



Publication Year	2015
Acceptance in OA @INAF	2020-02-27T13:42:39Z
Title	The 2014 KIDA Network for Interstellar Chemistry
Authors	Wakelam, V.; Loison, J. -C.; Herbst, E.; Pavone, B.; Bergeat, A.; et al.
DOI	10.1088/0067-0049/217/2/20
Handle	http://hdl.handle.net/20.500.12386/23074
Journal	THE ASTROPHYSICAL JOURNAL SUPPLEMENT SERIES
Number	217

THE 2014 KIDA NETWORK FOR INTERSTELLAR CHEMISTRY

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Received 2015 January 15; accepted 2015 February 20; published 2015 March 25

ABSTRACT

Chemical models used to study the chemical composition of the gas and the ices in the interstellar medium are based on a network of chemical reactions and associated rate coefficients. These reactions and rate coefficients are partially compiled from data in the literature, when available. We present in this paper *kida.uva.2014*, a new updated version of the *kida.uva* public gas-phase network first released in 2012. In addition to a description of the many specific updates, we illustrate changes in the predicted abundances of molecules for cold dense cloud conditions as compared with the results of the previous version of our network, *kida.uva.2011*.

Key words: astrochemistry – astronomical databases: miscellaneous – ISM: abundances – ISM: molecules

1. INTRODUCTION

Astrochemical models have been developed over the years to study the chemical composition of the interstellar medium (ISM, see Agúndez & Wakelam 2013, and references therein). Current models follow the abundances of hundreds of species through thousands of reactions (McElroy et al. 2013). Although the processes at the surface of the grains, such as sticking, surface reactions, and desorption, are crucial (Herbst & Yates 2013), gas-phase reactions are of prime importance and poor estimates of rate coefficients can induce large errors in the predicted abundances, as occurs for OCS (Loison et al. 2012). The rate coefficients for chemical reactions under the ISM conditions of low density and temperatures from about 10 K to hundreds of K can be studied in the laboratory for some systems or studied theoretically for others (Smith 2011; Larsson et al. 2012). Because each study on a specific reaction can take from a few months to several years, such studies are best undertaken for systems identified as the most important ones (Wakelam et al. 2010). For other systems, general rules can be used (with caution) to estimate the rate coefficients by similarities to other studied reactions (Loison et al. 2014c). Even for systems studied in detail, it is uncommon to explore temperatures as low as 10 K, so that some estimate or

extrapolation of the temperature dependence may be necessary but must then be performed with caution.

The KInetic Database for Astrochemistry (KIDA) online database²³ is a compilation of rate coefficients coming from various sources including published papers, and other databases or data sheets, which are of interest for the ISM or the modeling of planetary atmospheres. For “important” reactions, the appropriate KIDA experts can be asked to provide data sheets with recommendations on the rate coefficients to be used.²⁴ KIDA contains about 70 such data sheets and the number is increasing with time. The list of experts in physical chemistry is provided in Table 1 with their current coordinates. To help astrochemical users, we also provide a subset of chemical reactions, extracted from KIDA, to be used to model the chemistry in the ISM. The first release of this network, *kida.uva.2011*, was reported in Wakelam et al. (2012, herein-after W12). We are now presenting in this paper an updated version, labeled *kida.uva.2014*. The chemical updates of the network are described in Section 2 while the impact of the new chemistry is discussed in Section 3.

²³ <http://kida.obs.u-bordeaux1.fr/>

²⁴ <http://kida.obs.u-bordeaux1.fr/datasheets>

Table 1
List of KIDA Experts

Expert Name	Contact Information	Field of Expertise
Astrid Bergeat	University of Bordeaux, France astrid.bergeat@u-bordeaux.fr	(2)
Karine Béroff	University Paris-Sud, France karine.beroff@u-psud.fr	(1, 2, 4, 5)
Marin Chabot	University Paris-Sud, France chabot@ipno.in2p3.fr	(1, 2, 4, 5)
Alexandre Faure	University of Grenoble, France Alexandre.Faure@obs.ujf-grenoble.fr	(2)
Daniele Galli	INAF Arcetri Astrophysical Observatory, Italy galli@arcetri.astro.it	(1)
Wolf D. Geppert	University of Stockholm, Sweden wgeppert@hotmail.com	(2, 5, 6)
Dieter Gerlich	Technische Universitaet Chemnitz, Germany gerlich@physik.tu-chemnitz.de	(2, 3, 4, 6)
Eric Herbst	University of Virginia, USA ericherb@gmail.com	(2, 3, 5)
Kevin M. Hickson	University of Bordeaux, France km.hickson@ism.u-bordeaux1.fr	(1,2, 5)
Pascal Honvault	University of Franche-Comté/ Bourgogne, France pascal.honvault@univ-fcomte.fr	(2)
Stephen J. Klippenstein	Argonne National Laboratory, USA sjk@anl.gov	(2, 3)
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Jonathan Tennyson	University College London, UK j.tennyson@ucl.ac.uk	(3, 5, 6)
Roland Wester	University of Innsbruck, Austria roland.wester@uibk.ac.at	(1, 2, 4, 6)

Note. Field of expertise: (1) photo and cosmic-ray processes, (2) neutral-neutral and ion-neutral reactions, (3) radiative association, (4) charge exchange, (5) dissociative recombination, (6) associative detachment.

2. CHEMICAL UPDATES

This new network is based on the previously published kida.uva.2011 network (W12) with the updates posted in the KIDA database between 2011 October and 2014 October. The main updates of the network come from:

1. reactions from the high temperature network of Harada et al. (2010),
2. photo rates from van Dishoeck (1988), Roberge et al. (1991), van Dishoeck et al. (2006), van Hemert & van Dishoeck (2008),

Table 2
Species Added to the kida.uva.2014 Network

New Species
C ₅ O, C ₆ N, C ₂ H ₆ , C ₇ O, C ₈ N, C ₉ O, C ₁₀ N, HN ₂ O ⁺ , HC ₅ O ⁺ , C ₆ N ⁺ , HC ₆ N ⁺ , HC ₇ O ⁺ , C ₈ N ⁺ , H ₂ C ₆ N ⁺ , C ₂ H ₇ ⁺ , HC ₈ N ⁺ , HC ₉ O ⁺ , C ₁₀ N ⁺ , H ₂ C ₈ N ⁺ , HC ₁₀ N ⁺ , H ₂ C ₁₀ N ⁺

3. rate coefficients for the OCS chemistry from Loison et al. (2012),
4. new data sheets (Wakelam et al. 2013 and many others),
5. a review of the HCN/HNC chemistry by Loison et al. (2014b),
6. a review of the carbon chemistry by Loison et al. (2014c),
7. branching ratios for reactions forming C_{n=2-10}^(0,+), C_{n=2-4}H^(0,+), and C₃H₂^(0,+) from Chabot et al. (2013).

In addition to these updates, a number of individual reactions have been added or updated from a list of studies given in the Appendix. New species have been added to the network, and are listed in Table 2. A total of 446 rate coefficients have been changed and 1038 new reactions have been added. The final network contains 489 species composed of 13 elements and 7509 reactions. In addition to the gaseous species, neutral grains, negatively charged grains, grain-surface electrons and atomic hydrogen are included. The types of reactions and the formulas used to parameterize the rate coefficients are the same as described in W12. The complete network is available at <http://kida.obs.u-bordeaux1.fr/uploads/models/kida.uva.2014.zip> with a list of species and the bibliographic reference in bibtex format.

As for the previous version, kida.uva.2011, we expect the network to be used for the chemical modeling of the ISM at temperatures between 10 and 300 K. Despite the fact that we added reactions from Harada et al. (2010) for higher temperature conditions, including reactions with activation energy, and reverse reactions, we have not done any additional checks on its appropriateness for temperatures larger than 300 K. For some of the reactions, the parameter γ used in the temperature-dependent Arrhenius-Kooij expression for the rate coefficient— $k(T) = \alpha(T/300)^\beta \exp(-\gamma/T)$ —is negative. This sign change will produce strongly incorrect results if the calculation of the rate coefficient is extrapolated outside the temperature range of validity. Those reactions are listed in Table 3. Not extrapolating outside of the range of validity can also have consequences. In fact, the temperature dependence of rate coefficients is usually valid over a certain range of temperature, which can be a crucial piece of information. However, in many cases, the information is only partial and could lead to large errors if not carefully considered. This is particularly true for H-atom transfer reactions where quantum mechanical tunneling results in strong departure from Arrhenius behavior at low temperatures (Tizniti et al. 2014). As an example, consider the reaction $N + H_2 \rightarrow H + NH$, which has a very large activation energy. This reaction was already present in the previous OSU database (Harada et al. 2010) without any indication of the temperature range and, it is likely that common users would extrapolate the rate coefficient down to 10 K. In KIDA, we included the original rate coefficient from Davidson & Hanson (1990) with its measured temperature

Table 3
Reactions with Negative Gamma Parameters

Reaction	T Range (K)	Reference
$F + H_2 \rightarrow H + HF$	10–100	Neufeld et al. (2005)
$OH + OH \rightarrow O + H_2O$	200–350	datasheet
$C + NH_2 \rightarrow H + HNC/HNC$	10–300	datasheet
$O + OH \rightarrow O_2 + H$	150–500	datasheet
$H_2 + NH_3^+ \rightarrow NH_4^+ + H$	10–20	datasheet
$C + OH \rightarrow H + CO$	10–500	Zanchet et al. (2009)
$CH + OCS \rightarrow CO + H + CS$	301–667	Zabarnick et al. (1989)
$N + Si \rightarrow SiN + h\nu$	10–100	Gustafsson et al. (2012)
$H + F \rightarrow HF + h\nu$	100–2500	Gustafsson et al. (2014)

range of 1950–2850 K. The rate coefficient computed at the minimal temperature (1950 K) would then be $4 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1}$ (much larger than the 10 K extrapolation of $4 \times 10^{-82} \text{ cm}^3 \text{ s}^{-1}$). If only the measured temperature range for $N + H_2$ (1950–2850 K) were included in the network, the reaction rate coefficient for temperatures lower than the lowest measured temperature (1950 K) would be programmed to remain at the measured value for 1950 K. Likewise, the rate coefficient at temperatures higher than 2850 K would be programmed to remain at the 2850 K value. In dense cloud conditions where both N and H_2 are abundant, even the low 1950 K rate coefficient would be large enough to have a significant effect on the chemistry while the rate coefficient of this reaction at 10 K is clearly negligible. For this reason, in *kida.uva.2014*, we have used the original rate coefficient and reference but we have changed the temperature range to extend to 10 K to allow extrapolation. For reactions between ions and non-polar neutrals with measurements only at 300 K, we have assumed that the rate coefficients are independent of temperature, as in the Langevin approximation, and have used the measured total rate coefficients and product branching fractions over the temperature range 10–300 K.

3. MODELING RESULTS OF THE NEW NETWORK

3.1. Comparison with *kida.uva.2011*

To quantify the impact of the updates done on *kida.uva.2011*, we have compared the abundances computed with the chemical code Nahoon using *kida.uva.2011* (see W12) and *kida.uva.2014* with physical parameters typical for dense clouds: a temperature of 10 K, a total “proton” density, defined by the relation $n_H = n(H) + 2n(H_2)$, of $2 \times 10^4 \text{ cm}^{-3}$, a cosmic-ray ionization rate for H_2 of 10^{-17} s^{-1} , and a visual extinction of 30. The gas-phase abundances of the species are computed as a function of time starting from an atomic composition except for hydrogen, which is initially molecular. The elemental composition utilized is the same as used by Hincelin et al. (2011), except for elemental oxygen, which has an abundance with respect to H of 2.4×10^{-4} . Tables 4 and 5 give lists of abundant species, defined as those with abundances computed with at least one network larger than 10^{-12} compared with the total proton density. The lists contain only those abundant species with abundances modified by more than a factor of 2 at 10^5 and 10^6 yr with the change in reaction network. For each of these species, we also give the ratio of the abundance computed with *kida.uva.2014* to the one computed with *kida.uva.2011* in logarithmic terms. In Figure 1, we show

the abundances of a selection of species as functions of time computed with the two networks.

At 10^5 yr, the species that show a difference larger than two orders of magnitude are HC_2N^+ , $H C_n N$ (with $n = 4, 6$ and 8), CH_2NH , and CCS , and they are all decreased by the new network. The HC_2N^+ abundance is decreased by the newly added reaction $H_2 + HC_2N^+ \rightarrow H + CH_2CN^+$ while the $H C_n N$ species and CH_2NH are decreased by new destruction reactions with atomic carbon, all from Loison et al. (2014b). The strong decrease of the CCS abundance is due to the introduction of the destruction reaction $O + CCS \rightarrow CO + CS$, which possesses a rate coefficient of $10^{-10} \text{ cm}^3 \text{ s}^{-1}$ independent of temperature (Loison et al. 2012). The rate coefficient has been deduced from the similar $O + CCO$ reaction for which the rate coefficient has been measured to be $9 \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$ (Shackleford et al. 1972; Bauer et al. 1985) at room temperature. The high value of the rate coefficient is compatible with the fact that the $O + CCS$ reaction is a radical–radical reaction which usually shows no (or a submerged) barrier. Note that this reaction was also included in Harada et al. (2010) but with an activation barrier based on the rate coefficient from $O + CS$.

A significant fraction of the molecules listed in Table 4 are either nitrogen-bearing species or carbon-bearing species because a large number of the rate coefficients for these species have been changed, as mentioned in Section 2. The abundances of large carbon-chains have also been reduced. At 10^6 yr, the list of species is much smaller than at 10^5 yr and the differences are smaller than at earlier times, partly because the abundance of atomic carbon decreases with increasing time. Among the species that present a variation of more than a factor of 10, only NO was not already present in Table 3. This molecule is increased by approximately a factor of 10 because of the decrease in the $N + NO$ rate coefficient as recommended by the KIDA experts in a datasheet.

3.2. Comparison of Model Predictions with Observations

Although this is not the primary goal of this paper, we have compared the model results discussed in the previous section with the observations in TMC-1, as listed in Agúndez & Wakelam (2013, Table 4). We initially used only gas-phase chemistry and in a second attempt, we considered grain-surface chemistry as well. For this second test, we used the Nautilus gas-grain code as described in many previous papers (Semenov et al. 2010; Loison et al. 2014c; Reboussin et al. 2014). The grain surface network was adapted to include the new species introduced in *kida.uva.2014* but is basically the same as in Loison et al. (2014c). It consists mainly of diffusive Langmuir–Hinshelwood processes with adsorption and desorption mechanisms. In addition to thermal desorption, Nautilus includes cosmic-ray induced desorption, as described in Hasegawa & Herbst (1993), and the desorption by exothermicity of surface reactions following Garrod et al. (2007) with the parameter a set to 0.01.

The physical conditions and initial abundances are the same as described in the previous section. To compare with the observations, we have simply computed the differences between the logarithms of observed and modeled abundances using the two networks, and determined the time for which the mean logarithmic difference is at its minimum (Loison et al. 2014c). This logarithmic parameter is defined by the sum over all species of $|\log(X_{\text{mod}}/X_{\text{obs}})|/N_{\text{obs}}$, where X_{mod}

Table 4Species with Abundance Ratios $\log(X_{\text{new}}/X_{\text{old}})$ Smaller than -0.3 or Larger than 0.3 at 10^5 yr, and with an Abundance in at Least One of the Models Larger than 10^{-12} Compared with the Total Proton Density

Species	Ratio	Species	Ratio	Species	Ratio	Species	Ratio
HC ₂ N ⁺	-4.5	C ₁₀ H ₂	-1.2	N ₂ H ⁺	-0.7	C ₄ H ⁻	-0.4
HC ₈ N	-3.1	CH ₃ C ₃ N	-1.2	C ₅ H ₂	-0.7	l-C ₃ H	-0.4
HC ₆ N	-2.9	H ₃ C ₄ NH ⁺	-1.2	C ₅ H ₃ N ⁺	-0.7	C ₆ ⁻	-0.4
HC ₄ N	-2.9	C ₈ H ⁻	-1.2	Mg ⁺	0.7	Na ⁺	0.4
CH ₂ NH	-2.4	C ₉	-1.1	C ₅ H ⁻	-0.6	HC ₃ NH ⁺	-0.4
CCS	-2.2	C ₈ H	-1.1	C ₇	-0.6	NH ₃	-0.4
HNC	-1.7	C ₅ ⁻	-1.1	C ₇ ⁻	-0.6	OCS	-0.4
C ₁₀ H	-1.7	C ₉ N	-1.0	N ₂	-0.6	CCN	-0.4
C ₁₀ H ⁻	-1.7	C ₉ H ₂ N ⁺	-1.0	OCN	-0.6	C ₆ H ₂	-0.4
HC ₉ N	-1.6	C ₃ H ⁺	-1.0	C ₃ H	-0.6	H ₂ CCN	0.4
NC ₄ N	-1.6	C ₂ S ⁺	-0.9	C ₇ H ₂ N ⁺	-0.6	C ₈ H ₂ ⁺	-0.4
NC ₈ N	-1.6	C ₇ H	-0.9	l-C ₃ H ₂	0.6	H ₂ CCN	-0.4
NC ₆ N	-1.6	C ₇ H ⁻	-0.9	CNC ⁺	0.6	NH ₃ ⁺	-0.4
C ₁₁	-1.6	C ₈ H ₂	-0.9	C ₃ N ⁻	-0.6	C ₆	-0.4
CH ₃ C ₇ N	-1.5	NH	-0.9	c-C ₃ H	-0.6	C ₅ N	-0.4
HC ₇ N	-1.5	HC ₂ S ⁺	-0.9	NH ₂	-0.6	HNCCC	-0.3
H ₃ C ₇ N ⁺	-1.4	C ₈ ⁻	-0.9	HNO	-0.6	C ₆ H ₆	-0.3
CH ₃ C ₅ N	-1.4	C ₇ H ₂ ⁺	-0.8	C ₉ H ⁺	-0.5	C ₅ H ₄ ⁺	-0.3
C ₉ H	-1.4	C ₁₀ H ⁺	-0.8	CH ₃ CN ⁺	0.5	CN ⁻	-0.3
HC ₃ N	-1.3	C ₆ H	-0.8	SiC ₈ H	-0.5	HCNCC	-0.3
C ₉ H ₂	-1.3	CH ₂ CCH	-0.8	CH ₃ NH ₂	-0.5	C ₃ O ⁺	0.3
C ₉ H ⁻	-1.3	C ₆ H ⁻	-0.8	CH ₃ NH ₃ ⁺	-0.5	NS	0.3
C ₁₀	-1.3	Fe ⁺	0.8	C ₄ H	-0.5
HC ₅ N	-1.3	C ₇ N	-0.7	NH ₄ ⁺	-0.4
C ₁₀ ⁻	-1.3	C ₈	-0.7	CH ₃ C ₄ H	-0.4

Table 5Species with Abundance Ratios $\log(X_{\text{new}}/X_{\text{old}})$ Smaller than -0.3 or Larger than 0.3 at 10^6 yr, and with an Abundance in at Least One of the Models Larger than 10^{-12} Compared with the Total Proton Density

Species	Ratio	Species	Ratio
l-C ₃ H ₂	1.6	HC ₃ N	0.5
HC ₈ N	-1.5	SiS	-0.5
SiC ₈ H	-1.4	C ₃ S	0.5
CCS	-1.4	N ₂ O	0.5
HC ₆ N	-1.2	CH ₂ CHC ₂ H	-0.4
NO	1.1	C ₃ O	0.4
NC ₈ N	-1.1	SiO ₂	-0.4
SiC ₆ H	-1.0	NO ⁺	0.4
H ₂ CCN	-1.0	OCN	-0.4
NC ₆ N	-0.9	C ₄ H	-0.4
C ₆ H ₆	-0.8	H ₂ NC ⁺	0.3
C ₃ N	0.8	l-C ₃ H ₃ ⁺	0.3
OCS	-0.7	NH ₂	-0.3
CNC ⁺	0.7	HNO	-0.3
HNCCC	0.7	C ₃	0.3
HCCNC	0.6	N	0.3
HC ₄ N	-0.6	l-C ₃ H	-0.3
c-C ₃ H	-0.6	C ₄ H ₂	-0.3

and X_{obs} are the modeled and observed abundances while N_{obs} is the number of observed species (57) in TMC-1 used for the comparison. Considering only gas-phase chemistry, the general agreement with the model is slightly worse with the new network. When surface chemistry is considered, we obtain a similar degree of agreement but for different times. We now only discuss the comparison using the full gas-grain networks. Figure 2 shows the mean logarithmic difference as a function of time for both networks. We have ignored the species for which only upper limits have been constrained. At the best times, for

both models, the mean difference between modeled and observed abundances is smaller than a factor of 10. As already noted by Loison et al. (2014c), we now obtain a reasonable agreement with the observations in TMC-1 using a C/O elemental ratio smaller than 1. The best time is 2.5×10^5 yr using kida.uva.2011 while it is approximately 1.3×10^6 yr using the new network. For these best times, we have plotted in Figure 3 the difference between modeled and observed abundances for individual species. The difference between modeled and observed abundances is decreased for about half of the species and increased for the other half when comparing the two networks. This explains the fact that the general agreement is not changed.

The two species for which the changes are the strongest are CH₃CHO, for which the agreement with the new model is worse, and CCO, for which agreement with the new model is better. Figure 4 shows the abundance of these two species as a function of time predicted with the two networks. The TMC-1 abundance of CCO is 3×10^{-11} (compared to the total proton density; Ohishi & Kaifu 1998) while that of CH₃CHO is 3×10^{-10} (Matthews et al. 1985). Both modeled abundances are smaller than the observed ones at all times. The CCO predicted abundance is much smaller at 2.5×10^5 yr, the best time using the older network, than at 1.3×10^6 yr. After 10^6 yr however, the CCO abundance is also larger with the new network because of the larger abundance of atomic carbon since CCO is produced by $C + \text{HCO} \rightarrow \text{CCO} + \text{H}$. The better agreement between the new model and the observed CCO abundance is then due to the change in the best time rather than the chemistry itself. For CH₃CHO, the worse agreement with the new model is also due to the change in the best time: at later times, the CH₃CHO abundance is smaller. The decrease in the gas-phase abundance of this species is however much stronger

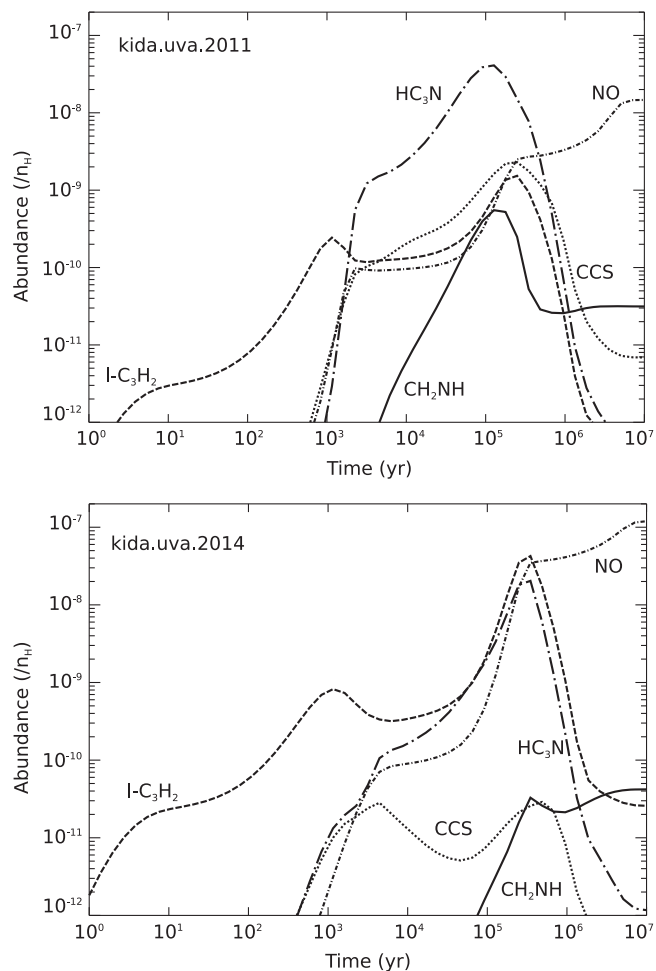


Figure 1. Abundances as a function of time for a selection of species for dense cloud conditions using kida.uva.2011 (upper panel) and kida.uva.2014 (lower panel).

with the new network as can be seen in Figure 4. At 10^6 yr, one of the main formation reactions of CH_3CHO is $\text{O} + \text{C}_2\text{H}_5 \rightarrow \text{H} + \text{CH}_3\text{CHO}$. The CH_3CHO abundance is then decreased with a decrease in the C_2H_5 abundance. The C_2H_5 molecule is more strongly destroyed using the new network because of the newly introduced reaction $\text{H} + \text{C}_2\text{H}_5 \rightarrow \text{CH}_3 + \text{CH}_3$ from Baulch et al. (1992). The rate coefficient for this reaction is $6 \times 10^{-11} \text{ cm}^{-3} \text{ s}^{-1}$ and was recommended by Baulch et al. (1992) for temperatures between 300 and 2000 K. Here we use the same rate coefficient down to 10 K.

4. CONCLUSION

The KIDA aims at providing to the community gas-phase kinetic data to study the chemistry under the extreme conditions of the ISM. From this database, a subset of reactions is extracted to be directly used in chemical models. The first release of this subset, kida.uva.2011, was included in W12. After a large number of updates, we are now presenting the new version: kida.uva.2014. A large number of gas-phase species are affected by these modifications at typical cloud chemical ages (10^5 – 10^6 yr). The mean ratio between modeled abundances and the ones observed in the TMC-1 dark cloud is a factor of six at best, using a full gas-grain model. This general

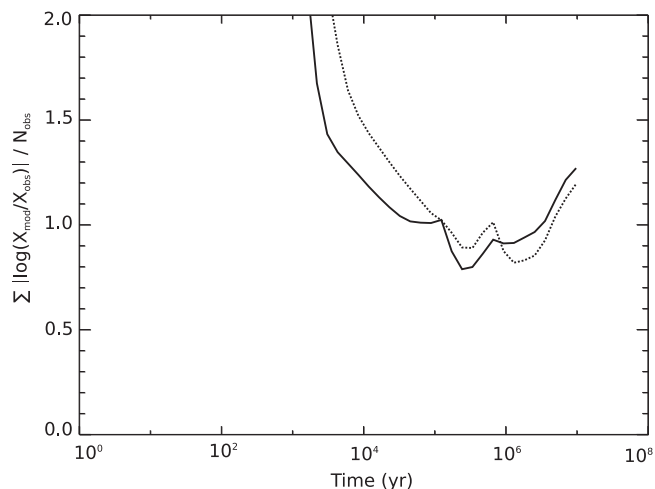


Figure 2. Mean logarithmic difference between the modeled and observed abundances over all observed species (see text) as a function of time using kida.uva.2011 (solid line) and kida.uva.2014 (dashed line).

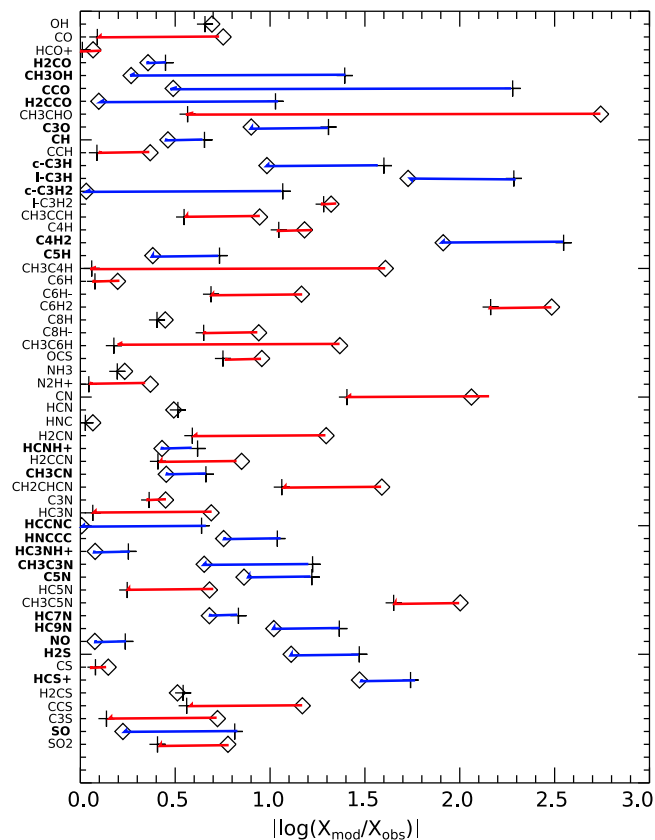


Figure 3. Absolute logarithmic difference between modeled and observed abundances for each species at the best time of each model using plus signs for kida.uva.2011 and diamonds for kida.uva.2014. Horizontal lines show the differences between the old and new values. Red lines indicate that the difference has been increased by the new network while blue lines indicate that it has been reduced. Boldface species are those with abundances improved by the new network.

agreement is not much affected by the new gas-phase network but the “best time” is older than obtained with the previous one.

The maintenance and development of the KIDA database are possible thanks to the European Research Council Starting Grant 3DICE (grant agreement 336474), the French program

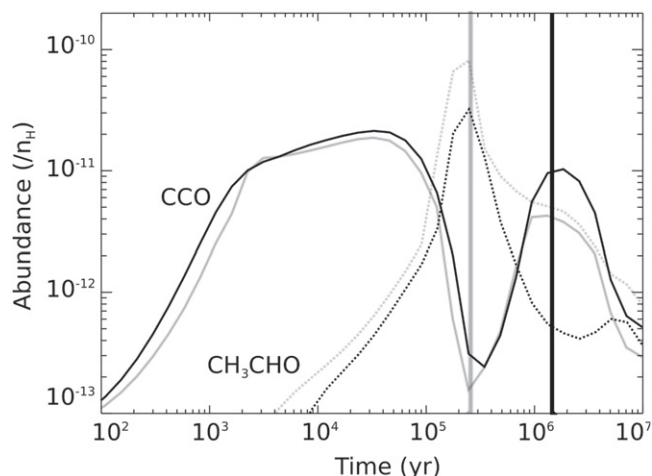


Figure 4. Abundances of CH_3CHO and CCO as a function of time computed with the kida.uva.2011 (gray lines) and kida.uva.2014 (black lines) networks. The vertical gray and black lines correspond to the best times constrained with the old and new networks respectively.

PCMI and the Observatoire Aquitain des Sciences de l'Univers. The KIDA team is also grateful to the persons who submitted data to the database. S.D.L.P. is grateful to the Institut Universitaire de France, while E.H. thanks the NSF and NASA for support. The work at Argonne is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences under Contract No. DE-AC02-06CH11357.

APPENDIX

REFERENCES FOR UPDATES

The references used to update the network are: Adams et al. (1984), Adusei et al. (1996), Anicich (1993), Arthur & Bell (1978), Avramenko & Krasnen'kov (1967), Azatyan et al. (1975), Bauerle et al. (1995a, 1995b), Baulch et al. (1992, 1994), Böhländ et al. (1985), Bryukov et al. (2001), Chabot et al. (2013), Cohen & Westberg (1991), Cole et al. (2012), Daranlot et al. (2011, 2012, 2013), Diau et al. (1995), Dombrowsky & Wagner (1992), Frank (1986), Freund & Palmer (1977), Fujii et al. (1987), Gustafsson et al. (2012), Hack et al. (1979), Hamberg et al. (2010), Hanson & Salimian (1984), Harada et al. (2010), Hemsworth et al. (1974), Henshaw et al. (1987), Herbrechtsmeier (1973), Hickson et al. (2013), Humpfer et al. (1995), Karkach & Osherov (1999), Kim (1975), Kim & Huntress (1975), Leen & Graff (1988), Lifshitz & Michael (1991), Lloyd (1974), Loison et al. (2012, 2014a, 2014b, 2014c), Mackay et al. (1980, 1981), Gustafsson et al. (2014), Maluendes et al. (1993), Mayer et al. (1966), Mebel et al. (1996), Millar et al. (1986, 1987, 1991), Miller & Melius (1988), Mitchell (1984a, 1984b), Miyoshi et al. (1993), Murrell & Rodriguez (1986), Neufeld & Wolfire (2009), Nguyen et al. (2004), Otto et al. (2008), Patterson & Greene (1962), Payzant et al. (1975), Peeters & Mahnen (1973), Roberge et al. (1991), Rodgers (1996), Schofield (1973), Shannon et al. (2014), Singleton & Cvetanovic (1988), Smith et al. (1984, 1992, 1994), Stewart et al. (1989), Tsang (1992), Tsang & Hampson (1986), Tsang & Herron (1991), Tsuboi & Hashimoto (1981), van Dishoeck (1988), pp. 49–72, van Dishoeck et al. (2006), van Hemert & van Dishoeck

(2008), Vandooren et al. (1994), Warnatz (1984), Yang et al. (1993), Zanchet et al. (2009), Zellner & Ewig (1988).

REFERENCES

- Adams, N. G., Smith, D., & Millar, T. J. 1984, *MNRAS*, **211**, 857
 Adusei, G. Y., Blue, A. S., & Fontijn, A. 1996, *JPhCh*, **100**, 16921
 Agúndez, M., & Wakelam, V. 2013, *ChRv*, **113**, 8710
 Anicich, V. G. 1993, *JPCRD*, **22**, 1469
 Arthur, N., & Bell, T. 1978, *Rev. Chem. Intermed.*, **2**, 37
 Avramenko, L. I., & Krasnen'kov, V. M. 1967, *Bull. Acad. Sci. USSR Div. Chem. Sci.*, **61**, 501
 Azatyan, V., Aleksandrov, E., & Troshin, A. 1975, *Kinet. Catal.*, **16**, 261
 Bauer, W., Becker, K. H., & Meuser, R. 1985, *Ber. Bunsenges. Phys. Chem.*, **89**, 340
 Bauerle, S., Klatt, M., & Wagner, H. 1995a, *Ber. Bunsenges. Phys. Chem.*, **99**, 870
 Bauerle, S., Klatt, M., & Wagner, H. G. 1995b, *Ber. Bunsenges. Phys. Chem.*, **99**, 97
 Baulch, D. L., Cobos, C. J., Cox, R. A., et al. 1992, *JPCRD*, **21**, 411
 Baulch, D. L., Cobos, C. J., Cox, R. A., et al. 1994, *JPCRD*, **23**, 847
 Böhländ, T., Dóbbé, S., Temps, F., & Wagner, H. G. 1985, *Ber. Bunsenges. Phys. Chem.*, **89**, 1110
 Bryukov, M. G., Slagle, I., & R. Knyazev, V. D. 2001, *JPCA*, **105**, 6900
 Chabot, M., Béroff, K., Gratier, P., Jallat, A., & Wakelam, V. 2013, *ApJ*, **771**, 90
 Cohen, N., & Westberg, K. 1991, *JPCRD*, **20**, 1211
 Cole, C. A., Wehres, N., Yang, Z., et al. 2012, *ApJL*, **753**, L1
 Daranlot, J., Hincelin, U., Bergeat, A., et al. 2012, *PNAS*, **109**, 10233
 Daranlot, J., Hu, X., Xie, C., et al. 2013, *PCCP*, **15**, 13888
 Daranlot, J., Jorfi, M., Xie, C., et al. 2011, *Sci*, **334**, 1538
 Davidson, D., & Hanson, R. 1990, *Int. J. Chem. Kinet.*, **22**, 843
 Diau, E., Halbgewachs, M., Smith, A., & Lin, M. 1995, *Int. J. Chem. Kinet.*, **27**, 867
 Dombrowsky, C., & Wagner, H. G. 1992, *Ber. Bunsenges. Phys. Chem.*, **96**, 1048
 Frank, P. 1986, in *Proc. 15th Int. Symp. Rarefied Gas Dynamics*, ed. V. Boffi, & C. Cercignani (Germany: Teubner), 422
 Freund, H., & Palmer, H. 1977, *Int. J. Chem. Kinet.*, **9**, 887
 Fujii, N., Kakuda, T., Takeishi, N., & Miyama, H. 1987, *JPhCh*, **91**, 2144
 Garrod, R. T., Wakelam, V., & Herbst, E. 2007, *A&A*, **467**, 1103
 Gustafsson, M., Antipov, S., Franz, J., & Nyman, G. 2012, *JPhCh*, **137**, 104301
 Gustafsson, M., Monge-Palacios, M., & Nyman, G. 2014, *JPhCh*, **140**, 184301
 Hack, W., Preuss, A., & Wagner, H. 1979, *Ber. Bunsenges. Phys. Chem.*, **83**, 212
 Hamberg, M., Österdahl, F., Thomas, R. D., et al. 2010, *A&A*, **514**, A83
 Hanson, R. K., & Salimian, S. 1984, *Combustion Chemistry*, ed. W. C. Gardiner, Jr. (New York: Springer), 361
 Harada, N., Herbst, E., & Wakelam, V. 2010, *ApJ*, **721**, 1570
 Hasegawa, T. I., & Herbst, E. 1993, *MNRAS*, **261**, 83
 Hemsworth, R. S., Payzant, J. D., Schiff, H., & Bohme, D. 1974, *CPL*, **26**, 417
 Henshaw, T. L., MacDonald, M. A., Stedman, D. H., & Coombe, R. D. 1987, *JPhCh*, **91**, 2838
 Herbrechtsmeier, P. 1973, *Combust. Inst. European Symp.*, ed. F. J. Weinberg (London: Academic), 13
 Herbst, E., & Yates, J. T., Jr. 2013, *ChRv*, **113**, 8707
 Hickson, K., Loison, J.-C., & Caubet, P. 2013, *JPCL*, **4**, 2843
 Hincelin, U., Wakelam, V., Hersant, F., et al. 2011, *A&A*, **530**, A61
 Humpfer, R., Oser, H., & Grotheer, H. 1995, *Int. J. Chem. Kinet.*, **27**, 577
 Karkach, S. P., & Osherov, V. I. 1999, *JChPh*, **110**, 11918
 Kim, J., & Huntress, W., Jr. 1975, *IJMIP*, **16**, 451
 Kim, J. K. 1975, *JChPh*, **62**, 2820
 Larsson, M., Geppert, W. D., & Nyman, G. 2012, *RPPH*, **75**, 066901
 Leen, T. M., & Graff, M. M. 1988, *ApJ*, **325**, 411
 Lifshitz, A., & Michael, J. 1991, *Symposium (International) on Combustion*, **23**, 59
 Lloyd, A. 1974, *Int. J. Chem. Kinet.*, **6**, 169
 Loison, J.-C., Halvick, P., Bergeat, A., Hickson, K. M., & Wakelam, V. 2012, *MNRAS*, **421**, 1476
 Loison, J.-C., Hu, X., Han, S., et al. 2014a, *PCCP*, **16**, 14212
 Loison, J.-C., Wakelam, V., & Hickson, K. M. 2014b, *MNRAS*, **443**, 398
 Loison, J.-C., Wakelam, V., Hickson, K. M., Bergeat, A., & Mereau, R. 2014, *MNRAS*, **437**, 930
 Mackay, G., Vlachos, G., Bohme, D., & Schiff, H. 1980, *IJMIP*, **36**, 259
 Mackay, G. I., Schiff, H. I., & Bohme, D. K. 1981, *CajCh*, **59**, 1771

- Maluendes, S. A., McLean, A. D., & Herbst, E. 1993, *ApJ*, **417**, 181
- Matthews, H. E., Friberg, P., & Irvine, W. M. 1985, *ApJ*, **290**, 609
- Mayer, S. W., Schieler, L., & Johnston, H. S. 1966, *JChPh*, **45**, 385
- McElroy, D., Walsh, C., Markwick, A. J., et al. 2013, *A&A*, **550**, A36
- Mebel, A., Lin, M., Morokuma, K., & Melius, C. 1996, *Int. J. Chem. Kinet.*, **28**, 693
- Millar, T. J., Adams, N. G., Smith, D., Lindinger, W., & Villinger, H. 1986, *MNRAS*, **221**, 673
- Millar, T. J., Bennett, A., & Herbst, E. 1987, *MNRAS*, **229**, 41P
- Millar, T. J., Herbst, E., & Charnley, S. B. 1991, *ApJ*, **369**, 147
- Miller, J., & Melius, C. 1988, *Symposium (International) on Combustion*, **21**, 919
- Mitchell, G. F. 1984a, *ApJS*, **54**, 81
- Mitchell, G. F. 1984b, *ApJ*, **287**, 665
- Miyoshi, A., Ohmori, K., Tsuchiya, K., & Matsui, H. 1993, *CPL*, **204**, 241
- Murrell, J., & Rodriguez, J. 1986, *JMoSt*, **39**, 267
- Neufeld, D. A., & Wolfire, M. G. 2009, *ApJ*, **706**, 1594
- Neufeld, D. A., Wolfire, M. G., & Schilke, P. 2005, *ApJ*, **628**, 260
- Nguyen, H. M. T., Zhang, S., Peeters, J., et al. 2004, *CPL*, **388**, 94
- Ohishi, M., & Kaifu, N. 1998, *FaDi*, **109**, 205
- Otto, R., Mikosch, J., Trippel, S., Weidemuller, M., & Wester, R. 2008, *PhRvL*, **101**, 063201
- Patterson, W. L., Jr., & Greene, E. F. 1962, *JChPh*, **36**, 1146
- Payzant, J. D., Schiff, H. I., & Bohme, D. K. 1975, *JChPh*, **63**, 149
- Peeters, J., & Mahnen, G. 1973, ed. F. J. Weinberg (New York: Academic)
- Reboussin, L., Wakelam, V., Guilloteau, S., & Hersant, F. 2014, *MNRAS*, **440**, 3557
- Roberge, W. G., Jones, D., Lepp, S., & Dalgarno, A. 1991, *ApJS*, **77**, 287
- Rodgers, A. 1996, *CPL*, **253**, 313
- Schofield, K. 1973, *JPCRD*, **2**, 25
- Semenov, D., Hersant, F., Wakelam, V., et al. 2010, *A&A*, **522**, A42
- Shackelford, W. L., Mastrup, F. N., & Kreye, W. C. 1972, *JChPh*, **57**, 3933
- Shannon, R. J., Cossou, C., Loison, J.-C., et al. 2014, *RSC Advances*, **4**, 26342
- Singleton, D. L., & Cvetanovic, R. J. 1988, *JPCRD*, **17**, 1377
- Smith, D., Adams, N. H., & Ferguson, E. E. 1984, *IJMSI*, **61**, 15
- Smith, D., Spanel, P., & Mayhew, C. 1992, *IJMSI*, **117**, 457
- Smith, D., Spanel, P., & Millar, T. J. 1994, *MNRAS*, **266**, 31
- Smith, I. W. M. 2011, *ARA&A*, **49**, 29
- Stewart, P., Larson, C., & Golden, D. 1989, *CoFI*, **75**, 25
- Tizniti, M., le Picard, S. D., Lique, F., et al. 2014, *NatCh*, **6**, 141
- Tsang, W. 1992, *JPCRD*, **21**, 753
- Tsang, W., & Hampson, R. F. 1986, *JPCRD*, **15**, 1087
- Tsang, W., & Herron, J. T. 1991, *JPCRD*, **20**, 609
- Tsuboi, T., & Hashimoto, K. 1981, *CoFI*, **42**, 61
- van Dishoeck, E. F. 1988, in *Rate Coefficients in Astrochemistry*, Vol. 146, ed. T. J. Millar, & D. A. Williams (Dordrecht: Kluwer)
- van Dishoeck, E. F., Jonkheid, B., & van Hemert, M. C. 2006, *FaDi*, **133**, 231
- van Hemert, M. C., & van Dishoeck, E. F. 2008, *CP*, **343**, 292
- Vandooren, J., Bian, J., & van Tiggelen, P. 1994, *CoFI*, **98**, 402
- Wakelam, V., Herbst, E., Loison, J.-C., et al. 2012, *ApJS*, **199**, 21
- Wakelam, V., Smith, I. W. M., Herbst, E., et al. 2010, *SSRv*, **156**, 13
- Wakelam, V., Smith, I. W. M., Loison, J.-C., et al. 2013, arXiv:1310.4350
- Warnatz, J. 1984, *Combustion Chemistry*, ed. W. C. Gardiner, Jr. (New York: Springer)
- Yang, D., Yu, T., Lin, M., & Melius, C. 1993, *CP*, **177**, 271
- Zabarnick, S., Fleming, J., & Lin, M. 1989, *Int. J. Chem. Kinet.*, **21**, 765
- Zanchet, A., Bussery-Honvault, B., Jorfi, M., & Honvault, P. 2009, *PCCP*, **11**, 61826191
- Zellner, R., & Ewig, F. 1988, *JPhCh*, **92**, 2971