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Ideal Gas Thermochemical Properties of Silicon containing Inorganic, Organic Compounds, Radicals and Ions.

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ABSTRACT

The ideal gas thermochemical properties such as standard heat of formation, entropy and heat capacities of 112 inorganic and 35 organic neutral compounds, radicals and ions containing silicon were calculated using molecular properties obtained with the G3B3 (or G3//B3LYP) method. Among them were linear and cyclic silanes, silenes, hydrocarbonsilanes, fluorine and oxygen containing compounds. Many of their molecular and thermodynamic properties were calculated for the first time and 16 of them had no CAS No.

Additionally the thermochemical properties were presented in the NASA 7-term polynomial format for the temperature range of 200 K to 6000 K commonly used in chemical kinetic modeling and simulation programs. The polynomials are available in the supplement to this article free of charge.

KEYWORDS

Thermodynamic data, Thermochemistry, Thermochemical properties, Heat of formation, Entropy, Enthalpy, Heat capacity, NASA format, Quantum chemical calculation, G3B3 composite approach, Silicon hydride, Silanes, Silicon fluoride, Silicon hydrocarbon, Silicon ions, Silicon compounds, Database

INTRODUCTION

Silicon containing substances are widely used and important for the mankind. For example silicon, a crystalline substance at room temperature, is used intensively in photovoltaic and solar cells, in light-emitting devices and by the electronic industry within semiconductors and integrated circuits and therefore silicon is used nearly in every electronic device such as mobile phones, computers and equipment containing control units. On the other hand the commonly known Silicons are polysiloxanes which are polymers. They are widely used as heat resistant rubber-like plastic compounds, but are not part of this publication.

Silicon has a high affinity to oxygen and therefore different silicon oxides exist in dusts and sands or as minerals. Silanes, the analogues compounds to hydrocarbons, are pyrophoric and used as reducing agents in organic and organometallic chemistry and as precursors to elemental silicon in chemical vapor decomposition processes used in the manufacturing of semiconductors and of solar photovoltaic modules. In chemical vapor deposition processes plasma or electric discharge can decompose silanes into more reactive compounds such as radicals, which react instantaneously with the surface. For etching of metal surfaces halogenated silanes as SiF_4 are used.

The thermochemistry of silicon containing substances has received a fair amount of publications which are usually restricted to small inorganic and organic molecules. To the best of our knowledge, ions were investigated before only for the inorganic species.

It was noted that due to experimental problems the calorimetric values reported before 1970 are erroneous [1].

The first publication including thermochemical tables of diatomic silicon hydride, deuteride and tritide was to our knowledge the NBS monograph No. 20 (1961) [2] by Haar, Friedman and Beckett, which did not include enthalpies of formation values. A few Silicon gaseous compounds were published in the JANAF tables during the 1960's and 1970's [3]. Glushko, Gurvich et al. (1970) [4] published a few tritide containing Silicon inorganic compounds. Gurvich published some Silicon compounds in his different editions (1989-

1996) [5]; Walsh recorded the thermochemistry of silicon containing substances in the second part of volume 1, which was edited by Rappoport (1989) [1]. In the same volume H. Schmidt discusses the structure of silicon cations and anions, but does not include thermochemical data. Rappoport and Apeloig updated the former title as volume 2 in three parts (1998) [6]. The thermochemical chapter of Walsh (now chapter 4) was updated by Becerra [6]. Wiberg and coworkers (1995) [7] included a few silicon compounds in their comparison of ab-initio methods; Boo and Armentrout (1987) [8] calculated monosiliconhydrides and deuterides; Broadbelt and coworkers (2004) [9] calculated 135 Silicon-Hydrogen compounds; Ho and Melius (1990) [10] calculated some fluorosilane compounds. Allendorf, Melius et al. (1995) [12] report calculations on Si-O-H compounds, and some of Melius's data from his internal Sandia database were incorporated in the Chemkin thermochemical database (1982) [13]. Lyman and Noda (2001) [14] calculated SiF_4 and Si_2F_6 compounds, and also Lias et al. (1988) [15] estimated some silicon compounds and cations. Katzer et al. (1997) [31] calculated thermochemical data for more than 140 silicon hydride compounds containing up to five silicon atoms using an validated empirically corrected ab initio methodology for the standard state at 298.15 K. Feller and Dixon (1999) [43] calculated ab initio enthalpies of formation for SiH to SiH_4, Si_2H_4 and SiF to SiF_4. They reported $\Delta_f H°(0$ K) values, which are common in quantum chemical studies, instead of the reference value of 298.15 K, which is commonly used by engineers. We provide calculated heat of formation values for both temperatures to make the comparison of data with different reference temperatures easier. Takhistov and Golovin (2006) [48] did not calculate any new data, but analyzed the existing literature for many elements including silicon and decided by comparison which is the best value. Sukkaew et al. (2014) [16] calculated some Si-C-H compounds. And finally M.C. Lin and coworkers published in 2013-2017 [60-64] articles about SiH_x and Si_2H_y family including some cations.

In 2007 Karton and Martin [52] published a revised value of the heat of formation of the gaseous Silicon atom i.e. $\Delta_f H°(298K) = 452.7 \pm 0.8$ kJ mol^{-1} calculated by their novel W4 *ab-initio* method. The value used in this article is $\Delta_f H°(298K) = 450 \pm 0.8$ kJ mol^{-1} [19]. Therefore the error bar was enlarged for molecules containing more than three Silicon atoms.

The Group Additivity (GA) contributions for the heat of formation of silicon compounds were discussed and published with reservations by Walsh (1989) [1], slightly extended by Becerra and Walsh [6], but they do not include GA coefficients for entropy S and heat capacities $C_p(T)$.

Swihart and Girshick (1999) [32] used the silicon hydrides ab initio data of Katzer et al. (1997) [31] to calculate reliable thermochemical group additivity values for temperatures up to 1500 K.

The MIT RMG thermochemical database has included lately (2016) [17] a limited number of silicon compounds, but most of their silicon containing data are at the moment out of context due to wrong connections to group additivity values of carbon compounds instead of silicon group data. On the other hand, West and coworkers (2016) [18] provide in their paper supplement much more reliable thermochemical data of silicon hydrides, which can be used with RMG and other estimating programs.

The aim of this article is to provide ideal gas thermochemical data for inorganic, and organic silicon containing species and their ions calculated by the G3//B3LYP method (G3B3) [21], which are available in the NASA polynomial format in the supplement and in a popular database [19]. The reason for the adherence where possible to the G3B3 method is to provide to the chemical simulation performer consistent thermochemical data, which are calculated by the same reliable common method as all other compounds before. The temperature dependent results were without exception polynomialyzed by the same program [20].

Use of unrealistic thermochemical data for some substances, for example through simultaneously use of thermochemical data of different quality, in combination with a reliable chemical reaction model, result normally in wrong model prediction outputs (e.g. species time profiles, global parameter as flame velocities, ignition temperatures and ignition delay times), due to the use of thermochemical data during the automatically calculation of backward reaction rates within the simulation programs.

The polynomial NASA format, described in detail in the Introduction to Reference 19, allows the user to calculate the original thermochemical ideal gas phase values of heat of formation, enthalpy, entropy, heat capacity and Gibbs free energy for temperatures between 200 K and 6000 K at a pressure of 1 bar. The maximal least square error due to the application of the fitting procedure to obtain the NASA polynomials was small; the highest value was less than 0.7% for the heat capacity values.

CALCULATION METHODS

The calculation of the thermochemistry data of the Silicon containing compounds was performed using Bonnie McBride´s NASA PAC program (last updated 2003) [20]. To perform the thermodynamic calculations, the vibrations of the molecule are needed, as well as the molecules moments of inertia, the symmetry of the molecule, its statistical weight (1

for neutral molecule 2 for a radical and the reverse value for the ion) and the standard enthalpy of formation of the molecule. If the molecule has internal hindered rotations, the rotor's moment of inertia, the rotor's symmetry and the rotation barrier were supplied instead of the pertinent low vibrations.

In most cases these molecular data were obtained by applying a variant of G3 theory, the G3//B3LYP variant or usually referred as G3B3 method, where the optimized structures, its moments of inertia, zero point vibrational energies and frequencies are calculated at the B3LYP/6-31G(d) level of theory. Following the recipe of Baboul et al. [21] the G3//B3LYP energy at 0 K can be calculated from the results obtained by sequential single point energy calculations with QCISDT(T,E4T)/6-31G(d); MP4/6-31+G(d); MP4/6-31G(2df,p) and at the end MP2(Full)/gen methods at the optimized structure obtained at the B3LYP/6-31G(d) level of theory. The data obtained were the atomization energies at 0 K and the enthalpies of formation at 0 K and 298.15 K. The moments of inertia and vibrational frequencies were taken from the optimized chemical structure obtained from B3LYP/6-31G(d) calculations and were used without scaling, because in most cases these vibrations were closer to the experimental vibrations. These quantum chemical calculations were performed with the Gaussian 03 set of programs [22].

To prepare the input for the G3B3 method the molecule was drawn with the Chem3D program [23] and relaxed with the built in MOPAC semi empirical PM3 method [23]. Since Chem3D does not include double bonds for the silicon element, in these cases, the bonding had to be adjusted by hand and the optimization was done solely by the B3LYP/6-31-G(d) level of theory.

The determination of thermochemical data of ions can be done from studies of ion/molecule reactions, by optical spectroscopy and identification of a Rydberg series in a spectrum to get the ionization energy, by different electron or photoionization techniques such as threshold photoelectron–photoion coincidence (TPEPICO) technique or by ab initio calculations. To our knowledge there exist only a very limited number of thermochemical group additivity (GA) values calculated for ions of any kind.

The ions in this study were calculated as the rest of compounds by the G3B3 method and reported by the thermal electron convention. [See Introduction p.17 of Ref. 19].

The compounds containing the isotopes deuterium and tritium (D and T) were calculated with the B3LYP/6-31G(d) to find their vibrations and moments of inertia. Their enthalpy of formation was calculated from the parent hydrogen molecule according to the formula:

$\Delta_f H°(0\ K)_{deuterated} =$

$\Delta_f H°(0\ K)_{undeuterated} + n[\Delta_f H°(0\ K)\ (D) - \Delta_f H°(0\ K)\ (H)]\ + E_{0\ deuterated} - E_{0\ undeuterated}$

where n is the number of isotope atoms in the molecule, and the zero point energy

$$E_0 = (\frac{1}{2}\sum_i v_i)(0.01196266)\ \text{kJ}\ \ \text{mol}^{-1}\ \text{using the vibrations}\ v_i\ \text{in cm}^{-1}.$$

A similar equation is used for tritium containing substances.

Since $\Delta_f H°(0\ K)\ (H)=216.034$ kJ mol^{-1}, $\Delta_f H°(0\ K)\ (D)=219.804$ kJ mol^{-1} [65] and $\Delta_f H°(0\ K)\ (T)=221.479$ kJ mol^{-1} [5], the difference $[\Delta_f H°(0\ K)\ (D) - \Delta_f H°(0\ K)\ (H)] =3.77$ kJ mol^{-1} and the according difference for tritium results in 5.445 kJ mol^{-1}.

The calculations of the values of isotopic species is listed in Table S6 in the Supplement of this publication.

RESULTS

Thermodynamic data of two groups of silicon containing compounds were calculated. In the first group properties such as standard heat of formation, entropy and heat capacity of 112 inorganic silicon neutral species, radicals and ions were calculated.
A lot of attention is placed on silanes, the silicon hydride species, which are analogues substances to the hydrocarbon compounds. At standard conditions (STP), which are 1 bar and 298.15 K, the monosilane and disilane are gaseous and very pyrophoric [53]. From trisilane on, the compounds are liquid at STP, but the pyrophoric property persists to hexasilane.

In the second group thermodynamic properties of 35 organic silicon containing species, including neutral radical and ionic compounds, were calculated.

The thermochemical properties of the species are listed in Tables 1 and 2 at 298.15 K at a standard pressure state of 1 bar. For the temperature range of 200 K to 6000 K the thermochemical properties of the species can be calculated from the 7 term NASA polynomials. They are listed for further use in chemical kinetics and computational fluid dynamics modelling software in Table S 5 in the supplement to this article, which is available free of charge.

DISCUSSION

The Silicon containing closed shell compounds, their radicals and ions have been divided into two categories:

- a) The inorganic 112 species
- b) The 35 organic species

All species will be individually discussed below.

In general it should be taken into account that due to experimental problems the calorimetric values reported before 1970 are erroneous [1] and sometimes persist in further publications. Also because the different JANAF publications are reprints of the earlier calculations with a minimal number of new species, the year of the calculation of the pertinent specie is reported, and not the specific edition.

SiF, SiF$^+$, SiF$^-$, **Monofluorosilicon and its ions.**

Monofluorosilicon was calculated according to the Huber and Herzberg constants for diatomic molecules [24] suggested by the NIST CCCBDB tables [25] with Irikura's [26] addition of $\omega_e Y_e$. Standard heat of formation $\Delta_f H°(298K) = -62.6 \pm 8$ kJ mol^{-1} and $\Delta_f H°(0 \text{ K}) = -63.78 \pm 8$ kJ mol^{-1} were calculated with the G3B3 method. Michels and Hobbs (1993) [47] report for using G2 theory a $\Delta_f H°(298K) = -56.1$ kJ mol^{-1}, Feller and Dixon (1999) [43] report in a theoretical study for 0 K $\Delta_f H°(0 \text{ K}) = -61.9 \pm 2.$ kJ mol^{-1} in contradiction to JANAF (1976) tables [3], which reported a value of $\Delta_f H°(298K) = -20.08$ kJ mol^{-1}, Gurvich in 1991 [5] reported $\Delta_f H°(298K) = -25.23$ kJ mol^{-1}. This value was corrected by B.McBride to -25.84 kJ mol^{-1}.

The heat of formation of the ions SiF$^+$ and SiF$^-$ were calculated from the single vibration obtained from the B3LYP/6-31G(d) method as $\Delta_f H°(298K) = 657.49 \pm 10.$ kJ mol^{-1} and $\Delta_f H°(298K) = -87.87 \pm 10.$ kJ mol^{-1} respectively, by the thermal electron convention. The error bar was enlarged, because only the single ω_e vibration was available. The literature values found were for the cation SiF$^+$ $\Delta_f H°(298K) = 712.90 \pm 9.2$ kJ mol^{-1} by Weber and Armentrout (1988) [28] and for the anion SiF$^-$ Michels and Hobbs (1993) [47] report for a calculation with Gaussian 2-theory transformed to thermal electron convention $\Delta_f H°(298K) = -140.9$ kJ mol^{-1}; $\Delta_f H°(298K) = -103 \pm 11$ kJ mol^{-1} was reported by Kawamata et al. (1996) [27].

SiF₂, SiF₂⁺, SiF₂⁻, Silicondifluoride (Difluorosilylene) F-Si-F and its ions.

JANAF (1977) [3] lists $\Delta_f H°$(298K) = -587.85 kJ mol^{-1}; Gurvich (1991) [5] $\Delta_f H°$(298K) = -592.8. kJ mol^{-1} and Becerra and Walsh (1998) [6] report $\Delta_f H°$(298K) = -638.±6. kJ mol^{-1} for difluorosilicon, which was calculated by Ho and Melius (1990) [10] as $\Delta_f H°$(298K) = -627.0±17. kJ mol^{-1}. Michels and Hobbs (1993) [47] report $\Delta_f H°$(298K) = -623.4 kJ mol^{-1}; Feller and Dixon (1999) [43] report $\Delta_f H°$(0 K) =-634.7±2. kJ mol^{-1} and the result of the present G3B3 calculation is $\Delta_f H°$(0 K) = -626.2 ±8. kJ mol^{-1} and $\Delta_f H°$(298K) = -630.8±8. kJ mol^{-1}.

The heat of formation of the cation SiF₂⁺ using the G3B3 method is $\Delta_f H°$(298K) =429.4±8. kJ mol^{-1}, and the anion results in $\Delta_f H°$(298K) = -661.±8. kJ mol^{-1} in thermal electron convention. Michels and Hobbs (1993) [47] report for the anion calculated by Gaussian 2-theory $\Delta_f H°$(298K) = - 651.8 kJ mol^{-1} in the thermal electron convention and Kawamata et al. (1996) [25] reports $\Delta_f H°$(298K) = -608±22. kJ mol^{-1} obtained from photoelectron spectroscopy experiments of binary cluster anions.

O=SiF₂, O=SiF₂⁺, O=SiF₂⁻ : Difluorooxysilane and ions.

Heat of formation of difluorooxysilane was first reported by JANAF (1963) [3] as $\Delta_f H°$(298K) =-966. kJ mol^{-1} and the present G3B3 value is $\Delta_f H°$(298K)=-899.0±8. kJ mol^{-1}. To our knowledge the thermochemical data of the ions were not published before, the thermal electron G3B3 values are $\Delta_f H°$(298K) =247.4±8. kJ mol^{-1} and $\Delta_f H°$(298K) = -1056.±8. kJ mol^{-1} for the cation and anion respectively. The anion has no CAS No.

SiF₃, Trifluorosilicon radical (Trifluorosilyl)

The heat of formation of the radical trifluorosilyl was published by JANAF (1977) [3] and Gurvich (1991) [5] as $\Delta_f H°$(298K) =-996.2. kJ mol^{-1}. The present calculation taken from Ho and Melius (1990) [10] lists $\Delta_f H°$(298K) =-993.3±8. kJ mol^{-1}. Michels and Hobbs (1993) [47] report for calculation with G2-theory $\Delta_f H°$(298K) = - 974.0 kJ mol^{-1}, Becerra and Walsh (1998) [6] reported $\Delta_f H°$(298K) = - 987±20. kJ mol^{-1}. The unused G3B3 results in $\Delta_f H°$(298K) =-988.47±8. kJ mol^{-1}.

SiHF₃, SiHF₃+, Trifluorosilane and cation:

JANAF (1976) [3] published for trifluorosilane $\Delta_f H°$(298K) =-1200.8 kJ mol^{-1}. The present calculation is based on Ho and Melius (1990) [10] $\Delta_f H°$(298K) =-1207.7 ±5.4. kJ

mol^{-1}. Becerra and Walsh (1998) [6] reported $\Delta_f H°$(298K) = -1200±21. kJ mol^{-1} and Takhistov and Golovin (2006) [48] propose $\Delta_f H°$(298K) = -1198.7 kJ mol^{-1}. The unused G3B3 value is $\Delta_f H°$(298K) = -1193.5 ±8. kJ mol^{-1}.

The thermal electron G3B3 value for the cation was found $\Delta_f H°$(298K) = 73.2±8 kJ mol^{-1}.

SiF$_4$, SiF$_4$+, SiF$_4$-, **Tetrafluorosilane and ions.**

The standard heat of formation of tetrafluorosilane was published by JANAF (1976) [3] $\Delta_f H°$(298K) = -1614.9 kJ mol^{-1}; Walsh (1983) [29] reports $\Delta_f H°$(298K) = -1615.±1. kJ mol^{-1} and CODATA (1984) [50] recommended $\Delta_f H°$(298K) = -1615.0±0.8 kJ mol^{-1}. Michels and Hobbs (1993) [47] report for G2-method $\Delta_f H°$(298K) = -1586.2 kJ mol^{-1}. Feller and Dixon (1999) [43] report $\Delta_f H°$(0 K) = -1608.7±4. kJ mol^{-1}. The present calculation comes from Ho and Melius (1990) [10] and also Takhistov and Golovin (2006) [48] report $\Delta_f H°$(298K) = -1615. ± 4.2 kJ mol^{-1}. In 2001 Lyman and Noda [14] used the same values for the heat of formation, but calculated the harmonic oscillator as well as the anharmonic oscillator and found no differences below 1000 K for the thermodynamical data. Above this temperature the small difference is probably of little importance in combustion processes because SiF$_4$ is normally not involved there, as well as in chemical vapor deposition processes, where the temperature is normally lower. The G3B3 calculation (unused) lists $\Delta_f H°$(298K) = -1606.±8. kJ mol^{-1}.

The thermal electron G3B3 result for the SiF$_4$ ions is $\Delta_f H°$(298K) = -81.09±8. kJ mol^{-1} and $\Delta_f H°$(298K) = -1544.08±8. kJ mol^{-1} for the cation and anion respectively.

SiH, SiH+, SiH-, SiD, SiD+, SiT, **: Silicon hydride (Silylidyne), deutride and tritide and ions.**

The thermochemical data of the non-ionic mono hydrides, deuterides and tritides up to temperatures of 5000 K were first published by Haar, Friedman and Beckett in the NBS Monograph 20 (1961) [2], but the enthalpy of formation was not reported. The diatomic constants were taken from Huber and Herzberg [24]. The JANAF tables (1976) [3] report first for SiH $\Delta_f H°$(298K) = 376.66±8.4 kJ mol^{-1}, a value repeated by Boo & Armentrout (1987) [8] and used here. Michels and Hobbs (1993) [47] report as G2-calculation result $\Delta_f H°$(298K) = 366.9 kJ mol^{-1}, Katzer et al. (1997) [31] calculated $\Delta_f H°$(298K) = 372.6 kJ mol^{-1}, Feller and Dixon (1999) [43] report from high level CCSD(T) calculation $\Delta_f H°$(0 K) = 366.0 ±1.7 kJ mol^{-1} and an experimental value of Berkowitz et al. (1987) [36] of $\Delta_f H°$(0 K) = 374.5 ±2.9 kJ mol^{-1} (compared with our value of $\Delta_f H°$(0 K) = 375.4 ±8. kJ mol^{-1}) and

Jursic (2000) [45,46] calculates $\Delta_f H°(0 K) = 369.0$ kJ mol^{-1}. Finally M.C. Lin and coworkers report (2013)[60] $\Delta_f H°(0 K) = 370.7$ to $374.9 \pm 5.$ kJ mol^{-1}.

Standard heat of formation of SiD is mentioned by HSC database (1999) [34] as $\Delta_f H°(298K) = 368.7$ kJ mol^{-1}. This value was adopted by us. The diatomic constants were taken from Huber & Herzberg [24].

SiT Silicontritide was reported by the HSC database [34] from a Russian unidentified reference as $\Delta_f H°(298K) = 369.1$ kJ mol^{-1} which was used here.

Grev and Schaefer (1992) [44] calculated for SiH$^+$ $\Delta_f H°(0 K) = 1139.5$ kJ mol^{-1}. M.C. Lin and Coworkers (2017) [61] found $\Delta_f H°(298K) = 1149.4$ kJ mol^{-1}. The heat of formation for SiH$^+$ was taken from Boo and Armentrout [8] as $\Delta_f H°(298K) = 1144.3 \pm 8.$ kJ mol^{-1} and for SiH$^-$ the G3B3 result in thermal electron convention is $\Delta_f H°(298K) = 298.8 \pm 8.$ kJ mol^{-1}. Michels and Hobbs (1993) [47] report for SiH$^-$ using the G2 method in thermal electron convention transformed value of $\Delta_f H°(298K) = 246.5$ kJ mol^{-1}.

SiD+ was suggested by Boo and Armentrout [8] as $\Delta_f H°(298K) = 1145.16$ kJ mol^{-1} and used here.

SiD_2 , SiD_2^+, SiD_2^-: Silylene-D2 and ions.

This compound was reported by Boo and Armentrout (1987) [8] as $\Delta_f H°(298K) = 295.4 \pm 10.$ kJ mol^{-1}. Based on $\Delta_f H°(0K)$ SiH$_2$ $= 265.5 \pm 8.$ kJ mol^{-1} we obtain for SiD$_2$ the value of $\Delta_f H°(0K) = 264.4 \pm 8.$ kJ mol^{-1} ($\Delta_f H°(298K) = 262.8 \pm 8.$ kJ mol^{-1}).

The cation SiD$_2^+$ was also reported by Boo and Armentrout [8] $\Delta_f H°(298K) = 1160.6 \pm 6.$ kJ mol^{-1}, and based on G3B3 $\Delta_f H°(0K)$ SiH$_2$+ $= 1152.34 \pm 8.$ kJ mol^{-1} we obtain for SiD$_2$+ $\Delta_f H°(0K) = 1150.9 \pm 8.$ kJ mol^{-1} ($\Delta_f H°(298K) = 1155.6 \pm 8.$ kJ mol^{-1}). The anion SiD$_2^-$ was not reported in the literature and the present calculation shows $\Delta_f H°(0K) = 161.2 \pm 8.$ kJ mol^{-1} ($\Delta_f H°(298K) = 147.3 \pm 8.$ kJ mol^{-1}) The ions at 298 K are reported in the thermal electron convention.

$SiHT_3$ Tritritiumsilane T3:

This tritium compound is published only by the Russian Glushko, Gurvich et al. edition (1970) [4] $\Delta_f H°(298K) = 27.5$ kJ mol^{-1}. The present calculation based on $\Delta_f H°(0K)$ (SiH$_4$)$= 44.3$ kJ mol^{-1} result in $\Delta_f H°(298K) = 27.610$ kJ mol^{-1} ($\Delta_f H°(0K) = 36.13$ kJ mol^{-1}).

SiH₂ Singlet and Triplet, SiH₂⁺, SiH₂⁻: **Silylene and their ions.**

The singlet of Silylene $^1SiH_2$ is reported by Boo and Armentrout (1987) [8] with $\Delta_fH°(298K) = 288.7 \pm 8.4$ kJ mol^{-1}; by Michels and Hobbs (1993) [47] as G2-calculation result $\Delta_fH°(298K) = 260.2$ kJ mol^{-1} , by Katzer et al. (1997) [31] as $\Delta_fH°(298K) = 272.9$ kJ mol^{-1}; by Becerra and Walsh (1998) [6] as $\Delta_fH°(298K) = 273 \pm 2.$ kJ mol^{-1}, by Feller and Dixon (1999) [43] $\Delta_fH°(0\ K) = 268.2 \pm 1.6$ kJ mol^{-1}, by Jursic (2000) [45] $\Delta_fH°(0\ K) = 279.0$ kJ mol^{-1}, by Sukkaew et al. (2014) [16] using G4 and G4(MP2) calculations as $\Delta_fH°(298K)$ $= 265.1$ and 262.0 kJ mol^{-1} respectively. A value of $\Delta_fH°(298K) = 263.$ kJ/mol (62.87 kcal/mol) is obtained within the RMG-SiliconHydrideLibary thermochemical data in NASA format as provided by West and coworkers (2016) [18] within the chem_annotated.inp- file of the supplement. The present G3B3 calculation result for the singlet Silylene is $\Delta_fH°(298K) = 263.8 \pm 8.$ kJ mol^{-1} ($\Delta_fH°(0K) = 265.5 \pm 8.$ kJ mol^{-1}).

The triplet Silylene $^3SiH_2$ is reported by Michels and Hobbs (1993) [47] for G2 method usage as $\Delta_fH°(298K) = 358.2$ kJ mol^{-1}; by Katzer et al. (1997) [31] as $\Delta_fH°(298K)$ $= 355.2$ kJ mol^{-1}; by Feller and Dixon (1999) [43] as $\Delta_fH°(0\ K) = 357.3 \pm 1.6$ kJ mol^{-1}, by Jursic (2000) [45,46] $\Delta_fH°(0\ K) = 362.8$ kJ mol^{-1}; by Sukkaew et al. (2014) [16] using G4 and G4(MP2) methods as $\Delta_fH°(298K) = 359.9$ and $355.2.$ kJ mol^{-1} respectively. The G3B3 value is $\Delta_fH°(298K) = 354.6 \pm 8.$ kJ mol^{-1}.

For the cation SiH₂⁺ the thermal electron value of Nguyen et al (2017) [61] is $\Delta_fH°(298K) = 1161.4.-1164.9$ kJ mol^{-1}. It was also reported by Boo and Armentrout [8] $\Delta_fH°(298K) = 1155.2 \pm 7.$ kJ mol^{-1}. and the G3B3 calculation results gives a value for the heat of formation of $\Delta_fH°(298K) = 1156.9. \pm 8.$ kJ mol^{-1}.

The anion SiH₂⁻ was calculated by Michels and Hobbs (1993) [47] with G2 method in ion convention. Transformation in thermal convention by subtraction of 6.197 kJ/mol per negative charge results in a value of $\Delta_fH°(298K) = 158.6$ kJ mol^{-1} , our G3B3 calculation produces a value of $\Delta_fH°(298K) = 153.7. \pm 8.$ kJ mol^{-1}. All ion values are reported in the thermal electron convention.

SiH₂T₂: **Silane-T₂, Ditritiumsilane.**

This tritium compound was reported only in the old Russian publication of Glushko, Gurvich, et al. (1970) [4] $\Delta_fH°(298K) = 29.6$ kJ mol^{-1}. The present calculation based on $\Delta_fH°(0K)(SiH_4) = 44.3$ kJ mol^{-1} lists $\Delta_fH°(298K)$ 30.09 kJ mol^{-1} ($\Delta_fH°(0K) = 39.08$ kJ mol^{-1}).

SiH_3, SiH_3^+, SiH_3^- : Silyl radical and ions.

Silyl was reported by Boo and Armentrout (1987) [8] as $\Delta_fH°(298K)=202.9$ kJ mol^{-1}; by Ho and Melius (1990) [10] $\Delta_fH°(298K)=198.5\pm4.2.$ kJ mol^{-1}; by Gurvich (1991) [5] $\Delta_fH°(298K)=197.7$ kJ mol^{-1}; Michels and Hobbs (1993) [47] report for G2 method $\Delta_fH°(298K)=194.6$ kJ mol^{-1}; Ochterski et al. (1995) [7] $\Delta_fH°(298K)=200.$ kJ mol^{-1} as well as Katzer et al (1997) [31], Beccerra and Walsh (1998) [6] report $\Delta_fH°(298K)=200.5\pm2.$ kJ mol^{-1}. Feller and Dixon (1999) [43] report $\Delta_fH°(0$ K$)=197.9$ kJ mol^{-1}; Jursic (2000) [45] $\Delta_fH°(0$ K$)=209.2$ kJ mol^{-1} and Sukkaew et al. (2014) [16] as $\Delta_fH°(298K)=197.7$ kJ mol^{-1} using G4 and $\Delta_fH°(298K)=193.7$ kJ mol^{-1} with G4(MP2) method. The present G3B3 result is $\Delta_fH°(298K)=195.6\pm8.$ kJ mol^{-1}.

The cation SiH_3^+ was listed by Boo and Armentrout (1987) [8] as $\Delta_fH°(298K)$ $=992.\pm8.$ kJ mol^{-1}, Grev and Schaefer (1992) [44] calculated $\Delta_fH°(0$ K$)=989.9\pm6.$ kJ mol^{-1}; Nguyen et al (2017) [61] using CCSD(T)/CBS report $\Delta_fH°(298K)=999.8\pm5.$ kJ mol^{-1}, and the present G3B3 lists $\Delta_fH°(298K)=988.9\pm8.$ kJ mol^{-1} all results of the ions are in thermal electron convention.

The anion SiH_3^- was reported by Michels and Hobbs (1993) [47] for G2 method in ion convention, which excludes the enthalpy of the electron. Transformation to thermal convention through subtraction of 6.197 kJ/mol per negative charge results in $\Delta_fH°(298K)$ $= 51.5$ kJ mol^{-1} and the G3B3 calculation was $\Delta_fH°(298K)=52.3\pm8.$ kJ mol^{-1}. The ions are reported in the thermal electron convention.

SiD_3 SiD_3+ SiD_3- Silyl-D3 and ions.

For the deuterated silyl radical. Boo and Armentrout (1987) [8] reported $\Delta_fH(298$ K$)=198.7\pm8.$ kJ mol^{-1}. The present calculation based on $\Delta_fH(0$ K$)(SiH_3)=201.090\pm8.$ kJ mol^{-1} is $\Delta_fH(0$ K$)=196.8\pm8.$ kJ mol^{-1} for SiD_3 ($\Delta_fH(298)==191.8\pm8.$ kJ mol^{-1}).

The cation SiD_3+ was reported by Boo and Armentrout [8] $\Delta_fH(298$ K$)=996.9\pm8.$ kJ mol^{-1}. The present calculation based on $\Delta_fH(0$ K$)(SiH_3+)=988.206\pm8.$ kJ mol^{-1} as a value obtained from G3B3 calculation results in $\Delta_fH(0$ K$)(SiD_3+)=988.839\pm8.$ kJ mol^{-1} ($\Delta f H(298$ K$)=996.13\pm8.$ kJ mol^{-1}).

The anion SiD_3^- is calculated for the first time from $\Delta_fH(0$ K$)SiH_3=64.053$ kJ mol^{-1} and the value obtained is $\Delta_fH°$ (298 K) $=37.431\pm8.$ kJ mol^{-1} ($\Delta_fH°$ (0 K)$=55.003\pm8.$ kJ mol^{-1}. The ions are reported in the thermal electron convention.

SiH₃T Silane-T (Monotritiumsilane).

Monotritiumsilane was reported in the Russian publication of Glushko, Gurvich et al. (1970) [4] as $\Delta_f H°(298K) = 32.2.$ kJ mol^{-1}. The calculation based on $\Delta_f H°(0K)(SiH_4)$ $_i$=44.319 kJ mol^{-1} resulted in $\Delta_f H°(0K) = 41.815 \pm 8.$ kJ mol^{-1} $\Delta_f H°(298K) = 32.451 \pm 8.$ kJ mol^{-1}.

SiH₄, SiH₄⁺, SiD₄, SiT₄,: Silane and Silane cation, Silane-D4 and Silane-T4.

SiH_4 is a pyrophoric gas at STP and was proposed to be used as igniter of Hydrogen jets instead of a spark. SiH_4 was calculated by JANAF (1976) [3] $\Delta_f H°(298K) = 34.3 \pm 2.$ kJ mol^{-1}. Ho and Melius (1990) [10] report $\Delta_f H°(298K) = 34.3$ kJ mol^{-1} as well as Takhistov and Golovin (2006) [48] . Michels and Hobbs (1993) [47] report for G2 method $\Delta_f H°(298K)$ = 24.7 kJ mol^{-1}, Katzer et al. (1997) [31] $\Delta_f H°(298K) = 34.4$ kJ mol^{-1} , Feller and Dixon (1999) [43] report $\Delta_f H°(0\ K) = 36.4 \pm 2.$ kJ mol^{-1}. Jursic (2000) [45] reports for the CBSQ calculation $\Delta_f H°(0\ K) = 42.3$ kJ mol^{-1}. Broadbelt and coworkers (2004) [9] calculated $\Delta_f H°(298K) = 33.9$ kJ mol^{-1} using bond additivity correction (BAC). Hidding and Pfitzner (2006) [53] report $\Delta_f H°(298K) = 34.5$ kJ mol^{-1} . Gurvich's (1991) [5] value $\Delta_f H°(298K)$ =34.7±1.5 kJ mol^{-1} was used for calculation of the polynomials. The G3B3 value found $\Delta_f H°(298K) = 30.1 \pm 8.$ kJ mol^{-1} was lower than all other values in literature although within the error range reported. The value of $\Delta_f H°(298K) = 23.3$ kJ mol^{-1} was calculated from the NASA polynomials of thermochemical data within the RMG-SiliconHydrideLibary taken from chem_annotated.inp-file of the supplement of West and coworkers 2016 [18] .

Boo and Armentrout [8] do not report a definite SiD_4 heat of formation. The calculation was based on $\Delta_f H°(0K)(SiH_4)$ which yields $\Delta_f H°(0K) = 31.6 \pm 8.$ kJ mol^{-1} ($\Delta_f H°(298K)= =22.8 \pm 8.$ kJ mol^{-1}).

Thermochemical data of SiT_4 Tetratritiumsilane is calculated for the first time based on $\Delta_f H°(0K)(SiH_4) = 44.3 \pm 8.$ kJ mol^{-1}, which result in $\Delta_f H°(0K) = 25.33 \pm 8.$ kJ mol^{-1} ($\Delta_f H°(298K) = 17.3 \pm 8.$ kJ mol^{-1}).

The cation SiH_4^+ was calculated by Nguyen et al (2017) [63] at the CCSD(T)/CBS method thermal electron is $\Delta_f H°(298K) = 1120.4$ kJ mol^{-1}. Our calculation was performed according to the NIST CCCBDB [25] B3LYP/6-31G(d) vibrations and moments of inertia. The present thermal electron G3B3 value is $\Delta_f H°(298K) = 1144.6 \pm 8.$ kJ mol^{-1}.

SiO, SiO$^+$, SiO$^-$: Oxosilyum and ions.

The constants for diatomic molecule SiO were taken from Huber and Herzberg (1977) [24]. The calculated G3B3 enthalpy of formation was $\Delta_f H°(298K) = -102.2\pm8.$ kJ mol^{-1}. JANAF (1967) [3] reports $\Delta_f H°(298K) = -100.4\pm8.$ kJ mol^{-1}. Gurvich (1994) [5] reports $\Delta_f H°(298K) = -98.7$ kJ mol^{-1}.

No mention in the literature was found for the ions. The calculated thermal electron G3B3 values for the cation SiO$^+$ and the anion SiO$^-$ is $\Delta_f H°(298K) = 1020.5\pm8.$ kJ mol^{-1} and $\Delta_f H°(298K) = -117.0\pm8.$ kJ mol^{-1} respectively.

SiO$_2$, SiO$_2^-$ Silica and anion.

The SiO$_2$ gas compound was calculated using the NIST CCCBDB [25] vibrations and B$_0$ rotation constant (for their G3B3 method). The enthalpy of formation was taken from Gurvich (1989) [5] $\Delta_f H°(298K) = -322.1\pm10.$ kJ mol^{-1}. McBride in the corrected NASA database reported the same value. JANAF (1967) [3] reports $\Delta_f H°(298K) = -305.4$ kJ mol^{-1} and Benson (1976) [33] by the Group Additivity method estimated $\Delta_f H°(298K) = -318.\pm12.$ kJ mol^{-1}.

The anion thermochemistry is mentioned in the literature by Wang, Wu et al. (1996) [51] $\Delta_f H°(298K) = -531.$ kJ mol^{-1} as an estimate, and the present thermal electron G3B3 lists $\Delta_f H°(298K) = -488.4\pm8.$ kJ mol^{-1}.

Si$_2$F$_6$, Si$_2$F$_6^+$,Si$_2$F$_6^-$: Hexafluorodisilane F$_3$Si-SiF$_3$ and ions.

Standard heat of formation of F$_3$Si-SiF$_3$ was reported by Ho and Melius (1990) [10] as $\Delta_f H°(298K) = -2383.3\pm14.5$ kJ mol^{-1}. This value vas used in 2001 by Lyman [14] as well as in the NASA database [37] where the value was erroneously referenced to Lymann and is included in the HSC database [34] too. The present G3B3 calculation lists $\Delta_f H°(298K) = -2346\pm7.$ kJ mol^{-1}.

The cation Si$_2$F$_6^+$ and anion Si$_2$F$_6^-$ thermochemistry are calculated for the first time and their thermal electron G3B3 values are $\Delta_f H°(298K) = -1205.\pm8.$ kJ mol^{-1} and $\Delta_f H°(298K) = -2401.7\pm8.$ kJ mol^{-1} respectively. The cation has no CAS number.

Si$_2$OF$_6$ Hexafluorodisiloxane F$_3$Si-O-SiF$_3$

This compound was listed in the HSC thermal database [34] as $\Delta_f H°(298K) = -2904.0\pm8.$ kJ mol^{-1} and the present G3B3 value is $\Delta_f H°(298K) = -2865.8\pm8.$ kJ mol^{-1}.

Si_2H, Si_2D Disilyne Hydride and Deuteride radicals HSi≡Si* DSi≡Si*.

Boo and Armentrout (1987) [8] quote Walsh for a value of $\Delta_fH°$(298K) =603.3±12.5. kJ mol^{-1}. Curtiss et al (1991) [57] using G2 method report $\Delta_fH°$(0K) =532.2 kJ mol^{-1}. The G3B3 calculation showed $\Delta_fH°$(0K) =492.25±8. kJ mol^{-1}. ($\Delta_fH°$(298K) =492.18±8. kJ mol^{-1}).

The enthalpy of formation of DSi≡Si* was calculated from the enthalpy $\Delta_fH°$(0K) of Si$_2$H and lists $\Delta_fH°$(0K) =491.3±8. kJ mol^{-1}. ($\Delta_fH°$(298K) =493.18±8. kJ mol^{-1}).

Si_2H_2, Si_2H_2+, Si_2D_2 Disilyne HSi≡SiH cation and disilyne-D2

This compound that resembles acetylene vas reported first by Katzer et. al (1997) [31] as $\Delta_fH°$(298K) =464.4 kJ mol^{-1}. Broadbelt and coworkers (2004) [9] report $\Delta_fH°$(298K) =454. kJ mol^{-1} using G3B3 calculation. $\Delta_fH°$(298K) =374.5. kJ mol^{-1} is reported by Boo and Armentrout (1987) [8]. The present G3B3 calculation lists $\Delta_fH°$(298K) =452.1.±8. kJ mol^{-1}.

Boo and Armentrout (1987) [8] suggested for the cation HSi≡SiH+ an upper limit of $\Delta_fH°$(298K) =1121.3±10.9 kJ mol^{-1} but obtained by analysis of a different reaction a higher upper limit $\Delta_fH°$(298K) =1278.±4.6. kJ mol^{-1}. The present G3B3 calculation is $\Delta_fH°$(298K) =1267.±8. kJ mol^{-1}. Both values are in thermal electron convention.

The Deuterated compound DSi≡SiD was calculated based on the standard heat of formation of HSi≡SiH $\Delta_fH°$(0K) =453.4.±8. kJ mol^{-1} to give for DSi≡SiD $\Delta_fH°$(0K) =451.96±8. kJ mol^{-1} ($\Delta_fH°$(298K) =451.3±8. kJ mol^{-1}).

Si_2H_4, $Si_2H_4^+$: Disilene (H$_2$Si=SiH$_2$) and cation.

The singlet compound disilene was calculated by Becerra and Walsh (1998) [6] with an heat of formation $\Delta_fH°$(298K) =261.±8. kJ mol^{-1}. Ruscic and Berkovitz (1991) [35] in a photo-ionization study report $\Delta_fH°$(298K) =275±4. kJ mol^{-1}. Ho and Melius (1990) [10] report $\Delta_fH°$(298K) =263.±10. kJ mol^{-1}. Katzer et al. (1997) [31] calculated $\Delta_fH°$(298K) =281.2 kJ mol^{-1}, Broadbelt and coworkers (2004) [9] report $\Delta_fH°$(298K) =274.9 kJ mol^{-1} (BAC method). Sukkaew et al (2013) [16] report $\Delta_fH°$(298K) =275.2-268.3 kJ mol^{-1}. The value of $\Delta_fH°$(298K) =270.1 kJ/mol^{-1} was calculated from the NASA polynomials of the Silicon Hydride Library of the chem_annotated.inp-file of the supplement of West and coworkers 2016 [18]. The present G3B3 calculation shows $\Delta_fH°$(298K) =273.1±8. kJ mol^{-1}.

The cation was reported by Curtiss et al (1991) [57] $\Delta_f H°(298K) = 1066.$ kJ mol^{-1}, by Ruscic and Berkowitz (1991) [35] $\Delta_f H°(298K) = 1070.6.\pm 2.5$ kJ mol^{-1} and the thermal electron G3B3 calculation resulted in $\Delta_f H°(298K) = 1066.\pm 8.$ kJ mol^{-1}.

Si$_2$H$_4$, Si$_2$H$_4$$^+$, Si$_2H_4$$^-$ DiSilanylidene SiH$_3$-SiH and ions.

Becerra and Walsh (1987) [56] have experimentally found $\Delta_f H°(298K) = 312.\pm 8.$ kJ mol^{-1} and report [6] calculated values of Pople and coworkers (1991) [57] $\Delta_f H°(298K)$ $= 300.$ kJ mol^{-1}, Ho and Melius (1990)[10] $\Delta_f H°(298K) = 313.\pm 11.$ kJ mol^{-1}, Sax and Kalcher (1991) [58] $\Delta_f H°(298K) = 317.$ kJ mol^{-1}, and Boatz and Gordon (1990) [59] $\Delta_f H°(298K) = 305.$ kJ mol^{-1}. Katzer et al. (1997) [31] calculated $\Delta_f H°(298K) = 318.8$ kJ mol^{-1}, Broadbelt and coworkers (2004) [9] calculated $\Delta_f H°(298K) = 306.7$ kJ mol^{-1}, Sukkaew et al (2013) [16] report $\Delta_f H°(298K) = 305.1$-$303.1$ kJ mol^{-1}, and Nguyen and M.C. Lin (2017) [62] using CCSD(T) method list $\Delta_f H°(0K) = 323.8$ kJ mol^{-1} The present G3B3 calculation lists $\Delta_f H°(298K) = 304.2.\pm 8.$ kJ mol^{-1} and $\Delta_f H°(0K) = 312.8 \pm 8.$ kJ mol^{-1}.

The cation Si$_2$H$_4$+ is calculated by Curtiss et al (1991) [57] $\Delta_f H°(0K) = 1117.5$ kJ mol^{-1} and our present thermal electron G3B3 calculation $\Delta_f H°(298K) = 1121.2.\pm 8.$ kJ mol^{-1}. The anion Si$_2$H$_4$- is not reported to our knowledge and our thermal electron G3B3 calculation is $\Delta_f H°(298K) = 138.97.\pm 8.$ kJ mol^{-1}.

Si$_2$H$_5$ Si$_2$H$_5$- Disilanyl and anion SiH$_3$-SiH$_2$*

The radical was experimentally measured by Ruscic and Berkowitz (1991) [35] $\Delta_f H°(0K) < 264.8$ kJ mol^{-1} and a less well defined value of 247.7 kJ mol^{-1} is given which is nearer to the calculated value by Nguyen and M.C. Lin (2017) [62] $\Delta_f H°(0K) = 248.9$ kJ mol^{-1}. The G3B3 present calculation reads $\Delta_f H°(298K) = 227.2 \pm 8.$ kJ mol^{-1} and $\Delta_f H°(0K) = 239.9 \pm 8.$ kJ mol^{-1}.

To our best knowledge the anion's SiH$_3$-SiH$_2$*- thermochemistry is not known. The thermal electron G3B3 value found is $\Delta_f H°(298K) = 39.3 \pm 8.$ kJ mol^{-1}

Si$_2$H$_6$, Si$_2$H$_6$$^+$ Disilane H$_3$Si-SiH$_3$ and cation.

The Disilane is also a pyrophoric gas at STP conditions like SiH$_4$. H$_3$Si-SiH$_3$ was listed first by Walsh in Rappoport's edited book (1989) [1] as $\Delta_f H°(298K) = 80.3 \pm 1.5$ kJ mol^{-1} and this value was used to calculate the polynomials. Katzer et al. (1997) [31] calculated $\Delta_f H°(298K) = 79.9$ kJ mol^{-1}, Broadbelt and coworkers (2004) [9] report

$\Delta_f H°(298K) = 80.8$ kJ mol^{-1}; Allendorf's database (2006) (now removed from the internet) listed $\Delta_f H°(298K) = 79.9 \pm 4.2$ kJ mol^{-1}; Hidding and Pfitzner (2006) [53] report $\Delta_f H°(298K) = 79.76$ kJ mol^{-1}, the present G3B3 (unused) calculation was $\Delta_f H°(298K) = 73.6 \pm 8.$ kJ mol^{-1}; the heat of formation value for RMG calculated from NASA polynomials in the supplement of West and coworkers 2016 [18] was $\Delta_f H°(298K) = 66.8$ kJ mol^{-1}

The cation H$_3$Si-SiH$_3$$^+$ was first reported by Lias et al (1988) [15] $\Delta_f H°(298K) = 1022.$ kJ mol^{-1} then by Ruscic and Berkowitz (1991) [35] $\Delta_f H°(298K) = 1041.7. \pm 25.$ kJ mol^{-1}, Curtiss et al (1991) [57] $\Delta_f H°(298K) = 1025.$ kJ mol^{-1} and the present thermal electron G3B3 calculation listed $\Delta_f H°(298K) = 1016. \pm 8.$ kJ mol^{-1} .

Si_3H_5, $Si_3H_5^+$, $Si_3H_5^-$ H$_2$Si=SiH-SiH$_2$* 2-Trisilenylium and ions.

The present G3B3 value for the radical is $\Delta_f H°(298K) = 433.3 \pm 8.$ kJ mol^{-1}.

The ions enthalpy of formation is not mentioned in the literature and the thermal electron G3B3 values are $\Delta_f H°(298K) = 1107.6 \pm 8.$ kJ mol^{-1} for the cation 2-Trisilenylium and $\Delta_f H°(298K) = 209. \pm 8.$ kJ mol^{-1} for the anion.

Si_3H_5, $Si_3H_5^+$, $Si_3H_5^-$ Cyclotrisilane Radical (cylcotrisilanyl) and ions.

This cyclic radical was reported by Katzer et al. (1997) [31] with $\Delta_f H°(298K) = 420.2$ kJ mol^{-1}. The present radical G3B3 calculation result in $\Delta_f H°(298K) = 387. \pm 8.$ kJ mol^{-1}.

No reports were found for the cyclotrisilane radical cation Si$_3$H$_5$$^+$ and anion Si$_3$H$_5$$^-$. The thermal electron G3B3 values are $\Delta_f H°(298K) = 1096.1 \pm 8.$ kJ mol^{-1} and $\Delta_f H°(298K) = 147.9 \pm 8$ kJ mol^{-1} respectively.

Si_3H_6, $Si_3H_6^+$, $Si_3H_6^-$ Cyclotrisilane and ions.

Heat of formation of cyclotrisilane was reported by Katzer et al. (1997) [31] as $\Delta_f H°(298K) = 281.6$ kJ mol^{-1} and by Broadbelt and coworkers (2004) [9] using bond additivity corrections as $\Delta_f H°(298K) = 269.0$ kJ mol^{-1}. The heat of formation value calculated from NASA polynomials of the SiliconHydrideLibrary in the supplement of West and coworkers 2016 [18] chem_annotated.inp-file is the same as that of Katzer et al. (1997) [31. The present G3B3 calculation lists $\Delta_f H°(298K) = 257.3 \pm 8$ kJ mol^{-1}.

The enthalpy of formation of the ions were not reported in literature to our knowledge and our thermal electron G3B3 value lists $\Delta_f H°$(298K) = 1063.5±8 kJ mol^{-1} for the cation and $\Delta_f H°$(298K) = 289.2±8 kJ mol^{-1} for the anion.

n-Si₃H₇ n-Si₃H₇+ n-Si₃H₇- **Trisilan-1-yl and ions SiH₃-SiH₂-SiH₂***

Katzer et al. (1997) [31] calculated $\Delta_f H°$(298K) = 274.8 kJ mol^{-1}, Ragunath and M.C. Lin (2013) [64] report $\Delta_f H°$(0K) = 287.4±4.2 kJ mol^{-1}. Nguyen and M.C. Lin (2017) [62] using CCSD(T) method list $\Delta_f H°$(0K) = 288,7 kJ mol^{-1}. The G3B3 value is $\Delta_f H°$(298K) = 262.4±8. kJ mol^{-1}, ($\Delta_f H°$(0K) = 280.1±8. kJ mol^{-1}).

The cation SiH₃-SiH₂-SiH₂*+ is not mentioned in the literature and has no CAS number. The thermal electron G3B3 value found is $\Delta_f H°$(298K) = 965.8±8. kJ mol^{-1}. The anion SiH₃-SiH₂-SiH₂*- has a G3B3 thermal electron value of $\Delta_f H°$(298K) = 56.2±8. kJ mol^{-1}.

i-Si₃H₇ i-Si₃H₇+ i-Si₃H₇- **Disilanyl-1-silyl (Trisilan-2-yl) SiH₃-SiH*-SiH₃ and ions.**

The *iso*-Si₃H₇ radical is listed by Katzer et al. (1997) [31] $\Delta_f H°$(298K) = 268.2 kJ mol^{-1}. Ragunath and M.C. Lin (2013) [64] report $\Delta_f H°$(0K) = 279.9±4.2 kJ mol^{-1}. Our G3B3 value is $\Delta_f H°$(298K) = 251.7±8. kJ mol^{-1}, ($\Delta_f H°$(0K) = 269.9±8. kJ mol^{-1}).

The ions of the *iso*-Si₃H₇ radical were not reported and the thermal electron G3B3 values calculated are $\Delta_f H°$(298K) = 977.6±8. kJ mol^{-1} and $\Delta_f H°$(298K) = 28.8±8. kJ mol^{-1} for the cation SiH₃-SiH*-SiH₃+ and anion SiH₃-SiH*-SiH₃-, respectively.

Si₃H₈ , Si₃H₈⁻ **Trisilane H₃Si-SiH₂-SiH₃ and anion .**

Trisilane was listed by Ho et al (1986) [11] $\Delta_f H°$(298K) = 118.4±12. kJ mol^{-1}; by Bercerra and Walsh (1998) [6] as $\Delta_f H°$(298K) = 121.±4.4 kJ mol^{-1}. Katzer et al. (1997) [31] calculated $\Delta_f H°$(298K) = 120.6 kJ mol^{-1}, Ochterski et al. (1995) [7] report $\Delta_f H°$(298K) = 120.5 kJ mol^{-1}. Allendorf et al. (1992) [30] report $\Delta_f H°$(298K) = 120.9 kJ mol^{-1}. Hidding and Pfitzner (2006) [53] list $\Delta_f H°$(298K) = 120.95 kJ mol^{-1}. Sukkaew et al. (2014) [16] $\Delta_f H°$(298K) = 111.5 kJ mol^{-1} using the G4 method. Heat of formation of $\Delta_f H°$(298K) = 126.4 kJ mol^{-1}, is calculated from NASA polynomials in the supplement of West and coworker (2016) [18], which uses group additivity values of silicon species. The present G3B3 calculation is $\Delta_f H°$(298K) = 109.2±8. kJ mol^{-1} in very good agreement with Sukkaew et al. [16].

The anion is not reported in the literature and the thermal electron value obtained from use of G3B3 method result in $\Delta_f H°(298K) = 122.12 \pm 8.$ kJ mol^{-1}. No CAS number was found for the anion.

Si_4H_7 , $Si_4H_7^+$, $Si_4H_7^-$ Cyclotetrasilane radical (Cyclotetrasilanyl) and ions.

The heat of formation of this cyclic radical was calculated by Katzer et al. (1997) [31] as $\Delta_f H°(298K) = 372.8$ and 369.5 kJ mol^{-1}, depending on the used basis set in their quantum chemical calculations. The present G3B3 result is $\Delta_f H°(298K) = 339.2 \pm 12.$ kJ mol^{-1}.

No quotations for the enthalpy of formation of the ions was found in the literature, and the thermal electron G3B3 results are $\Delta_f H°(298K) = 1026.2 \pm 12.$ kJ mol^{-1} for the cation and $\Delta_f H°(298K) = 108.8 \pm 12.$ kJ mol^{-1} for the anion.

Si_4H_8 , $Si_4H_8^+$ Cyclotetrasilane and cation.

Heat of formation of cyclotetratilane was reported first by Katzer et al (1997) [31] $\Delta_f H°(298K) = 231.4$ kJ mol^{-1}; Broadbelt and coworkers (2004) [9] report $\Delta_f H°(298K) = 215.9$ kJ mol^{-1} by the BAC method and the present G3B3 result is $\Delta_f H°(298K) = 201.06 \pm 12.$ kJ mol^{-1}. West and coworkers 2016 [18] provide NASA polynomials in the chem_annotated.inp-file of the supplement, which result in $\Delta_f H°(298K) = 255.4$ kJ mol^{-1} .

No calculation of the cation was found in the literature and its thermal electron G3B3 calculation lists $\Delta_f H°(298K) = 1062.1 \pm 12.$ kJ mol^{-1}. No CAS number is available.

n-Si_4H_9 n-Si_4H_9+ n-Si_4H_9- Tetrasilanyl and ions SiH$_3$-SiH$_2$-SiH$_2$-SiH$_2$*

The enthalpy of formation of tetrasilane-1-yl was reported first by Katzer et al (1997) [31] $\Delta_f H°(298K) = 312.8$ kJ mol^{-1}; The G3B3 value calculated is $\Delta_f H°(298K) = 293.8 \pm 12.$ kJ mol^{-1}.

The cation SiH$_3$-SiH$_2$-SiH$_2$-SiH$_2$*+ is not reported in the literature and has no CAS number.   The thermal electron G3B3 value calculated for the cation is $\Delta_f H°(298K) = 940. \pm 12.$ kJ mol^{-1}. The anion SiH$_3$-SiH$_2$-SiH$_2$-SiH$_2$*- got a G3B3 value of $\Delta_f H°(298K) = 77.12 \pm 12.$ kJ mol^{-1}.

i-Si$_4$H$_9$ i-Si$_4$H$_9$+ i-Si$_4$H$_9$- Tetrasilenyl-1-silyl and ions SiH$_3$-SiH*-SiH$_2$-SiH$_3$

The heat of formation of Tetrasylenyl-1-silyl (Tetrasilane-2-yl) was reported by Katzer et al (1997) [31] $\Delta_f H°(298K) = 306.2$ kJ mol^{-1}; The G3B3 value found is $\Delta_f H°(298K) = 285.9 \pm 12.$ kJ mol^{-1}.

The cation SiH$_3$-SiH*-SiH$_2$-SiH$_3$+ has no CAS number. The thermal electron G3B3 value found is $\Delta_f H°(298K) = 984.9 \pm 12.$ kJ mol^{-1}. The anion SiH$_3$-SiH*-SiH$_2$-SiH$_3$- got a G3B3   value of $\Delta_f H°(298K) = 47.9 \pm 12.$ kJ mol^{-1}.

Si$_4$H$_9$ Si$_4$H$_9$+ Si$_4$H$_9$- Trisilanyl-2-silyl and ions (SiH$_3$)$_2$-SiH-SiH$_2$*

The heat of formation of Trisilanyl-2-silyl (2-silyltrisilan-1-yl) was reported by Katzer et al (1997) [31] $\Delta_f H°(298K) = 312.1$ kJ mol^{-1}; The G3B3 value found is $\Delta_f H°(298K) = 287.5 \pm 12.$ kJ mol^{-1}.

The cation (SiH$_3$)$_2$-SiH-SiH$_2$*+ has no CAS number. The thermal electron G3B3 value calculated is $\Delta_f H°(298K) = 993.9 \pm 12.$ kJ mol^{-1}. The anion (SiH$_3$)$_2$-SiH-SiH$_2$*- got a G3B3 value of $\Delta_f H°(298K) = 66.3 \pm 12.$ kJ mol^{-1}.

Si$_4$H$_9$ Si$_4$H$_9$- Disilanyl-1,1-disilyl and anion (SiH$_3$)$_3$-Si*

The G3B3 value calculated was $\Delta_f H°(298K) = 270.6 \pm 12.$ kJ mol^{-1}.

The thermal electron G3B3 value of the anion Trisilane-2-silyl (SiH$_3$)$_3$-Si*- is $\Delta_f H°(298K) = 17.85 \pm 12.$ kJ mol^{-1}.

n-Si$_4$H$_{10}$ n-Si$_4$H$_{10}^-$, Tetrasilane SiH$_3$-SiH$_2$-SiH$_2$-SiH$_3$ and anion.

The heat of formation of Tetrasilane is reported by Katzer et al (1997) [31] as $\Delta_f H°(298K) = 160.3$ kJ mol^{-1}, by Broadbelt and coworkers (2004) [9] as $\Delta_f H°(298K) = 147.7$ and 158.6 kJ mol^{-1} for using atomization energy and bond additivity corrections, respectively, and by Hidding & Pfitzner (2006) [53] as $\Delta_f H°(298K) = 160.64$ kJ mol^{-1}. The present G3B3 calculation lists $\Delta_f H°(298K) = 142.86 \pm 12.$ kJ mol^{-1}.

The anion appears to be calculated for the first time and the thermal electron G3B3 results in $\Delta_f H°(298K) = 128.33 \pm 12.$ kJ mol^{-1}.

Si_5H_9, $Si_5H_9{}^+$, $Si_5H_9{}^-$ Cyclopentasilane radical [-SiH$_2$-SiH$_2$-SiH$_2$-SiH$_2$-SiH*-] and ions.

This radical is reported by Katzer et al (1997) [31] as $\Delta_f H°(298K) = 365.6$ kJ mol^{-1}. The present G3B3 result is $\Delta_f H°(298K) = 327.4 \pm 15.$ kJ mol^{-1}.

The thermochemistry of the cation and anion was not published to our knowledge and the thermal electron G3B3 calculation is $\Delta_f H°(298K) = 1027.4 \pm 15.$ kJ mol^{-1} and $\Delta_f H°(298K) = 79.8 \pm 15.$ kJ mol^{-1} respectively. The cation has no CAS number.

Si_5H_{10}, $Si_5H_{10}{}^+$ Cyclopentasilane [-SiH$_2$-SiH$_2$-SiH$_2$-SiH$_2$-SiH$_2$-] and cation.

Katzer et al. (1997) [31] reported for cyclopentasilane a heat of formation value $\Delta_f H°(298K) = 221.4$ kJ mol^{-1}. Swihart and Girshick (1999) [32] report $\Delta_f H°(298K) = 220.08$ kJ mol^{-1}. Broadbelt and coworkers (2004) [9] reported $\Delta_f H°(298K) = 193.7$ kJ mol^{-1} for using atomization energies and 207.9 kJ mol^{-1} for using bond additivity corrections. The present G3B3 calculation result in $\Delta_f H°(298K) = 189.4 \pm 15.$ kJ mol^{-1}.

The thermochemistry of the cation $Si_5H_{10}{}^+$ was not listed in the literature and the thermal electron value calculated is $\Delta_f H°(298K) = 1058.6 \pm 15.$ kJ mol^{-1}.

Si_5H_{12}, $Si_5H_{12}{}^-$ n-Pentasilane SiH$_3$-SiH$_2$-SiH$_2$-SiH$_2$-SiH$_3$ and anion.

Heat of formation of linear pentasilane was calculated by Katzer et al. (1997) [31] as $\Delta_f H°(298K) = 199.7$ kJ mol^{-1}, by Broadbelt and coworkers (2004) [9] as $\Delta_f H°(298K) = 182.4$ kJ mol^{-1} using atomization energies and as 195.8 kJ mol^{-1} using bond additivity corrections based on G3B3 calculations, and by Hidding and Pfitzer (2006) [53] $\Delta_f H°(298K) = 200.60$ kJ mol^{-1}. The present G3B3 calculation results in $\Delta_f H°(298K) = 177.37 \pm 15.$ kJ mol^{-1}.

The anion $Si_5H_{12}{}^-$ has not been reported and the present G3B3 thermal calculation reads $\Delta_f H°(298K) = 144.5 \pm 15.$ kJ mol^{-1}.

Si_6H_{11}, $Si_6H_{11}{}^+$, $Si_6H_{11}{}^-$ Cyclohexasilane radical [-SiH$_2$-SiH$_2$-SiH$_2$-SiH$_2$-SiH$_2$-SiH*-] (Cyclohexasilyl) and ions.

The present G3B3 calculation gives $\Delta_f H°(298K) = 351.6 \pm 20.$ kJ mol^{-1} for cyclohexasilyl.

The ions were not reported in the literature and the cation does not have a CAS number. The thermal electron G3B3 calculation results in $\Delta_f H°(298K) = 1039.4\pm20.$ kJ mol^{-1} and $\Delta_f H°(298K) = 99.1\pm20.$ kJ mol^{-1} for cation and anion respectively.

Si_6H_{12} , $Si_6H_{12}^+$, $Si_6H_{12}^-$ Cyclohexasilane [-SiH$_2$-SiH$_2$-SiH$_2$-SiH$_2$-SiH$_2$-SiH$_2$-] and ions.

Katzer et al. (1997) [31] reports $\Delta_f H°(298K) = 227.6$ kJ mol^{-1}; Broadbelt and coworkers (2004) [9] report $\Delta_f H°(298K) = 211.3$ kJ mol^{-1} using atomization energies and $\Delta_f H°(298K) = 227.6$ kJ mol^{-1} by using bond additivity corrections, and the present G3B3 result is $\Delta_f H°(298K) = 212.5\pm20.$ kJ mol^{-1}.

The cation and anion were not mentioned in the literature, the anion has no CAS number, and the present thermal electron G3B3 values are $\Delta_f H°(298K) = 1074.2\pm20.$ kJ mol^{-1} and $\Delta_f H°(298K) = 204.2\pm20.$ kJ mol^{-1} respectively.

Results for organic carbon containing silicon species:

CH_2Si, CH_2Si^- Silynemethylidyne HC≡SiH and anion.

The enthalpy of formation of this acetylene type compound was not found in literature, although its structure was calculated [54]. Our G3B3 calculation shows $\Delta_f H°(298K) = 452.4\pm8.$ kJ mol^{-1}.

The thermal electron G3B3 value for the anion HC≡SiH$^-$ is $\Delta_f H°(298K) = 338.6\pm8.$ kJ mol^{-1}.

CH_4Si, CH_4Si^+ , CH_4Si^- Methylenesilene H$_2$C=SiH$_2$ and ions.

This compound was published in the Chemkin thermochemical database (1982) [13] and by Allendorf et al. (1992) [30] $\Delta_f H°(298K) = 170.3$ kJ mol^{-1}. Wiberg and coworkers (1995) [7] report for calculations with CBS-Q method $\Delta_f H°(298K) = 193.7$ kJ mol^{-1}. Becerra and Walsh (1998) [6] reported $\Delta_f H°(298K) = 187.\pm6.$ kJ mol^{-1}. Sukkaew et al. (2014) [16] report for calculation results using G4 and G4(MP2) method $\Delta_f H°(298K) = 188.9$ and 184.3 kJ mol^{-1} respectively. The present G3B3 calculation reports $\Delta_f H°(298K) = 187.3\pm8.$ kJ mol^{-1}.

The ions were not reported in the literature and the thermal electron G3B3 value obtained was $\Delta_f H°(298K) = 1051.4\pm8.$ kJ mol^{-1} for the cation H$_2$C=SiH$_2^+$ and $\Delta_f H°(298K) = 177.4\pm8.$ kJ mol^{-1} for the anion H$_2$C=SiH$_2^-$.

CH₅Si , CH₅Si⁺ CH₅Si⁻ **Methylsilyl radical (H₃C-SiH₂*** ***) and ions.***

The heat of formation of the radical methylsilyl is reported by Wiberg and coworkers (1995) [7] as $\Delta_f H°(298K) = 149.4\pm8.$ kJ mol⁻¹. Allendorf et al. (1992) [30] report $\Delta_f H°(298K) = 139.1$ kJ mol⁻¹; Becerra and Walsh (1998) [6] report $\Delta_f H°(298K) = 141.4\pm6.$ kJ mol⁻¹. Sukkaew et al. report (2014) [16] for calculations with G4 and G4MP2 method $\Delta_f H°(298K) = 142.1$ and 138.2 kJ mol⁻¹ respectively. The present G3B3 calculation resulted in $\Delta_f H°(298K) = 141.9\pm8.$ kJ mol⁻¹.

The cation $CH_3SiH_2^{*+}$ and anion $CH_3SiH_2^{*-}$ are presented here for the first time and their thermal electron G3B3 calculations resulted in $\Delta_f H°(298K) = 864.9\pm8.$ kJ mol⁻¹ and $\Delta_f H°(298K) = 22.4\pm8.$ kJ mol⁻¹.

CH₆Si , CH₆Si⁺ **Methylsilane H₃C-SiH₃ and cation.**

Heat of formation of methylsilane is reported by Becerra and Walsh (1998) [6] as $\Delta_f H°(298K) = -29.1\pm4.$ kJ mol⁻¹. Wiberg and coworkers (1995) [7] report $\Delta_f H°(298K) = -25.1$ kJ mol⁻¹. Sukkaew et al. (2014) [16] report $\Delta_f H°(298K) = -26.6$ kJ mol⁻¹ and the present G3B3 calculation results in $\Delta_f H°(298K) = -27.4\pm8.$ kJ mol⁻¹.

The heat of formation of the cation $CH_3SiH_3^+$ was reported by Lias et al. (1988) [15] as $\Delta_f H°(298K) = 1009.$ kJ mol⁻¹ and the present G3B3 lists $\Delta_f H°(298K) = 1001.1\pm8.$ kJ mol⁻¹, both are thermal electron values.

CH₆Si₂ , CH₆Si₂⁺ , CH₆Si₂⁻ **1-Methyldisilydenyl H₃C-SiH₂SiH and ions**

This radical is reported by Sukkaew et al. (2014) [16] with $\Delta_f H°(298K) = 248.4$ and 247.7 kJ mol⁻¹ using G4 and G4MP2 methods. An erroneous value of $\Delta_f H°(298K) = -42.3$ kJ mol⁻¹ is in the NASA polynomials of the thermochemical data of the Chemkin database [13] The present G3B3 value is $\Delta_f H°(298K) = 247.9\pm8.$ kJ mol⁻¹, like the Sukkaew et al. [16] results.

The cation $H_3CSiH_2SiH^+$ and anion $H_3CSiH_2SiH^-$ were not reported and the anion has no CAS number. Their thermal electron G3B3 calculation results in $\Delta_f H°(298K) = 1038.3\pm8.$ kJ mol⁻¹ and $\Delta_f H°(298K) = 82.4\pm8.$ kJ mol⁻¹ respectively.

C₂H₄Si, C₂H₄Si⁺, C₂H₄Si⁻ , **Ethylidenesilylene H₂C=CH-SiH and ions.**

The heat of formation of ethylidenesilylene obtained from G3B3 calculation results in $\Delta_f H°(298K) = 307.4\pm8.$ kJ mol⁻¹. The same value is given by Allendorf et al. [12], and

Sukkaev et al. (2014) [16] reports $\Delta_f H°(298K) = 309.3$ and 306.8 kJ mol^{-1} using G4 and G4MP2 methods.

The heat of formation of the cation CH$_2$=CH-SiH$^+$ and anion CH$_2$=CH-SiH$^-$ obtained in thermal electron convention from G3B3 calculations are $\Delta_f H°(298K) = 1122.6\pm8.$ kJ mol^{-1} and $\Delta_f H°(298K) = 200.9\pm8.$ kJ mol^{-1} respectively. The anion has no CAS number

C_2H_6Si , $C_2H_6Si^+$, $C_2H_6Si^-$ Vinylsilane H$_2$C=CH-SiH$_3$ and ions.

 Heat of formation of vinylsilane was estimated by Lias et al. (1988) [15] $\Delta_f H°(298K) = 4.2\pm12.5.$ kJ mol^{-1}; by Allendorf et al. (1992) [30] $\Delta_f H°(298K) = 86.6$ kJ mol^{-1}; reported by Sukkaew et al. (2014) [16] $\Delta_f H°(298K) = 88.4$ and 90.2 kJ mol^{-1} using G4 and G4MP2 methods. The present G3B3 result is $\Delta_f H°(298K) = 90.2\pm8.$ kJ mol^{-1}.

The cation is estimated by Lias et al. (1988) [15] in thermal electron convention as $\Delta_f H°(298K) = 984.$ kJ mol^{-1} and the present thermal electron G3B3 value is $\Delta_f H°(298K) = 1062.6\pm8.$ kJ mol^{-1}. The anion is not reported and has no CAS number. The thermal electron G3B3 value is $\Delta_f H°(298K) = 165.2\pm8.$ kJ mol^{-1}.

C_2H_6Si , $C_2H_6Si^+$, $C_2H_6Si^-$ Methylmethylenesilane H$_2$C=SiH-CH$_3$ and ions.

This compound is listed by Allendorf et al.(1992)[30] with $\Delta_f H°(298K) = 86.6$ kJ mol^{-1}; and by Sukkaew et al. (2014) [16] with $\Delta_f H°(298K) = 92.6$ and 90.2 kJ mol^{-1} for using G4 and G4MP2 methods. The present G3B3 calculation lists $\Delta_f H°(298K) = 125.8\pm8.$ kJ mol^{-1}.

Both ions were not reported in the literature and have no CAS numbers. The thermal electron G3B3 values are $\Delta_f H°(298K)=938.1\pm8.$ kJ mol^{-1} for the cation H$_2$C=SiH-CH$_3$$^+$ and $\Delta_f H°(298K) = 131.6\pm8.$ kJ mol^{-1} for the anion H$_2$C=SiH-CH$_3$$^-$.

C_2H_8Si , $C_2H_8Si^+$, $C_2H_8Si^-$ Dimethylsilane CH$_3$-SiH$_2$-CH$_3$ and ions.

Heat of formation of dimethylsilane is reported by Becerra and Walsh (1998) [6] as $\Delta_f H°(298K) =-94.7\pm4.$ kJ mol^{-1}.The present G3B3 value is $\Delta_f H°(298K) = -88.2\pm8.$ kJ mol^{-1}.

The cation CH$_3$-SiH$_2$-CH$_3$$^+$ and anion CH$_3$-SiH$_2$-CH$_3$$^-$ were not reported and their thermal electron G3B3 values are $\Delta_f H°(298K) = 893.3\pm8.$ kJ mol^{-1} and $\Delta_f H°(298K) = 68.7\pm8.$ kJ mol^{-1} respectively. The anion has no CAS No.

C_2H_8Si , C_2H_8Si ⁺ Ethylsilane $C_2H_5SiH_3$ and cation.

Thermochemical data of ethylsilane was reported in the literature by Gordon, Boatz and Walsh (1989) [38] as $\Delta_fH°(298K) = -37.7$ kJ mol⁻¹; by Tel'noi and Rabinovitch (1980) [39] $\Delta_fH°(298K) = -34.3$ kJ mol⁻¹ and the present G3B3 calculation reads $\Delta_fH°(298K) = -36.1\pm8$. kJ mol⁻¹.

The cation $C_2H_5SiH_3$⁺ thermal electron G3B3 value reads $\Delta_fH°(298K) = 930.\pm8$. kJ mol⁻¹.

C_3H_9Si Trimethylsilyl radical $(CH_3)_3Si$*.

The radical trimethylsilyl is reported in the Chemkin database (1982) [13] with $\Delta_fH°(298K) = 13$. kJ mol⁻¹. Kalinovski, Gutman et al. (1994) [40] report $\Delta_fH°(298K) = 68.6\pm25$. kJ mol⁻¹. Becerra and Walsh (1998) [6] report $\Delta_fH°(298K) = 15.\pm7$. kJ mol⁻¹. The present G3B3 value is $\Delta_fH°(298K) = 24.2.\pm8$. kJ mol⁻¹.

$C_3H_{10}Si$ Trimethylsilane $(CH_3)_3SiH$.

Trimethylsilane was published in the Chemkin thermochemical database (1982) [13] with $\Delta_fH°(298K) = -164.8$ kJ mol⁻¹. Doncaster and Walsh (1986) [41] report an experimental value of $\Delta_fH°(298K) = -163.4\pm4$. kJ mol⁻¹. Allendorf and Melius (1992) [30] report $\Delta_fH°(298K) = -163.6$ kJ mol⁻¹. The present G3B3 value lists $\Delta_fH°(298K) = -153.2\pm8$. kJ mol⁻¹.

$C_4H_{12}Si$, $C_4H_{12}Si$⁺ Tetramethylsilane $(CH_3)_4Si$ and cation.

The heat of formation of tetramethylsilane is reported by JANAF (1960) [3] as $\Delta_fH°(298K) = -286.6$ kJ mol⁻¹. Becerra and Walsh (1998) [6] report $\Delta_fH°(298K) = -229.\pm3$. to -233.2 ±3. 2 kJ mol⁻¹. The present G3B3 calculation lists $\Delta_fH°(298K) = -219.3\pm8$. kJ mol⁻¹.

The tetramethylsilane cation $C_4H_{12}Si$⁺ is calculated for the first time and thermal electron G3B3 value is $\Delta_fH°(298K) = 706.5\pm8$. kJ mol⁻¹.

$C_4H_{12}Si$, $C_4H_{12}Si$⁺ Diethylsilane $(C_2H_5)_2SiH_2$ and cation.

Thermochemical data of diethylsilane was reported by Pedley and Rylance (1977) [42] as $\Delta_fH°(298K) = -182.\pm6$. kJ mol⁻¹; by Walsh and coworkers (1989) [38] $\Delta_fH°(298K) = -117.2$ kJ mol⁻¹. The G3B3 calculation result in $\Delta_fH°(298K) = -106.0\pm8$. kJ mol⁻¹.

The thermal electron G3B3 value of the cation $(C_2H_5)_2SiH_2^+$ is $\Delta_fH°(298K) =$ 821.3±8. kJ mol^{-1}.

C_6H_8Si, $C_6H_8Si^-$, Phenylsilane C_6H_5-SiH_3 and anion

To the best of our knowledge the enthalpy of formation of phenylsilane, diphenylsilane, triphenylsilane and tetraphenylsilane were never published. Therefore this is the first calculation of phenylsilane using the G3B3 method, which gives $\Delta_fH°(298K) =$ 123.06±8. kJ mol^{-1}. The multi phenylsilanes exceed our computational capacities.

The thermal electron G3B3 value of the phenylsilane anion C_6H_5-SiH_3^- lists $\Delta_fH°(298K) =$ 164.7±8. kJ mol^{-1}.

As can be seen from the above report in some cases the results differ between different authors very much and in other cases they agree around some value. Mostly the differences are coming from different advanced experimental as well as computational techniques and resources, which were available at the time of reporting. There are explanations in the different cited articles about this behavior. The most interesting article in this category is that of Prascher et al. (2009) [49] where calculations were performed with the CCSD(T) method using 29 different basis sets and differences of 8 kcal mol^{-1} for SiH; 5 kcal mol^{-1} for SiF; 23 kcal mol^{-1} for SiH_4; 48 kcal mol^{-1} for SiF_2; 90 kcal mol^{-1} for SiF_4, etc. were obtained. Many of the data obtained by GA (group additivity) calculations differ from the rest as already pointed out by Becerra and Walsh [6]. Most of them were not quoted for this reason in the article. The most striking case is the RMG database [17] where the silicon data are relatively new (2016), and where the difference from other data usually is the highest, due to the erroneously use of carbon instead of silicon group additivity data.

ERRORS

The errors reported in this article are the original values reported in the literature cited. Where no error was given the values were published as it was found. In our G3B3 calculation we have assigned the mean absolute deviation assigned by Baboul et al. [21] "slightly less than 1 kcal/mol or better". The result uncertainty that represents ±2σ of the statistical normal distribution curve which is ~96% confidence limit of the data should be therefore ±8. kJ mol^{-1} [66]. However as explained in the introduction, because of some uncertainty in the value of the enthalpy of formation of the pure elementary silicon in

gaseous state, the error of all compounds containing more than three silicon atoms was increased.

CONCLUSION

The thermochemistry of 112 inorganic silicon containing species and 35 organic silicon containing species were calculated for ideal gas conditions in the temperature range of 200 K to 6000 K and 1 bar by the G3B3 composite method. The enthalpy of formation at 298.15 K was compared with literature values, if available. The thermochemical data calculated are presented as NASA 7 term format polynomials in the supplement of this article.

SUPPLEMENTARY MATERIAL

The supplement to this article contains the vibrations and moments of inertia used to calculate the thermochemical data reported. It also contains the NASA 7 term polynomials for calculation of the thermochemical data of all the species reported. The supplement can be found in the online version of this article.

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BIBLIOGRAPHY

1. Walsh, R. In The Chemistry of Organic Silicon Compounds; Patai, S.; Rappoport, Z., Eds.; Wiley, 1989; Thermochemistry, Chapter 5, pages 371-391.

2. Haar L.; Friedman, A.S.; Beckett C.W.; Ideal Gas Thermodynamic Functions and Isotope Exchange Functions for the Diatomic Hydrides, Deuterides, and Tritides; NBS Monograph 20, United States Department of Commerce, National Bureau of Standards, Washington, DC, 1961.

3. JANAF thermochemical tables, series of loose leaves, distributed within US government agencies, 1960 and following years.
3a. Stull, D.R.; Prophet, H.; JANAF thermochemical tables, second edition, NBS National Standard Reference Data Series (NSRDS) – NBS 37, 1971.
3b. Chase M.W. Jr.; Curnutt, J.L.; McDonald, R.A.; Syverud, A.N.; JANAF Thermochemical Tables, J Phys Chem Ref Data 1978, Supplement, Vol. 7, No. 3, 793-940.

3c. Chase, M. W. Jr.; Curnutt, J. L.; Downey, J. R. Jr.; McDonald, R. A.; Syverud, A. N.; Valenzuela, E. A.; JANAF Thermochemical Tables, J Phys Chem Ref Data 1982 Supplement, Vol. 11, No. 3, 695-940.

3d. Chase, M. W. Jr.; Davies, C.A.; Downey, J. R. Jr.; Frurip, D. J.; McDonald, R. A.; Syverud, A. N. JANAF thermochemical tables; 3rd edition; J Phys Chem Ref Data 1985, 14, 1-1856, Suppl. No. 1.

4. Glushko, *V. P.;* Gurvich, *L.V.;* Bergman, G.A.; Veyts, I.V.; Medvedev , V.A.; Khachkuruzov, G.A.; Yungman, V.S. Thermodynamic Properties of Pure Substances 1970 (in Russian).

5. Gurvich, V. N.; Veyts, L. V.; Alcock, C. B. Thermodynamic Properties of Individual Substances; 4th edition; Hemisphere; New York, 1992.

6. Becerra, R.; Walsh, R. In The Chemistry of Organic Silicon Compounds; Rappoport, Z.; Appeloig, Y., Ed.; Wiley, 1998, Vol 2, Chapter 4 (Thermochemistry), pages 153-180.

7. Ochterski, J. W.; Petersson G. A.; Wiberg K. B.; A Comparison of Model Chemistries, J Am Chem Soc 1995, 117, 11299-11308. DOI: 10.1021/ja00150a030

8. Boo, B. H; Armentrout P.B.; Reaction of Silicon Ion (^{2}P) with Silane (SiH_4, SiD_4). Heats of Formation of SiH_n, SiH_n^+ (n=1, 2, 3) and $Si_2H_n^+$ (n=0, 1, 2, 3). Remarkable Isotope Exchange Reaction Involving Four Hydrogen Shifts. J Am Chem Soc 1987, 109, 3549-3559. **DOI:** 10.1021/ja00246a010

9. Wong H.-W.; Nieto J. C. A.; Swihart M. T.; Broadbelt L. J.; Thermochemistry of Silicon-Hydrogen Compounds Generalized From Quantum Chemical Calculations; J Phys Chem A 2004, 108, 874-897. **DOI:** 10.1021/jp030727k

10. Ho, P.; Melius, C. F.; A theoretical Study of the thermochemistry of SiF_n and SiH_nF_m compounds and Si_2F_6; J Phys Chem 1990, 94, 5120-5127.

11. Ho, P.; Coltrin, M. E.; Binkley, J. S.; Melius; C. F., Theoretical study of the heats of formation of Si_2H_n (n = 0-6) compounds and trisilane, J Phys Chem 1986, 90, 3399–3406. DOI: 10.1021/j100406a019

12. Allendorf, M. D.; Melius, C. F.; Ho, P.; Zachariah, M. R.; Theoretical study of the Thermochemistry of Molecules in the Si-O-H System; J Phys Chem 1995, 99, 15285-15293.

13. CHEMKIN, a program to calculate chemical kinetics problems, developed by SANDIA and marketed by "Reaction Design" San Diego, CA, USA. Includes a Thermochemical database and Fitdat, a program to calculate NASA type thermochemical polynomials.

14. Lyman J.L.; Noda T., Thermochemical Properties of Si_2F_6 and SiF_4 in Gas and Condensed Phases, J Phys Chem Ref Data, 2001, 30, 165-186. Doi: 10.1063/1.1364519

15. Lias, S. G.; Bartmess, J. E.; Liebman, J. F.; Holmes, J. L.; Levin, R.D.; Mallard, W.G., *Gas-Phase Ion and Neutral Thermochemistry*, J Phys Chem Ref Data 1988, Vol 17, Supplement 1, 1-861.

16. Sukkaew, P; Ojamäe L.; Danielsson Ö.; Kordina O.; Janzén, E.; Revisiting the Thermochemical Database of Si-C-H System Related to SiC CVD Modeling, Material Science Forum 2014, Volumes 778-780, 175-178. DOI 10.4028/www.scientific.net/MSF.778-780.175

17. Green, W.H. and West R.H.; RMG (Reaction Mechanism Generator) program. 2017 <rmg.mit.edu>. RMG Molecule search : http://rmg.mit.edu/molecule_search

18. Slakman, B. L.; Simka, H.; Reddy, H.; West; R. H., Extending Reaction Mechanism Generator to Silicon Hydride Chemistry; Ind Eng Chem Res 2016, 55, 12507–12515.
DOI: 10.1021/acs.iecr.6b02402

19. Goos E., Burcat A., Ruscic, B. Extended Third Millennium Ideal Gas and Condensed Phase Thermochemical Database for Combustion with Updates from Active Thermochemical Tables, 2017, <http://burcat.technion.ac.il>
Electronic update of Burcat A., Ruscic, B. Third Millennium Ideal Gas and Condensed Phase Thermochemical Database for Combustion with Updates from Active Thermochemical Tables, Report ANL-05/20 and TAE 960, Argonne National Laboratory, and Technion, Israel Institute of Technology, 2005.

20. McBride B. J.; Gordon, S., Computer Program for Calculating and Fitting Thermodynamic Functions, NASA RP-1271; 1992.

21. Baboul, A. G.; Curtiss, L.A.; Redfern, P.C.; Raghavachari, K.; Gaussian-3 theory using density functional geometries and zero point energies. J Chem Phys 1999, 110, 7650-7657. Doi 10.1063/1.478676

22. Gaussian 03, Revision B.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, J.A. Pople et al. Gaussian, Inc, Pittsburg PA, 2003**.**

23. Chem3D is a "CambrigeSoft" program for molecular modelling and display with semi-empirical calculations built in with the Mopac 2000 application.

24. Huber, K. P.; Herzberg, G., Molecular Spectra and Molecular Structure, IV. Constants of Diatomic Molecules, Van Nostrand Reinhold, New York, (1977) as reprinted in <Webbook.NIST.GOV>

25. NIST Computational Chemistry Comparison and Benchmark Database, NIST Standard Reference Database Number 101, Release 18, October 2016, Editor: Russell D. Johnson III, <http://cccbdb.nist.gov/>.

26. Irikura K. K.; Johnson III, R. D.; Kacker, R. N., Uncertainties in Scaling Factors for ab Initio Vibrational Frequencies, J Phys Chem A 2005, 109, 8430-8437. **DOI:** 10.1021/jp052793n

27. Kawamata, H.; Negishi, Y.; Kishi, R.; Iwata S.; Nakajima, A.; Kaya K., Photoelectron spectroscopy of silicon–fluorine binary cluster anions ($Si_nF_m^-$), J Chem Phys 1996, 105, 5369-5376. http://dx.doi.org/10.1063/1.472377

28. Weber, M. E.; Armentrout, P. B. Energetics and dynamics in the reaction of Si^+ with SiF_4. Thermochemistry of SiF_x and SiF_x^+ (x=1, 2, 3), J Chem Phys 1988, 88, 6898-6910. DOI 10.1063/1.454387

29. Walsh R., Thermochemistry of Silicon-containing Compounds. Part 1.-Silicon-Halogen Compounds, an Evaluation, J Chem Soc Faraday Trans 1, 1983, 79, 2233-2248. DOI 10.1039/F19837902233

30. Allendorf M. D.; Melius, C.F., Theoretical Study of the Thermochemistry of Molecules in the Si-C-H System, J Phys Chem 1992, 96, 428-437. DOI 10.1021/j100180a080

31. Katzer, G.; Ernst, M. C.; Sax, A. F.; Kalcher, J.; Computational thermochemistry of medium-sized silicon hydrides, J Phys Chem A 1997, 101, 3942-3958. DOI 10.1021/jp9631947

32. Swihart M. T., Girshick S. L., Thermochemistry and Kinetics of Silicon Hydride Cluster Formation during Thermal Decomposition of Silane, J Phys Chem B 1999,103, 64-76.

33. Benson, S.W. *Thermochemical Kinetics*, Wiley, New York, 1976.

34. HSC Thermochemical database (1999)

35. Ruscic B.; Berkowitz, J.; Photoionization mass spectrometric studies of the transient species Si_2H_n (n=2–5), J Chem Phys 1991, 95, 2416-2432. http://dx.doi.org/10.1063/1.460947

36. Berkowitz, J; Greene, J. P.; Cho, H.; Ruscic B. Photoionization mass spectrometric studies of SiH_n (n=1-4), J Chem Phys 1987, 86, 1235-1248.

37. McBride B.J. The NASA Thermochemical database, last updated in 2003. https://www.grc.nasa.gov/www/CEAWeb/ceaThermoBuild.htm

38. Gordon, M. S.; Boatz, J. A.; Walsh, R., Heats of Formation of Alkylsilanes, J Phys Chem 1989, 93, 1584-1585.

39. Tel'noi, V. I.; Rabinovich I. B., Thermochemistry of Organic Derivatives of Non-transition Elements, Russ Chem Review 1980, 49, 603-622.

40. Kalinovski, I. J.; Gutman, D.; Krasnoperov, L. N.; Goumri, A.; Yuan, W.-J.; Marshall, P., Kinetics and Thermochemistry of the Reaction $Si(CH_3)_3$ + HBR$\rightleftharpoons$ $Si(CH_3)_3$H + Br: Determination of the $(CH_3)_3$Si-H Bond Energy, J Phys Chem 1994, 98, 9551-9557.

41. Doncaster, A. M.; Walsh, R., Thermochemistry of Silicon-containing Compounds. Part 2. -The Enthalpies of Formation of the Methylsilanes, an Experimental Study and Review, J Chem Soc Faraday Trans 2, 1986, 82, 707-717. DOi 10.1039/F29868200707

42. Pedley J. B.; Rylance, J., Sussex-N.P.L. Computer Analyzed Thermochemical Data: Organic and Organometallic Compounds; University of Sussex, 1977.

43. Feller, D.; Dixon, D. A., Theoretical Study of the Heats of Formation of Small Silicon-Containing Compounds; J Phys Chem A 1999, 103, 6413-6419. DOI 10.1021/jp990596g

44. Grev, R. S.; Schaefer III, H. F., Thermochemistry of CH_n, SiH_n (n = 0-4), and the cations SiH^+, SiH_2^+ and SiH_3^+: A converged quantum mechanical approach, J Chem Phys 1992, 97, 8389-8406.

45. Jursic B.S., A B3LYP hybrid density functional theory study of structural properties, energies, and heats of formation for silicon–hydrogen compounds, J Mol Struct THEOCHEM 2000, 497, 65-73. DOI: 10.1016/S0166-1280(99)00197-9

46. Jalbout, A.F.; Swihart, M. T.; Jursic, B.S.; Corrigendum to "Potential energy surface for H_2Si_2 isomers explored with complete basis set ab initio method" [J. Mol. Struct. (Theochem) 1999, 459, 221–228.], J Mol Struct: THEOCHEM, 2001, 571 (1–3), 231-232. https://doi.org/10.1016/S0166-1280(01)00584-X

47. Michels, H. H.; Hobbs, R. H., Electronic structure and thermochemistry of silicon hydride and silicon fluoride anions, Chem Phys Letters 1993, 207, 389-396. https://doi.org/10.1016/0009-2614(93)89019-E

48. Takhistov, V. V.; Golovin, A. V., Thermochemistry of organic, heteroorganic and inorganic species. XV. The enthalpies of formation for halogenides of main group elements, J Molec Struct 2006, 784, 47-68. https://doi.org/10.1016/j.molstruc.2005.06.028

49. Prascher, B. P.; Lucente-Schultz, R. M.; Wilson, A. K.; A CCSD(T) and ccCA study of mixed silicon hydrides and halides: Structures and thermochemistry, Chem Phys 2009, 359, 1-13. https://doi.org/10.1016/j.chemphys.2009.02.009

50. Cox, J. D.; Wagman, D. D.; Medvedev, V. A., CODATA Key Values for Thermodynamics, Hemisphere Publishing Corp., New York, 1984.

51. Wang, L.-S.; Wu, H.; Desai, S. R.; Fan, J.; Colson, S. D.; A Photoelectron Spectroscopic Study of Small Silicon Oxide Clusters: SiO_2, Si_2O_3, and Si_2O_4, J Phys Chem 1996, 100, 8697-8700. DOI: 10.1021/jp9602538

52. Karton A.; Martin J. M. L.; Heats of Formation of Beryllium, Boron, Aluminum, and Silicon Re-examined by Means of W4 Theory; *J Phys Chem A* 2007, 111, 5936-5944. **DOI:** 10.1021/jp071690x

53. Hidding, B; Pfitzner, M., Rocket Propellant Characteristics of Silanes/O_2, J Propulsion Power 2006, 22, 786-789. DOI 10.2514/1.17996

54. Danovich, D.; Ogliaro, F.; Karni, M.; Apeloig, Y.; Cooper, D. L.; Shaik, S.; Silynes (RC≡SiR') and Disilynes (RSi≡SiR'): Why Are Less Bonds Worth Energetically More ?, Angew Chem Int Ed 2001, 40(21), 4023-4026. DOI 10.1002/1521-3773(20011105)40:21<4023::AID-ANIE4023>3.0.CO;2-Z

55. Dolgonos, G.; Relative stability and thermodynamic properties of Si_2H_4 isomers; Chem Phys Letters 2008, 466(1-3), 11-15. **DOI:** 10.1016/j.cplett.2008.10.017

56. Becerra, R.; Walsh, R.; Mechanism of Formation of Tri- and Tetrasilane in the Reaction of Atomic Hydrogen with Monosilane and the Thermochemistry of the

Si_2H_4 Isomers, J Phys Chem 1987, 91(22), 5765-5770. https://pubs.acs.org/doi/abs/10.1021/j100306a049

57. Curtis, L. A.; Raghavachari, K.; Deutsch, P. W.; Pople, J. A.; Theoretical study of Si_2H_n (n =0-6)and $Si_2H^+_n$ (n =0--7): Appearance potentials, ionization potentials, and enthalpies of formation J Chem Phys 1991, 95,2433-2444.

58. Sax, A. F.; Kalcher, J.; Theoretical enthalpies of formation for small silicon hydrides; J Phys Chem 1991, 95, 1768-1783. https://pubs.acs.org/doi/abs/10.1021/j100157a052

59. Boatz, J. A.; Gordon, M. S.; Predicted enthalpies of formation for silaethylene, disilene, and their silylene isomers; J Phys Chem 1990, 94, 7331-7333. https://pubs.acs.org/doi/abs/10.1021/j100382a001

60. Raghunath, P.; Lee, Y.-M.; Wu, S.-Y.; Wu, J.-S.; Lin, M.-C.; Ab Initio Chemical Kinetics for reactions of H atoms with SiH_x(x=1-3) Radicals and Related Unimolecular Decomposition Processes, Int J Quantum Chem 2013, 113, 1735-1746. DOI: 10.1002/qua.24396

61. Nguyen, T.-N.; Lee, Y.-M.; Wu, J.-S.; Lin, M.-C.; Capturing H and H_2 by SiH_x^+ (x≤4) ions: Comparison between Langevin and quantum statistical models, Jpn J Appl Phys 2017, 56, 026101. http://stacks.iop.org/1347-4065/56/i=2/a=026101

62. Nguyen, T.-N.; Lin, M.C.; Ab Initio Chemical Kinetics for SiH_x Reactions with Si_2H_y (x=1,2,3,4; y=6,5,4,3; x+y=7) under a-Si:H CVD Condition; Int J Chem Kinet 2017, 49, 197-208. DOI: 10.1002/kin.21067

63. Nguyen, T. N.; Lee, Y. M.; Wu, J. S.; Lin, M. C; Ab Initio Chemical Kinetics for the Thermal Decomposition of SiH_4^+ Ion and Related Reverse Ion-Molecule Reactions of Interest to PECVD of a-Si:H Films, Plasma Chem Plasma Process 2017, 37, 1249-1264. https://doi.org/10.1007/s11090-017-9825-7

64. Raghunath, P.; Lin, M.C. ; Ab Initio Chemical Kinetics for SiH_2 + Si_2H_6 and SiH_3 + Si_2H_5 Reactions and the Related Unimolecular Decomposition of Si_3H_8 under a-Si/H CVD Conditions, J Phys Chem A 2013, 117, 10811-10823. DOI: 10.1021/jp407553a

65. Ruscic, B.; Bross, D.H. Active Thermochemical Tables (ATcT) version 1.122 of the Thermochemical Network (2016); https://atct.anl.gov

66. Ruscic B. Uncertainty Quantification in Thermochemistry, Benchmarking Electronic Structure Computations, and Active Thermochemical Tables Int. J. Quantum Chem. 2014, 114, 1097–1101. DOI: 10.1002/qua.24605

Table 1 Thermochemical properties of Inorganic Si containing compounds:

Molecular Weights, $\Delta_f H_{298}$, $\Delta_f H_0$, C_{p298}, S_{298}, H_{298}-H_0. The standard state corresponds to a pressure of 1 bar and 298.15 K.

Compounds	Mol. Wgt. g/mol	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/ mol	C_{p298} J/(mol K)	S_{298} J/(mol K)	H_{298}-H_0 kJ/mol
SiF Monofluorosilicon radical	47.08390	-62.555	-63.776	±8.	31.551	220.615	8.851
SiF$^+$ Monofluorosilicon cation	47.08335	657.491	650.143	±20.	30.593	214.001	8.765
SiF$^-$ Monofluorosilicon anion	47.08445	-87.869	-83.036	±20.	32.550	216.367	8.968
SiF$_2$ Difluorosilylene	66.08231	-630.8	-626.2	±8	44.396	262.954	11.231
SiF$_2^+$ Difluorosilylene cation	66.08176	429.400	423.96	±8.	43.488	261.852	11.247
SiF$_2^-$ Difluorosilylenene anion	66.08285	-661.0	-654.7	±8.	47.004	266.168	11.614
SiOF$_2$ O=SiF$_2$ DiFluorooxysilane	82.08171	-899.008	-895.73	±8.	57.762	277.687	13.109
SiOF$_2^+$ O=SiF$_2$ cation	82.08116	247.409	243.780	±8.	59.201	281.730	13.649
SiOF$_2^-$ O=SiF$_2$ anion	82.08225	-1056.07	-1047.1	±8.	60.504	279.970	13.461
SiF$_3$ Trifluorosilyl radical	85.08071	-993.365	-990.4	±8.	59.613	282.433	13.398
SiHF$_3$ Trifluorosilane	86.08865	-1207.67	-1200.5	±5.4	63.486	277.351	13.545
SiHF$_3$+ Trifluorosilane cation	86.08810	73.200	71.818	±8.	74.988	291.332	15.874
SiF$_4$ Tetrafluorosilane	104.07911	-1614.98	-1609.4	±4.2	73.534	282.615	15.325
SiF$_4$+ Tetrafluorosilane cation	104.07856	-81.09	-83.341	±8.0	79.002	297.107	16.636
SiF$_4$- Tetrafluorosilane anion	104.07966	-1544.08	-1534.93	±8.	82.680	317.359	18.190
SiH	29.09344	376.660	375.355	±8.	29.209	192.745	8.656
SiH$^+$	29.09289	1144.3	1136.89	±8.	29.555	192.472	8.686
SiH$^-$	29.09399	298.812	303.800	±8.	29.259	187.615	8.660
SiD	30.09960	368.749	367.565	±8.	29.555	198.661	8.686
SiD$^+$	30.09905	1145.161	1125.31	±8.	29.516	193.017	8.684
SiT	31.10155	369.096	367.882		29.982	201.971	8.716
SiD$_2$ D-Si-D	32.11370	262.855	264.418	±8.	37.031	217.458	10.193
SiD$_2^+$ cation	32.11315	1155.624	1150.938	±8.	37.518	222.013	10.276
SiD$_2^-$	32.11425	147.281	161.210	±8.	37.761	224.001	10.252
SiD3	34.12781	191.761	196.765	±8.	45.928	229.809	11.067
SiD3+ cation	34.12726	996.129	988.839	±8.	45.179	223.200	10.967
SiD3- anion	34.12835	37.431	55.003	±8.	45.331	224.113	10.894
SiHT$_3$ Tritritiumsilane	38.14159	27.610	36.134	±8.	53.868	234.262	11.781

Compounds	Mol. Wgt. g/mol	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/ mol	C_{p298} J/(mol K)	S_{298} J/(mol K)	H_{298}-H_0 kJ/mol
$^1SiH_2$ Silicon dihydride singlete radical	30.10138	263.843	265.527	±8.	34.742	207.584	10.001
$^3SiH_2$ Silicon dihydride triplete radical	30.10138	354.623	356.244	±8.	35.460	215.360	10.065
SiH_2^+ Silicon dihydride cation	30.10083	1156.920	1152.34	±8.	35.343	211.902	10.054
SiH_2^- Silicon dihydride anion	30.10193	153.720	161.565	±8.	35.067	213.949	10.023
SiH_2T_2 Ditritiumsilane	36.13348	30.086	39.077	±8.	49.675	226.033	11.263
SiH_3 Silyl	31.10932	195.569	201.090	±8.	40.077	217.058	10.398
SiH_3^+ Silyl cation	31.10877	988.889	988.206	±8.	39.544	210.564	10.342
SiH_3^- Silyl anion	31.10987	52.253	64.053	±8.	38.758	211.838	10.260
SiH_3T Monotritiumsilane	34.89487	32.451	41.815	±8.	45.939	222.416	10.840
SiH_4 Silane	32.11726	34.7	44.319	±8.2	42.787	204.208	10.535
SiH_4^+ Silane cation	32.11671	1144.596	1147.03	±8.	51.119	215.286	11.525
SiD_4 Tetradeuteriunsilane	36.14191	22.792	31.610	±8.	52.240	219.352	11.537
SiT_4 Tetratritiumsilane	40.14970	17.344	25.330	±8.	58.469	226.904	12.370
SiO	44.08490	-102.223	-103.381	±8.	29.899	211.591	8.715
SiO^+ cation	44.08435	1020.495	1013.110	±8.	30.185	217.702	8.734
SiO^- anion	44.08545	-117.002	-112.018	±8.	30.459	218.277	8.754
SiO_2 gas	60.08430	-322.070	-321.432	±10.	45.674	233.390	11.260
SiO_2^- anion	60.08485	-488.386	-481.398	±8.	42.656	256.257	11.039
Si_2F_6 Hexafluorodisilane	170.16142	-2346.72	-2340.59	±8.	128.567	404.351	26.782
$Si_2F_6^+$ Hexafluorodisilane cation	170.16087	-1205.09	-1207.48	±8.	130.849	433.135	28.747
$Si_2F_6^-$ Hexafluorodisilane anion	170.16197	-2401.73	-2391.39	±8.	136.436	411.445	28.461
Si_2OF_6 $F_3Si-O-SiF_3$	186.16082	-2865.85	-2857.61	±8.	138.522	446.199	29.015

Compounds	Mol. Wgt. g/mol	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/ mol	C_{p298} J/(mol K)	S_{298} J/(mol K)	H_{298}-H_0 kJ/mol
Si$_2$H HSi≡Si Disilene monohydrid	57.17894	492.176	492.246	±8.	40.409	254.305	10.599
Si$_2$D DSi≡Si Disilene monodeuterid	58.18510	493.18	491.35	±8.	46.438	284.446	12.607
Si$_2$H$_2$ HSi≡SiH Disilyne	58.18688	452.119	453.439	±8.	57.192	262.489	13.583
Si$_2$H$_2$+ HSi≡SiH+ Disilyne cation	58.18633	1267.00	1261.208	±8.	59.584	276.578	14.357
Si$_2$D$_2$ DSi≡SiD Disilyne-d2	60.19920	451.340	451.964	±8.	59.768	272.843	14.380
Si$_2$H$_4$ H$_2$Si=SiH$_2$	60.20276	273.136	282.273	±8.	70.016	262.567	14.234
Si$_2$H$_4$$^+$ H$_2$Si=SiH$_2$ cation	60.20221	1066.000	1068.288	±8.	71.846	265.111	14.613
Si$_2$H$_4$ H$_3$Si-SiH	60.20276	304.231	312.848	±8.	69.895	280.449	14.754
Si$_2$H$_4$+ H$_3$Si-SiH+ cation	60.20276	1121.250	1122.709	±8.	72.353	286.811	14.975
Si$_2$H$_4$- H$_3$Si-SiH- anion	60.20331	138.975	153.737	±8.	69.440	284.039	14.468
Si$_2$H$_5$ H$_3$Si-SiH$_2$*	61.21070	227.220	239.884	±8.	76.052	295.764	14.942
Si$_2$H$_5$- H$_3$Si-SiH$_2$*- radical anion	61.21125	39.329	57.710	±8.	75.852	295.424	14.810
Si$_2$H$_6$ Disilane H$_3$Si-SiH$_3$	62.21864	80.3	96.502	±1.5	77.260	274.605	15.638
Si$_2$H$_6$$^+$ H$_3$Si-SiH$_3$ cation	62.21809	1016.014	1022.833	±8.	90.949	302.371	17.963
Si$_3$H$_5$ SiH$_2$=SiH-SiH$_2$	89.29620	433.257	444.025	±8.	103.073	336.958	20.055
Si$_3$H$_5$$^+$ SiH$_2$=SiH-SiH$_2$ cation	89.29565	1107.610	1111.848	±8.	100.783	340.465	19.973
Si$_3$H$_5$$^-$ SiH$_2$=SiH-SiH$_2$ anion	89.29675	209.000	225.513	±8.	101.867	331.845	20.079
Si$_3$H$_5$ Cyclotrisilanyl	89.29620	387.024	399.641	±8.	99.539	314.302	18.206
Si$_3$H$_5$$^+$ Cyclotrisilanyl cation	89.29565	1096.095	1101.488	±8.	98.930	318.325	18.785
Si$_3$H$_5$$^-$ Cyclotrisilanyl anion	89.29675	147.948	166.494	±8.	98.121	307.705	18.005
Si$_3$H$_6$ Cyclotrisilane	90.30414	257.314	273.626	±8.	105.306	304.512	18.965

Compounds	Mol. Wgt. g/mol	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/ mol	C_{p298} J/(mol K)	S_{298} J/(mol K)	H_{298}-H_0 kJ/mol
$Si_3H_6^+$ Cyclotrisilane cation	90.30359	1063.513	1071.472	±8.	111.575	319.427	20.369
$Si_3H_6^-$ Cyclotrisilane anion	90.30469	289.248	310.386	±8.	108.758	314.228	19.588
Si_3H_7 n-SiH_3-SiH_2-SiH_{2*}	91.31208	262.379	280.452	±8.	114.942	354.048	21.217
Si_3H_7+ n-SiH_3-SiH_2-SiH_{2*}+	91.31153	965.767	996.160	±8.	116.509	347.994	21.336
Si_3H_7- n-SiH_3-SiH_2-SiH_{2*}-	91.31263	56.170	79.445	±8.	113.947	346.165	20.944
Si_3H_7 i-SiH_3-SiH_*-SiH_3	91.31208	251.718	269.829	±8.	113.162	339.966	21.188
Si_3H_7+ i-SiH_3-SiH_*-SiH_3+ cation	91.31153	977.584	987.432	±8.	115.382	344.968	22.331
Si_3H_7- i-SiH_3-SiH_*-SiH_3- anion	91.31263	28.806	52.471	±8.	110.578	334.645	21.152
Si_3H_8 Trisilane	92.32002	109.228	131.052	±8.	112.552	343.103	21.700
$Si_3H_8^-$ Trisilane anion	92.32057	122.122	147.101	±8.	123.630	346.629	23.036
Si_4H_7 Cyclotetrasilanyl	119.39758	339.182	358.382	±12.	132.552	360.528	23.309
$Si_4H_7^+$ Cyclotetrasilanyl radical cation	119.39703	1026.227	1038.433	±12.	134.837	350.763	23.408
$Si_4H_7^-$ Cyclotetrasilanyl radical anion	119.39813	108.800	133.735	±12.	131.810	351.163	23.105
Si_4H_8 Cyclotetrasilane	120.40552	201.058	224.213	±12.	137.843	342.156	23.587
$Si_4H_8^+$ Cyclotetrasilane cation	120.40497	1062.080	1075.116	±12.	147.644	385.233	26.790
Si_4H_9 SiH_3-SiH_2-SiH_2-SiH_2*	121.41346	293.750	317.669	±12.	149.814	409.481	27.658
Si_4H_9+ SiH_3-SiH_2-SiH_2-SiH_2+	121.41291	939.986	958.090	±12.	146.722	380.952	25.276
Si_4H_9- SiH_3-SiH_2-SiH_2-SiH_2-	121.41401	77.123	105.169	±12.	149.771	394.291	27.658
Si_4H_9 SiH_3-SiH*-SiH_2-SiH_3	121.41346	285.869	309.074	±12.	151.369	405.267	27.761
Si_4H_9+ SiH_3-SiH*-SiH_2-SiH_3+	121.41291	984.922	1006.100	±12.	147.899	399.839	28.157
Si_4H_9- SiH_3-SiH*-SiH_2-SiH_3-	121.41401	47.910	76.253	±12.	148.389	386.626	27.427

Compounds	Mol. Wgt. g/mol	Δ_fH_{298} kJ/mol	Δ_fH_0 kJ/mol	± kJ/ mol	C_{p298} J/(mol K)	S_{298} J/(mol K)	$H_{298}-H_0$ kJ/mol
Si_4H_9 $(SiH_3)_2$-SiH-SiH$_2$*	121.41346	287.550	310.681	±12.	153.868	403.944	27.845
Si_4H_9+ $(SiH_3)_2$-SiH-SiH$_2$*+	121.41291	993.951	1008.415	±12.	151.507	404.473	28.292
Si_4H_9- $(SiH_3)_2$-SiH-SiH$_2$*-	121.41401	66.328	93.914	±12.	153.044	397.181	27.769
Si_4H_9 $(SiH_3)_3$Si*	121.41346	270.596	293.485	±12.	148.452	398.748	28.087
Si_4H_9- $(SiH_3)_3$Si*- anion	121.41401	17.853	46.024	±12.	150.442	381.591	27.264
Si_4H_{10} n-Tetrasilane	122.42140	142.863	170.592	±12.	152.455	407.440	27.482
$Si_4H_{10}^-$ n-Tetrasilane anion	122.42195	128.330	159.870	±12.	159.029	430.902	29.868
Si_5H_9 Cyclopentasilanyl radical	149.49896	327.406	352.193	±15.	168.977	414.872	29.407
$Si_5H_9^+$ Cyclopentasilanyl cation	149.49841	1027.423	1044.105	±15.	172.120	421.981	30.445
$Si_5H_9^-$ Cyclopentasilanyl anion	149.49951	79.813	109.943	±15.	168.489	408.458	29.396
Si_5H_{10} Cyclopentasilane	150.50690	189.397	218.051	±15.	173.967	401.697	29.774
$Si_5H_{10}^+$ Cyclopentasilane cation	150.50635	1058.569	1076.882	±15.	185.851	430.374	32.990
Si_5H_{12} n-Pentasilane	152.52278	177.37	210.79	±15.	178.296	488.638	33.477
$Si_5H_{12}^-$ n-Pentasilane anion	152.52333	144.50	181.94	±15.	184.268	508.548	35.649
Si_6H_{11} Cyclohexasilanyl	179.60034	351.611	381.832	±20.	205.391	465.188	35.658
$Si_6H_{11}^+$ Cyclohexasilanyl cation	179.59979	1039.444	1061.152	±20.	208.642	468.661	36.538
$Si_6H_{11}^-$ Cyclohexasilanyl anion	179.60089	99.118	134.541	±20.	204.763	457.281	35.598
Si_6H_{12} Cyclohexasilane	180.60828	212.476	246.543	±20.	210.583	447.199	36.045
$Si_6H_{12}^+$ Cyclohexasilane cation	180.60773	1074.209	1098.128	±20	222.369	474.835	38.858
$Si_6H_{12}^-$ Cyclohexasilane anion	180.60883	204.191	241.492	±20.	216.896	465.731	37.900

Table 2 Thermochemical properties of Organic Si containing compounds. Molecular Weights, $\Delta_f H_{298}$, $\Delta_f H_0$, C_{p298}, S_{298}, H_{298}-H_0. The standard state corresponds to a pressure of 1 bar and 298.15K.

Compound	Mol. Wgt. g/mol	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/(mol K)	S_{298} J/(mol K)	H_{298}-H_0 kJ/mol
CH_2Si HSi≡CH	42.11208	452.424	453.661	±8.	47.841	241.991	11.503
CH_2Si^- HSi≡CH anion	42.11263	338.644	346.284	±8.	47.098	248.026	11.170
CH_4Si $H_2C=SiH_2$	44.12796	187.276	196.311	±8.	56.872	245.568	12.168
CH_4Si^+ $H_2C=SiH_2$	44.12741	1051.435	1053.766	±8.	58.636	253.837	12.464
CH_4Si^- $H_2C=SiH_2$ anion	44.12851	177.426	191.439	±8.	62.287	264.645	13.165
CH_5Si^* CH_3-SiH_2^* radical	45.13590	141.879	154.470	±8.	61.598	258.522	12.851
CH_5Si^{*+} CH_3-SiH_2^{*+} cation	45.13535	864.938	869.895	±8.	58.975	263.859	13.358
CH_5Si^{*-} CH_3-SiH_2^{*-} anion	45.13645	22.434	40.694	±8.	61.340	256.661	12.773
CH_3SiH_3 CH_3SiH_3 Methylsilane	46.14384	-27.420	-11.579	±8.	66.009	267.332	13.827
$CH_3SiH_3^+$ $CH_3SiH_3^+$ Methylsilane cation	46.14329	1001.110	1007.766	±8.	81.219	285.168	16.670
CH_6Si_2 CH_3SiH_2SiH	74.22934	247.902	262.599	±8.	93.052	313.855	18.196
$CH_6Si_2^+$ CH_3SiH_2SiH cation	74.22879	1038.277	1045.198	±8.	95.143	343.868	18.756
$CH_6Si_2^-$ CH_3SiH_2SiH anion	74.22989	82.365	108.692	±8.	92.630	338.515	18.053
C_2H_4Si $CH_2=CH-SiH$	56.13866	307.432	315.538	±8.	65.371	278.892	14.155
$C_2H_4Si^+$ $CH_2=CH-SiH$ cation	56.13111	1122.630	1124.454	±8.	65.910	276.057	13.997
$C_2H_4Si^-$ $CH_2=CH-SiH$ anion	56.13921	200.882	214.961	±8.	67.638	276.355	14.121
C_2H_6Si $CH_2=CH-SiH_3$	58.15454	90.174	106.267	±8.	75.903	280.937	14.636
$C_2H_6Si^+$ $CH_2=CH-SiH_3$ cation	58.15399	1062.586	1070.361	±8.	80.135	300.154	16.145
$C_2H_6Si^-$ $CH_2=CH-SiH_3$ anion	58.15509	165.192	183.899	±8.	89.718	303.118	17.357
C_2H_6Si $CH_2=SiH-CH_3$	58.15454	125.817	140.865	±8.	82.212	287.045	15.681
$C_2H_6Si^+$ $CH_2=SiH-CH_3$ cation	58.15399	938.099	945.379	±8.	81.677	302.032	16.633
$C_2H_6Si^-$ $CH_2=SiH-CH_3$ anion	58.15509	131.628	151.072	±8.	87.328	299.695	16.631
C_2H_8Si $H_3C-SiH_2CH_3$	60.17042	-88.190	-65.677	±8.	90.149	289.540	16.683
$C_2H_8Si^+$ $CH_3SiH_2CH_3^+$ cation	60.16987	893.340	906.884	±8.	104.302	313.942	19.455
$C_2H_8Si^-$ $CH_3SiH_2CH_3^-$ anion	60.17097	68.684	96.104	±8.	98.317	303.243	17.974
C_2H_8Si $C_2H_5SiH_3$	60.17042	-36.116	-12.942	±8.	85.192	291.590	16.023
$C_2H_8Si^+$ $C_2H_5SiH_3^+$ cation	60.16987	929.961	943.743	±8.	96.348	307.231	17.853
C_3H_9Si $Si(CH_3)_3$ radical	73.18906	24.175	48.091	±8.	112.449	324.106	20.568
$C_3H_{10}Si$ $(CH_3)_3SiH$	74.1970	-153.193	-125.366	±8.	117.339	319.711	20.891
$C_4H_{12}Si$ $Si(CH_3)_4$	88.22358	-219.338	-186.489	±8.	145.448	344.106	25.391
$C_4H_{12}Si^+$ $Si(CH_3)_4^+$ cation	88.22303	706.536	728.016	±8.	156.214	361.645	27.654
$C_4H_{12}Si$ $(C_2H_5)_2SiH_2$	88.22358	-106.002	-72.329	±8.	129.567	372.008	24.567
$C_4H_{12}Si^+$ $(C_2H_5)_2SiH_2^+$ cation	88.22303	821.349	845.565	±8.	140.733	386.178	26.787

Compound	Mol. Wgt. g/mol	Δ_fH_{298} kJ/mol	Δ_fH_0 kJ/mol	± kJ/mol	C_{p298} J/(mol K)	S_{298} J/(mol K)	H_{298}-H_0 kJ/mol
C_6H_8Si C_6H_5-SiH_3 Phenylsilane	108.21322	123.056	146.625	±8.	114.369	337.995	19.842
$C_6H_8Si^-$ C_6H_5-SiH_3^- Phenylsilane anion	108.21377	164.700	191.615	±8.	128.950	349.744	22.002