 -2.275E+23 -2.473 28592.3 /

PLOG/ 1.000E+00 4.100E+14 0.000 8765.0 /

PLOG/ 1.000E+00 -2.454E+24 -2.473 28692.3 /

PLOG/ 1.000E+02 1.100E+14 0.133 10140.0 /

PLOG/ 1.000E+02 -1.391E+24 -2.419 30990.9 /

OCHCO=H+CO+CO 2.454E+24 -2.473 28692.3

```
PLOG/     1.000E-02   7.988E+21   -2.359   27419.6 /
PLOG/     1.000E-01   2.275E+23   -2.473   28592.3 /
PLOG/     1.000E+00   2.454E+24   -2.473   28692.3 /
PLOG/     1.000E+02   1.391E+24   -2.419   30990.9 /

OCHCO+O2=CO+CO2+OH                3.3E14   0.000    2075 ! 1.0 atm
 PLOG/  0.01                       1.6E14   0.000    1540/
 PLOG/  0.1                        1.1E14   0.000    1300/
 PLOG/  1.0                        3.3E14   0.000    2075/
! kinf                           3.4E04   1.929     344 !
! da Silva, G. Phys. Chem. Chem. Phys. 12 (2010) 6698-6705.
! ---------- HOCHO ...
CH2O+OH=HOCH2O                                                                  6.3E06   1.63
          4282
! Xu, et al., Int. J. Chem. Kinet. 38 (2006) 322–326:
HOCH2O=HOCHO+H                    1.000E+14  0.00  1.490E+04
! Z. Zhao, M. Chaos, A. Kazakov, F. L. Dryer, Int. J. Chem. Kinet. 40 (2008) 1–18.

HOCHO(+M)=CO+H2O(+M)              7.5E14   0.000   68710 !
 LOW  /4.1E15 0 52980/                        !
! J.-G. Chang, H.-T. Chen, S. Xu, M.C. Lin, J. Phys. Chem. A 111 (2007) 6789-6797.
!
HOCHO(+M)=CO2+H2(+M)              4.5E13   0.000   68240 !
 LOW  /1.7E15 0 51110/                          !
! J.-G. Chang, H.-T. Chen, S. Xu, M.C. Lin, J. Phys. Chem. A 111 (2007) 6789-6797.
!
HOCHO+H=HOCO+H2                   2.3E02   3.272    4858 !
! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.
!
HOCHO+H=OCHO+H2                   4.2E05   2.255   14091 !
! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.
!
HOCHO+O=HOCO+OH                   5.1E01   3.422    4216 !
! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.
!
HOCHO+O=OCHO+OH                   1.7E05   2.103    9880 !
! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.
!
HOCHO+OH=HOCO+H2O                 7.8E-6   5.570   -2365 !
```

! J.M. Anglada, J. Am. Chem. Soc. 126 (2004) 9809-9820.

! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.

!

HOCHO+OH=OCHO+H2O 4.9E-5 4.910 -5067 !

! J.M. Anglada, J. Am. Chem. Soc. 126 (2004) 9809-9820.

! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.

!

HOCHO+HO2=HOCO+H2O2 4.7E-1 3.975 16787 !

! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.

!

HOCHO+HO2=OCHO+H2O2 3.9E01 3.080 25206 !

! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.

!

HOCO+HO2=HOCHO+O2 4.0E11 0.000 0 !

! H.G. Yu, G. Poggi, J.S. Francisco, J.T. Muckerman, J. Chem. Phys. 129 (2008) 214307.

!

HOCHO+O2=OCHO+HO2 3.0E13 0.000 63000 !

! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.

! ---------- OCHO ...

OCHO=CO2+H 1.0E10 0.000 0 !

! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.

!

OCHO+O2=CO2+HO2 5.0E13 0.000 0 !

! P. Marshall, P. Glarborg, Proc. Combust. Inst. 35 (2015) 153-160.

! ---------- CH3C(O)OOH ...

CH3C(O)OOH=CH3C(O)O+OH 5.0E14 0.000 40142 !

! Sahetchian, K.A.; Rigny, R.; Tardieu de Maleissye, J.; Batt, L.; Anwar Khan, M.; Mathews, S., Proc. Combust. Inst. 24, 637-643, 1992.

!

CH3C(O)OOH+H=CH3C(O)OO+H2 5.4E10 0.000 1860 !

! est ch3ooh+h

!

CH3C(O)OOH+O=CH3C(O)OO+OH 8.7E12 0.000 4750 !

! est ch3ooh+o

!

CH3C(O)OOH+OH=CH3C(O)OO+H2O 1.1E12 0.000 -437 !

! est ch3ooh+o

!

CH3C(O)OOH+HO2=CH3C(O)OO+H2O2 4.1E04 2.500 10206 !

! est ch2o+ho2

!

CH3C(O)OO+H=CH3C(O)O+OH 1.0E14 0.000 0 !

! est ch3oo+h

!

CH3C(O)OO+O=CH3+CO2+O2 5.0E12 0.000 0 !

! A. Miyoshi, H. Matsui, N. Washida, J. Phys. Chem. 1989, 93, 5813-5818.

! est

!

CH3C(O)OO+O=CH3O+CO+O2 1.5E13 0.000 0 !

! A. Miyoshi, H. Matsui, N. Washida, J. Phys. Chem. 1989, 93, 5813-5818.

! est

!

CH3C(O)OO+OH=CH3C(O)O+HO2 4.0E11 0.600 0 !

! est ch3oo+oh

!

CH3C(O)OO+HO2=CH3C(O)O+OH+O2 1.9E11 0.000 -1950 !

! C.B.M. Gross, T.J. Dillon, G. Schuster, J. Lelieveld, J. N. Crowley, J. Phys. Chem. A 2014, 118, 974-985.

! R. Atkinson, D.L. Baulch, R.A. Cox, J.N. Crowley, R.F. Hampson, R.G. Hynes, M.E. Jenkin, M.J. Rossi, J. Troe, Atmos. Chem. Phys., 6, 3625-4055, 2006

!

CH3C(O)OO+HO2=CH3C(O)OOH+O2 1.2E11 0.000 -1950 !

! C.B.M. Gross, T.J. Dillon, G. Schuster, J. Lelieveld, J. N. Crowley, J. Phys. Chem. A 2014, 118, 974-985.

! R. Atkinson, D.L. Baulch, R.A. Cox, J.N. Crowley, R.F. Hampson, R.G. Hynes, M.E. Jenkin, M.J. Rossi, J. Troe, Atmos. Chem. Phys., 6, 3625-4055, 2006

!

CH3C(O)OO+CH3O2=CH3C(O)O+CH3O+O2 1.1E12 0.000 -1000 !

! R. Atkinson, D.L. Baulch, R.A. Cox, J.N. Crowley, R.F. Hampson, R.G. Hynes, M.E. Jenkin, M.J. Rossi, J. Troe, Atmos. Chem. Phys., 6, 3625-4055, 2006

!

!CH3C(O)OO+CH3O2=CH3C(O)OH+CH2O+O2 1.2E11 0.000 -1000 !

! R. Atkinson, D.L. Baulch, R.A. Cox, J.N. Crowley, R.F. Hampson, R.G. Hynes, M.E. Jenkin, M.J. Rossi, J. Troe, Atmos. Chem. Phys., 6, 3625-4055, 2006

!

CH3CHO+CH3C(O)OO=CH3CO+CH3C(O)OOH 1.7E13 0.000 16293 !

! est ch3cho+ho2

!

CH3CHO+CH3C(O)OO=CH2CHO+CH3C(O)OOH 1.1E13 0.000 23248 !

! est ch3cho+ho2

!

CH3C(O)O=CH3+CO2 2.2E11 0.290 4579 !

! Zhou, Y.Z.; Li, S.; Li, Q.S.; Zhang, S.W. J. Mol. Struct. Theochem 854, 40-45, 2008

HOCH2CH2OO=CH2O+CH2O+OH 2.0E15 -2.030 15913.0 ! 1 atm

PLOG/ 1.30E-02 5.6E13 -1.900 14338.0/

PLOG/ 1.00E-01 2.2E14 -1.920 14870.0/

PLOG/ 1.00E+00 2.0E15 -2.030 15913.0/

PLOG/ 1.00E+01 5.0E16 -2.260 17552.0/

PLOG/ 1.00E+02 3.8E18 -2.600 19972.0/

! Zador J Fernandes RX Georgievskii Y Meloni G Taatjes CA Miller JA Proc Combust Inst 2009 32 271-277

HOCH2CH2OO=CH2CHOH+HO2 1.4E10 -0.780 14836 ! 1 atm

PLOG/ 1.30E-02 2.0E09 -1.010 13160.0/

PLOG/ 1.00E-01 2.1E09 -0.810 13598.0/

PLOG/ 1.00E+00 1.4E10 -0.780 14836.0/

PLOG/ 1.00E+01 8.5E11 -1.010 17045.0/

PLOG/ 1.00E+02 5.8E14 -1.510 20561.0/

! Zador J Fernandes RX Georgievskii Y Meloni G Taatjes CA Miller JA Proc Combust Inst 2009 32 271-277

HOCH2CH2OO+HO2=>CH2OOH+CH2OH+O2 2.5E11 0.000 -1490

! GIM/GLA09 est CH3OO+HO2

HOCH2CH2OO+CH2O=>CH2OOH+CH2OH+HCO 4.1E04 2.500 10206

! GIM/GLA09 CH2O+HO2

HOCH2CH2OO+C2H4=>CH2O+CH2OH+CH3CHO 2.2E12 0.000 17200

! JIM/GLA08 est=C2H4+HO2

! Nuevas ARTICULO H-C-S

SH+CH3=CH2S+H2 1.018E+12 0.000 0.000 ! No afecta

!H2S=SH+H 4.6E14 0.00 82155.00 ! Importante

!H2S=SH+H 4.E14 0.00 82155.00 ! Importante

!H2S+M=SH+H+M 1.76E16 0.00 66200.00 ! Nemirovskii 1990

!H2S=SH+H 1.0E2 0.0 0.0

!H2S+H=SH+H2 1.078E13 0.00 2969.67

!SH+CH3=CH3SH 9.998E12 0.00 0.00

!SH+CH3=H2+CH2S 1.018E12 0.00 0.00

!H+CH3SH=CH3+H2S 6.929E12 0.00 1664.00

!H+CH3SH=CH3S+H2 2.903E13 0.00 2593.00

H+CH3S=CH2S+H2 1.988E13 0.00 0.00 ! No afecta

H+CH2S=HCS+H2 5.252E12 1.77 2989.29 ! Afecta minimamente

H+HCS=H2+CS 1.211E14 0.00 0.00 ! No afecta

!SH+CS=H+CS2 3.232E10 1.5 495.00

!H+SH=H2+S 1.301E13 0.0 0.00

!CH4+S=CH3+SH 2.042E14 0.0 19796

!H2S+S=SH+SH 5.704E14 0.00 15045.00

!S+S+M=S2+M 1.2E17 -1.00 0.00

!SH+S=S2+H 2.409E13 0.00 0.00

!SH+SH=H2+S2 3.012E10 0.00 0.00

! Clayton R. 2018

!H2O+H2O=H+OH+H2O 1.01E+26 -2.4 120180

!O+O2+M=O3+M 1.88E+21 -2.8 0

!O+O3=O2+O2 4.80E+12 0 4090

!H+O3=OH+O2 8.43E+13 0 950

!OH+O3=HO2+O2 1.14E+12 0 2000

!HO2+O3=OH+O2+O2 8.43E+09 0 1200

HSO+SH=SO+H2S 1.00E+13 0 0

!HOSO(+M)=OH+SO(+M) 9.90E+21 -2.5 75891

!LOW /1.2E46 -9.020 52953/

! TROE/0.95 2989 1.1/

!! Ningun efecto las de CS de abajo

CS2+OH(+M)=>CS2OH(+M) 4.80E+12 0 0

LOW / 2.9E17 0 0 /

CS2OH(+M)=>CS2+OH(+M) 1.60E+13 0 10250

LOW / 9.6E17 0.0 10250/

CS2+O2=COS+SO 1.60E+13 0 61600

CS2+O2=COS+SO(S) 3.60E+11 0 35574

CS2+S(+M)=CS3(+M) 1.30E+12 0 0

LOW / 2.5E21 -1.600 0 /

CS2+SO=CS+S2O 1.00E+12 0 10000

CS2+SO2=COS+S2O 7.80E+12 0 48600

CS+OH=COS+H 1.00E+14 0 0

CS+OH=CO+SH 2.00E+13 0 0

CS+O3=COS+O2 4.50E+12 0 6000

CS+COS=CS2+CO 2.00E+12 0 37700

CS+SO=COS+S 3.60E+05 2.2 3465

CS+SO2=COS+SO 2.70E+12 0 24300

COS+O2=CO+SO2	1.00E+12	0	32000	
COS+SO=S2O+CO	2.00E+12	0	37700	
COS2+O=COS+SO	6.00E+13	0	0	
COS2+S=COS+S2	6.00E+13	0	0	
COS2+O2=COS+SO2	1.00E+12	0	0	
CS3+O=CS2+SO	6.00E+13	0	0	
CS3+S=CS2+S2	6.00E+13	0	0	
CS2OH+O2=>COS+HOSO	1.40E+10	0	0	
CS2OH+O2=>HCO+SO2+S	3.00E+09	0	0	
!! C/S				
CH3+H2S2=CH4+HS2	2.20E+13	0	3900	
C2H5+H2S=C2H6+SH	9.90E+11	0	5470	
C2H5+H2S2=C2H6+HS2	1.40E+12	0	2770	
C2H3+H2S2=C2H4+HS2	2.80E+13	0	1360	
C2H3+H2S=C2H4+SH	1.80E+13	0	3900	
CH3SH+O3=CH2S+H2O+O2	3.90E+11	0	14900	
CH3SH+C2H5=CH3S+C2H6	6.70E+11	0	5250	
CH3SH+C2H5=CH2SH+C2H6	7.50E+11	0	7500	
CH3SH+C2H3=C2H4+CH2SH	6.40E+12	0	10400	
CH3SH+C2H3=C2H4+CH3S	1.20E+13	0	3580	
CH2SH+H2S=CH3SH+SH	2.30E+12	0	7620	
CH3S+H2S2=CH3SH+HS2	7.40E+13	0	3730	
CH2SH+H2S2=CH3SH+HS2	1.50E+12	0	3270	
CH3SH+CH2SH=CH3SH+CH3S	1.60E+12	0	6800	
CH3SH+CHS=CH2S+CH2SH	2.50E+13	0	21900	
CH3SH+CHS=CH2S+CH3S	4.90E+12	0	6110	
CH3S+H=CH3+SH	2.00E+13	0	0	
CH3S+OH=CH2S+H2O	1.80E+13	0	0	
CH3S+HO2=CH2S+H2O2	3.00E+11	0	0	
CH3S+CH3=CH2S+CH4	2.40E+13	0	0	
CH3S+SH=CH3SSH	9.00E+11	0.2	-1432	
CH3S+CS=CH3+CS2	5.90E+04	1.7	1080	
C2H6S+H=CH3SH+CH3	5.74E+13	0	6568	
C2H6S+CH3=CH4+C2H5S	1.41E+13	0	15190	
C2H6S+C2H5=C2H6+C2H5S	2.34E+12	0	16002	
C2H6S+CHS=CH2S+C2H5S	4.93E+13	0	21877	
C2H6S+CH2SH=CH3SH+C2H5S	2.03E+12	0	18677	
C2H6S(1)+H=H2S+C2H5	6.31E+13	0	6591.8	

C2H6S(1)+CH3=CH4+C2H5S(1)	1.42E+13	0	13446
C2H6S(1)+CH3=CH4+C2H5S(2)	3.00E+13	0	17674
C2H6S(1)+CH3=CH4+C2H5S(3)	9.78E+12	0	6114.2
C2H6S(1)+C2H5=C2H6+C2H5S(1)	2.09E+12	0	14187
C2H6S(1)+C2H5=C2H6+C2H5S(2)	4.35E+12	0	18892
C2H6S(1)+C2H5=C2H6+C2H5S(3)	6.68E+11	0	5254.4
C2H6S(1)+C2H3=C2H4+C2H5S(1)	1.28E+13	0	8645.8
C2H6S(1)+C2H3=C2H4+C2H5S(2)	2.72E+13	0	12873
C2H6S(1)+C2H3=C2H4+C2H5S(3)	1.21E+13	0	3582.5
C2H6S(1)+SH=H2S+C2H5S(3)	1.20E+14	0	5923.1
C2H6S(1)+HS2=H2S2+C2H5S(3)	1.85E+13	0	17268
C2H6S(1)+CH3S=CH3SH+C2H5S(3)	5.21E+13	0	6902.3
C2H6S(1)+CHS=CH2S+C2H5S(1)	5.15E+13	0	20134
C2H6S(1)+CHS=CH2S+C2H5S(2)	9.62E+13	0	24361
C2H6S(1)+CHS=CH2S+C2H5S(3)	4.89E+12	0	6114.2
C2H6S(1)+CH2SH=CH3SH+C2H5S(1)	2.05E+12	0	16456
C2H6S(1)+CH2SH=CH3SH+C2H5S(2)	7.99E+12	0	22235
C2H6S(1)+CH2SH=CH3SH+C2H5S(3)	1.56E+12	0	6806.8
C2H6S(1)+C2H5S=C2H6S+C2H5S(1)	2.05E+12	0	16456
C2H6S(1)+C2H5S=C2H6S+C2H5S(2)	7.99E+12	0	22235
C2H6S(1)+C2H5S=C2H6S+C2H5S(3)	1.56E+12	0	6806.8
C2H6S(1)+C2H5S(2)=C2H6S(1)+C2H5S(1)	2.09E+12	0	14187
C2H5S+H2S=C2H6S+SH	2.27E+12	0	7618.8
C2H5S+H2S2=C2H6S+HS2	1.51E+12	0	3272
C2H5S+CH3SH=C2H6S+CH3S	1.56E+12	0	6806.8
C2H5S+CH3SSH=C2H6S+CH3S2(1)	7.55E+11	0	3224.3
C2H5S(1)+H2S=C2H6S(1)+SH	4.33E+12	0	6233.6
C2H5S(1)+H2S2=C2H6S(1)+HS2	2.63E+12	0	1719.6
C2H5S(1)+CH3SH=C2H6S(1)+CH3S	3.02E+12	0	5517.1
C2H5S(1)+C2H6S(1)=C2H6S(1)+C2H5S(3)	3.02E+12	0	5517.1
C2H5S(2)=C2H5S(3)	7.94E+01	3	11703
C2H5S(2)=C2H4+SH	3.02E+13	0	8263.7
C2H5S(2)+H2S=C2H6S(1)+SH	9.86E+11	0	5469.3
C2H5S(2)+H2S2=C2H6S(1)+HS2	1.38E+12	0	2770.5
C2H5S(2)+CH3SH=C2H6S(1)+CH3S	6.68E+11	0	5254.4
C2H5S(2)+C2H6S(1)=C2H6S(1)+C2H5S(3)	6.68E+11	0	5254.4
C2H5S(3)=CH2S+CH3	3.98E+15	0	41557
CH3SSH+H=CH3S2(1)+H2	2.22E+04	3.1	-644.9

CH3SSH+CH3=CH3S2+CH4	7.06E+12	0	15190	
CH3SSH+CH3=CH3S2(1)+CH4	1.12E+13	0	3845.2	
CH3SSH+C2H5=C2H6+CH3S2	1.17E+12	0	16002	
CH3SSH+C2H5=CH3S2(1)+C2H6	6.91E+11	0	2722.7	
CH3SSH+C2H3=C2H4+CH3S2	6.39E+12	0	10389	
CH3SSH+C2H3=C2H4+CH3S2(1)	1.38E+13	0	1313.6	
CH3SSH+SH=H2S+CH3S2(1)	1.31E+14	0	3009.3	
CH3SSH+HS2=H2S2+CH3S2(1)	9.51E+12	0	7475.5	
CH3SSH+CH3S=CH3SH+CH3S2(1)	3.69E+13	0	3725.8	
CH3SSH+CH2SH=CH3SH+CH3S2(1)	7.55E+11	0	3224.3	
CH3SSH+CHS=CH2S+CH3S2	2.47E+13	0	21877	
CH3SSH+CHS=CH2S+CH3S2(1)	5.60E+12	0	3845.2	
CH3SSH+C2H5S(1)=C2H6S(1)+CH3S2(1)	1.32E+12	0	1671.8	
CH3SSH+C2H5S(2)=C2H6S(1)+CH3S2(1)	6.91E+11	0	2722.7	
CH3SSH+CH3S2=CH3SSH+CH3S2(1)	7.55E+11	0	3224.3	
CH3S2+H2S=CH3SSH+SH	2.27E+12	0	7618.8	
CH3S2+H2S2=CH3SSH+HS2	1.51E+12	0	3272	
CH3S2+CH3SH=CH3SSH+CH3S	1.56E+12	0	6806.8	
CH3S2+C2H6S=CH3SSH+C2H5S	2.03E+12	0	18677	
CH3S2+C2H6S(1)=CH3SSH+C2H5S(1)	2.05E+12	0	16456	
CH3S2+C2H6S(1)=CH3SSH+C2H5S(2)	7.99E+12	0	22235	
CH3S2+C2H6S(1)=CH3SSH+C2H5S(3)	1.56E+12	0	6806.8	
CH3S2+CH2S2=CH3SSH+CHS2	2.08E+12	0	6090.3	
S2+CH3=CH3S2(1)	1.53E+03	3	23.9	
CH3S2(1)+C2H6S(1)=CH3SSH+C2H5S(3)	1.77E+13	0	17268	
CH3S2(1)+CH2S2=CH3SSH+CHS2	5.06E+13	0	17029	
CH2S2+H=CHS2+H2	1.74E+04	2.9	1402	
CH2S2+C2H5=C2H6+CHS2	8.87E+11	0	4537.9	
CH2S2+C2H3=C2H4+CHS2	1.61E+13	0	2866	
CH2S2+SH=H2S+CHS2	5.28E+13	0	4179.6	
CH2S2+HS2=H2S2+CHS2	5.25E+13	0	17029	
CH2S2+CHS=CH2S+CHS2	6.49E+12	0	5397.7	
CH2S2+CH2SH=CH3SH+CHS2	2.08E+12	0	6090.3	
CH2S2+C2H5S=C2H6S+CHS2	2.08E+12	0	6090.3	
CH2S2+C2H5S(1)=C2H6S(1)+CHS2	4.01E+12	0	4800.6	
CH2S2+C2H5S(2)=C2H6S(1)+CHS2	8.87E+11	0	4537.9	
CHS2=CS2+H	1.14E+14	0	32768	
CHS2+C2H6S(1)=CH2S2+C2H5S(3)	6.97E+13	0	13470	

C2H6S2+CH3=CH4+C2H5S2	1.42E+13	0	13446	
C2H6S2+CH3=CH4+C2H5S2(1)	3.00E+13	0	17674	
C2H6S2+CH3=CH4+C2H5S2(2)	1.12E+13	0	3845.2	
C2H6S2+C2H5=C2H6+C2H5S2	2.09E+12	0	14187	
C2H6S2+C2H5=C2H6+C2H5S2(1)	4.35E+12	0	18892	
C2H6S2+C2H3=C2H4+C2H5S2	1.28E+13	0	8645.8	
C2H6S2+C2H3=C2H4+C2H5S2(1)	2.72E+13	0	12873	
C2H6S2+C2H3=C2H4+C2H5S2(2)	1.38E+13	0	1313.6	
C2H6S2+C2H5=C2H6+C2H5S2(2)	6.91E+11	0	2722.7	
C2H6S2+SH=H2S+C2H5S2(2)	1.31E+14	0	3009.3	
C2H6S2+HS2=H2S2+C2H5S2(2)	9.51E+12	0	7475.5	
C2H6S2+CH3S=CH3SH+C2H5S2(2)	3.69E+13	0	3725.8	
C2H6S2+CH2SH=CH3SH+C2H5S2(2)	7.55E+11	0	3224.3	
C2H6S2+CH2SH=CH3SH+C2H5S2	2.05E+12	0	16456	
C2H6S2+CH2SH=CH3SH+C2H5S2(1)	7.99E+12	0	22235	
C2H6S2+CHS=CH2S+C2H5S2	5.15E+13	0	20134	
C2H6S2+CHS=CH2S+C2H5S2(1)	9.62E+13	0	24361	
C2H6S2+CHS=CH2S+C2H5S2(2)	5.60E+12	0	3845.2	
C2H6S2+C2H5S=C2H6S+C2H5S2	2.05E+12	0	16456	
C2H6S2+C2H5S=C2H6S+C2H5S2(1)	7.99E+12	0	22235	
C2H6S2+C2H5S=C2H6S+C2H5S2(2)	7.55E+11	0	3224.3	
C2H6S2+C2H5S(1)=C2H6S(1)+C2H5S2(2)	1.32E+12	0	1671.8	
C2H6S2+C2H5S(2)=C2H6S(1)+C2H5S2(2)	6.91E+11	0	2722.7	
C2H6S2+CH3S2=CH3SSH+C2H5S2	2.05E+12	0	16456	
C2H6S2+CH3S2=CH3SSH+C2H5S2(1)	7.99E+12	0	22235	
C2H6S2+CH3S2=CH3SSH+C2H5S2(2)	7.55E+11	0	3224.3	
C2H6S2+CH3S2(1)=CH3SSH+C2H5S2(2)	1.39E+14	0	15859	
C2H6S2+CHS2=CH2S2+C2H5S2(2)	8.31E+13	0	10556	
C2H5S2+H2S=C2H6S2+SH	4.33E+12	0	6233.6	
C2H5S2+H2S2=C2H6S2+HS2	2.63E+12	0	1719.6	
C2H5S2+CH3SH=C2H6S2+CH3S	3.02E+12	0	5517.1	
C2H5S2+C2H6S(1)=C2H6S2+C2H5S(1)	3.84E+12	0	15739	
C2H5S2+C2H6S(1)=C2H6S2+C2H5S(2)	1.43E+13	0	21997	
C2H5S2+CH3SSH=C2H6S2+CH3S2(1)	1.32E+12	0	1671.8	
C2H5S2+CH2S2=C2H6S2+CHS2	4.01E+12	0	4800.6	
C2H5S2+C2H6S(1)=C2H6S2+C2H5S(3)	3.02E+12	0	5517.1	
C2H5S2+C2H6S2=C2H6S2+C2H5S2(2)	1.32E+12	0	1671.8	
C2H5S2(1)+H2S=C2H6S2+SH	9.86E+11	0	5469.3	

C2H5S2(1)+H2S2=C2H6S2+HS2 1.38E+12 0 2770.5
C2H5S2(1)+CH3SH=C2H6S2+CH3S 6.68E+11 0 5254.4
C2H5S2(1)+C2H6S(1)=C2H6S2+C2H5S(1) 2.09E+12 0 14187
C2H5S2(1)+C2H6S(1)=C2H6S2+C2H5S(2) 4.40E+12 0 18892
C2H5S2(1)+C2H6S(1)=C2H6S2+C2H5S(3) 6.68E+11 0 5254.4
C2H5S2(1)+CH3SSH=C2H6S2+CH3S2(1) 6.91E+11 0 2722.7
C2H5S2(1)+CH2S2=C2H6S2+CHS2 8.87E+11 0 4537.9
C2H5S2(1)+C2H6S2=C2H6S2+C2H5S2 2.09E+12 0 14187
C2H5S2(1)+C2H6S2=C2H6S2+C2H5S2(2) 6.91E+11 0 2722.7
C2H5S2(2)+C2H6S(1)=C2H6S2+C2H5S(3) 1.77E+13 0 17268
!!
HS2+O2=HSSO+O 1.00E+13 0 26000
HS2+SO3=HSSO+SO2 1.00E+13 0 10000
HS2+HSO=HSSO+SH 1.00E+13 0 7000
S2O+H+M=HSSO+M 6.40E+22 -2.6 287
S2O+HSO2=HSSO+SO2 1.00E+13 0 32000
HSSO+H=S2O+H2 1.00E+13 0 0
HSSO+H=HS2+OH 1.00E+13 0 0
HSSO+O=S2O+OH 1.00E+13 0 0
HSSO+O=SH+SO2 1.00E+13 0 0
HSSO+OH=S2O+H2O 1.00E+13 0 0
HSSO+OH=HS2+HO2 1.00E+13 0 27000
HSSO+HO2=S2O+H2O2 1.00E+13 0 0
HSSO+S=HS2+SO 1.00E+13 0 0
HSSO+S=S2O+SH 1.00E+13 0 0
HSSO+SH=S2O+H2S 1.00E+13 0 0
HSSO+HS2=S2O+H2S2 1.00E+13 0 0
HSSO+S2=S2O+HS2 1.00E+13 0 0
!!!!!******Gersen et al. '17********
!CH3+H2S=CH4+SH 6.8E7 1.2 1434 ! Importante para H2S y SO2
CH3+SH=CH3SH 7.3E12 0.230 -139 ! Importante para H2S y SO2
CH3O2+SH=CH3O+HSO 2.5E7 1.477 -2169 !
CH3OOH+SH=CH3O2+H2S 5.6E3 2.823 8668 !
CH3SH+H=CH3S+H2 1.3E8 1.729 986 !
CH3SH+H=CH2SH+H2 4.1E3 2.925 4750 !
CH3SH+H=CH3+H2S 7.1E10 0.766 3220 !
CH3SH+H=CH4+SH 7.0E6 1.983 16530 !
CH3SH+O=CH3S+OH 4.2E7 1.818 80 !

CH3SH+O=CH2SH+OH 3.3E3 2.864 1224 !

CH3SH+OH=CH3S+H2O 1.3E7 1.770 -1689 !

CH3SH+OH=CH2SH+H2O 1.9E5 2.220 718 !

!CH3SH+HO2=CH3S+H2O2 9.1E12 0.0 14300 !

CH3SH+HO2=CH2SH+H2O2 2.0E11 0.0 14500 !

CH3S+HO2=CH3SH+O2 1.7E-15 7.49 -12060 !

CH3SH+CH3=CH3S+CH4 8.1E5 1.9 1700 !

CH3SH+CH3=CH2SH+CH4 1.5E12 0.0 6500 !

CH3SH+SH=CH3S+H2S 1.2E14 0.0 5920 !

CH3S=CH2S+H 2.5E38 -7.8 62053 !

!CH3S+O2=CH3+SO2 9.5E25 -3.8 12300 !

! ****** CS2 formation

!

CH2S+H=CH2SH 9.5E08 1.700 -700 ! R Van de Vijver, NM Vandewiele, AG Vandeputte, KM Van Geem, M-F Reyniers, WH Green, GB Marin Chem Eng J 278 (2015) 385-393

CH2SH+O2=CH2S+HO2 3.8E10 -0.280 4113 !

DUP

CH2SH+O2=CH2S+HO2 6.1E19 -2.820 5124 !Xin Zheng, J.W. Bozzelli, E.M. Fisher, F.C. Gouldin, Li Zhu, Proc Combust Inst 33 (2011) 467-475.

DUP

CH2S+H=CHS+H2 2.8E07 2.020 7760 !Xin Zheng, J.W. Bozzelli, E.M. Fisher, F.C. Gouldin, Li Zhu, Proc Combust Inst 33 (2011) 467-475.

!CH2S+H=CHS+H2 9.5E04 2.720 3580 ! ! R Van de Vijver, NM Vandewiele, AG Vandeputte, KM Van Geem, M-F Reyniers, WH Green, GB Marin Chem Eng J 278 (2015) 385-393

CH2S+O=CHS+OH 2.1E13 0.000 3000 ! Xin Zheng, J.W. Bozzelli, E.M. Fisher, F.C. Gouldin, Li Zhu, Proc Combust Inst 33 (2011) 467-475.

CH2S+OH=CHS+H2O 5.2E12 0.000 500 !Xin Zheng, J.W. Bozzelli, E.M. Fisher, F.C. Gouldin, Li Zhu, Proc Combust Inst 33 (2011) 467-475.

CH2S+CH3=CHS+CH4 2.3E04 2.370 12280 ! Xin Zheng, J.W. Bozzelli, E.M. Fisher, F.C. Gouldin, Li Zhu, Proc Combust Inst 33 (2011) 467-475.

CHS+H2S=CH2S+SH 7.3E12 0.000 6425 ! R Van de Vijver, NM Vandewiele, AG Vandeputte, KM Van Geem, M-F Reyniers, WH Green, GB Marin Chem Eng J 278 (2015) 385-393

CHS+SH=CH2S2 7.3E12 0.230 -578 ! R Van de Vijver, NM Vandewiele, AG Vandeputte, KM Van Geem, M-F Reyniers, WH Green, GB Marin Chem Eng J 278 (2015) 385-393

CHS+S=CS2+H 2.0E13 0.000 0 ! Xin Zheng, J.W. Bozzelli, E.M. Fisher, F.C. Gouldin, Li Zhu, Proc Combust Inst 33 (2011) 467-475. #161105#

CHS+H2S2=CH2S+HS2 1.1E13 0.000 3900 ! R Van de Vijver, NM Vandewiele, AG Vandeputte, KM Van Geem, M-F Reyniers, WH Green, GB Marin Chem Eng J 278 (2015) 385-393

CHS+S2=CS2+SH 3.0E11 0.000 4000 ! Xin Zheng, J.W. Bozzelli, E.M. Fisher, F.C. Gouldin, Li Zhu, Proc Combust Inst 33 (2011) 467-475. #161105#

CHS+C2H6=CH2S+C2H5 2.0E14 0.000 24360 ! R Van de Vijver, NM Vandewiele, AG Vandeputte, KM Van Geem, M-F Reyniers, WH Green, GB Marin Chem Eng J 278 (2015) 385-393

!CHS+CH4=CH2S+CH3 1.1E14 0.000 26845 ! R Van de Vijver, NM Vandewiele, AG Vandeputte, KM Van Geem, M-F Reyniers, WH Green, GB Marin Chem Eng J 278 (2015) 385-393

!CH2S+CH3=CHS+CH4 1.4E12 0.000 9480 ! VANMAR12

!***Bibliography***

!

! * Abian ea 2015: Abian M, Millera A, Bilbao R, Alzueta MU, FUEL 159, 550-558, 2015

! * Atkinson 2004: Atkinson R, J Atmos Chem Phys, 4, 2004

! * Blitz 2002: Hughes KJ Blitz MA, Proc Combust Inst, 29, 2002

! * Blitz 2006: MA Blitz, J Phys Chem A, 110, 2006

! * Du 2008: Du SY, J Chem Phys, 128, 2008

! * Ellingson ea, JACS2007: Ellingson BA, J Am Chem Soc, 129, 2007

! * Frenklach ea 1981: Frenklach M, Combustion Flame, 41, 1981

! * Gao ea 2011: Y Gao CR Zhou K Sendt BS Haynes P Marshall Proc Combust Inst, 33, 2011

! * Glarborg 1996: P Glarborg, Int J Chem Kinet, 28, 1996

! * Goumri ea 95: Goumri A, J Chem Phys, 102, 1995

! * Goumri ea 99: A Goumri, J.-D.R. Rocha, D. Laakso, C.E. Smith, P. Marshall, J. Phys. Chem. A 1999, 103, 11328-11335.

! * MOU/MORJPCA2013: Mousavipour SH, Hematti O, J Phys Chem A, 117, 2013

! * Lu 2003: Lu C-W Wu Y-J Lee Y-P Zhu RS Lin MC J Phys Chem A, 107, 2003

! * Peng eaJPCA1999: Jingping Peng, J. Phys. Chem. A, 103, 1999

! * Plach/Troe 1994: Plach HJ, Troe J, Int J Chem Kinet, 16, 1984

! * Rasmussen 2007: Rasmussen CL, Proc Combust Inst, 31, 2007

! * Sendt ea 2002: Sendt K Jazbec M Haynes BS PROC COMBUST INST, 29, 2002

! * Sendt ea 2005: Sendt K Haynes BS J PHYS CHEM A 109, 2005

! * Sendt ea 2007: Sendt K Haynes BS Proc Combust Inst, 31, 2007

! * Singleton 1988: Singleton DL Cvetanovic RJ JPCRD 17:1377 1988

! * Song ea 2016: Song Yu, Int J Chem Kinetics, 49, 2016

! * Shiina+98 (9911): Shiina H, J Phys Chem A, 102, 1998

! * Yilmaz 2006: A Yilmaz, J. Phys. Chem. A, 110, 2006

! * Zhou 2009: CR Zhou K Sendt BS Haynes J. Phys. Chem. A 2009, 113, 2975–2981

! * Zhou 2009: CR Zhou K Sendt BS Haynes J. Phys. Chem. A 2009, 112, 3239-3247

!

!

END