Predictions of Entropy and Gibbs Energy for Carbonyl Sulfide

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ABSTRACT: Many chemical and physical equilibrium conditions can be determined from minimizing the Gibbs free energies of the system. Efficient analytical representations of the entropy and Gibbs free energy of carbonyl sulfide remain elusive in the communality of science and engineering. Here, we report two analytical representations of the entropy and Gibbs free energy for carbonyl sulfide, and the prediction procedures only involve six molecular constants of the carbonyl sulfide molecule. In the temperature range from 300 to 6000 K, the average relative deviations of the predicted molar entropy and reduced Gibbs free energy values of carbonyl sulfide from the National Institute of Standards and Technology database are arrived at 0.150 and 0.189%, respectively.

1. INTRODUCTION

Carbonyl sulfide (COS or OCS, hereafter COS) is a colorless and toxic organic sulfur compound, which widely exists in natural gas, petroleum gas, water gas, and semewater gas. COS also originates from the volcanic activity and biomass burning. COS passes through the same diffusion pathway into the leaf chloroplasts as carbon dioxide (CO₂) and is consumed by the enzyme carbonic anhydrase. Plants do not produce COC, and plant leaves directly consume COS. Observations of COS have appeared as an efficient tool for understanding terrestrial carbon uptake and plant physiology. As natural gas has economic and ecological advantages, this leads it to become more attractive for many countries. In order to transport natural gas and utilize commercially, it is usually necessary to remove acid gases, including CO₂ and hydrogen sulfide (H₂S), and impurities such as COS and mercaptans. Emission of toxic COS without treatment in coal gas, biogas, tail gas, and other industrial gas will yield air pollution and can also lead to equipment corrosion and poisoning the catalysts. Therefore, the industry has developed strict specifications for the transportation and utilization of sulfur compounds, limiting the total content of sulfur to 35−50 ppm. To prevent equipment damage and catalystempoisoning in various processes such as methane reforming and oil refining, the efficient removal of COS can be achieved by adsorption using aqueous solutions of various amines. The removal of COS and reducing its emission have aroused much attention. The knowledge of Gibbs free energy plays an important role for understanding adsorbate−adsorbent interactions. A higher negative value of the change in the Gibbs free energy implies a more energetically favorable adsorption process. The accurate prediction of the Gibbs free energy change in an adsorption process is useful for the design and fabrication of suitable adsorbents.

In order to carry out optimization of COS recovery and emissions, one requires accurate and reliable thermochemical property data on COS. An accurate and efficient analytical representation of the Gibbs free energy for COS can afford direct and rapid pathways to determine the change in Gibbs free energy and minimization of Gibbs free energy for a system containing COS. However, obtaining efficient analytical representations of the entropy and Gibbs free energy for COS remains a perennial challenging task in science and engineering community. Based on the effective descriptions of molecular internal vibrations in terms of several improved oscillators, including the improved Tietz oscillator, improved Manning−Rosen oscillator, and Rosen−Morse oscillator, some authors have successfully predicted thermochemical properties of some gaseous diatomic substances. In the previous work, our group investigated two analytical representations of the entropy and Gibbs free energy of carbon dioxide (CO₂), which is a triatomic linear symmetric molecule. Here, we further extend our treatment approach proposed in ref 53 to the triatomic linear nonsymmetric molecule COS. Span and Wagner suggested that all the thermodynamic properties of a pure substance can be obtained by combining the Helmholtz free energy and its derivatives. Although Lemmon and Span proposed an empirical analytical representation for the ideal-gas part of the Helmholtz free energy of COS, it contains 13 adjustable coefficients which were determined by fitting many
experimental data points. Here, we report two efficient analytical representations to our knowledge of the molar entropy and Gibbs free energy of COS from the first principles. To check the effectiveness of the proposed prediction models, a comparison of the predicted values with the available data from the National Institute of Standards and Technology (NIST) database is also performed.

2. RESULTS AND DISCUSSION

In order to test the proposed models, calculations of the molar entropy and reduced Gibbs free energy are performed and compared to available data from the NIST database, where six molecular constants of the COS molecule are collected from the work made by Lochte-Holtgreven et al. and Robinson and Tubergen et al. $D_e = 76 \text{kcal/mol}^{-1}$, $r_{\text{rCO}} = 1.16 \text{Å}$, $r_{\text{rCS}} = 1.56 \text{Å}$, $\omega_{\text{aCO}} = 859 \text{ cm}^{-1}$, $\omega_{\text{aCS}} = 2062 \text{ cm}^{-1}$, and $\omega_{\text{ab}} = 521 \text{ cm}^{-1}$. The reduced Gibbs free energy is represented as $G_i = -(G - H_{298.15})/T$; here, $H_{298.15}$ denotes the molar enthalpy of COS at 298 K. The molar Gibbs free energy determined from expression for COS is 231.6 J·mol$^{-1}$ at 298 K. The NIST value of reduced molar Gibbs free energy is 1.56 Å, and Tubergen et al.: $59$ $\epsilon_{r} = 859 \text{ cm}^{-1}$, $\epsilon_{os} = 2062 \text{ cm}^{-1}$, and $\epsilon_{ab} = 521 \text{ cm}^{-1}$. The values in the NIST-JANAF Tables are taken from the NIST-JANAF Thermochemical Tables compiled by Chase. $60$ The values in the NIST-JANAF Tables are determined by using plenty of theoretical or experimental spectroscopic constants. In the future, we will expand the applications of the proposed prediction models under the conditions of different pressures.

The conventional prediction treatment of entropy and Gibbs free energy values of substances involves a large number of experimental spectroscopy data. The present procedure involves only six molecular constant of the COS molecule and calculations begin by inputting directly the molecular constant values to the analytical representations. This merit can help engineers to acquire directly and quickly thermochemical property data of COS. Because acid gas COS is toxic and corrosive, the experimental thermochemical data are scarce. The reason is that performing experimental measurements on COS is fraught with difficulties as breath of it can injure people at concentrations researchers sometimes encounter. The present prediction models provide available computational means as the alternatives to obtain the required thermochemical property data.

3. CONCLUSIONS

We present two analytical representations for the entropy and Gibbs free energy calculations of COS. The proposed procedure merely rely on experimental values of six molecular constants of the COS molecule. The average relative deviations of molar entropy and reduced molar Gibbs free energy values for COS from the NIST database are 0.150 and 0.189%, respectively. The agreement of the predictions with the NIST data is very good. The new prediction strategy for the entropy and Gibbs free energy can be adapted to other substances such as methane.

4. COMPUTATIONAL METHODS

The COS molecule is a linear nonsymmetric triatomic molecule. As shown in Figure 2, the COS molecule contains internal symmetric stretching vibration, antisymmetric stretching vibration, and a degenerate pair of bending vibrations. Our strategy to treat these vibrations is to choose the improved Tietz oscillator and harmonic oscillator to represent symmetric vibration and other vibrations, respectively. An expression for the vibrational partition function subject to the symmetric stretching mode of COS can be derived based on the utilization of the improved Tietz oscillator and reaches the following form from eq 14 of ref $37$

$$Q_{\lambda} = \frac{1}{2} e^{-D_e/kT} \left[ e^{\lambda^2/kT} e^{\lambda^2/kT} + \sqrt{\frac{2\pi kT}{\lambda}} \left( e^{-\lambda^2/kT} - e^{-\lambda^2/kT} \right) - e^{-2\lambda^2/kT} \left( 2\lambda + a \right) + e^{-2\lambda^2/kT} \left( 2\lambda + b \right) \right] \times e^{1/13}$$

where $D_e$ denotes the energy to dissociate COS into CO and S, $k$ denotes the Boltzmann constant, $T$ denotes the absolute temperature, $\lambda = \frac{n^2}{2\pi^2 \sigma_{\text{CS}}}$, $a = \frac{1}{\sigma_1^2} - \frac{1}{\sigma_2^2}$, and $b = \frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}$.

Figure 1. Temperature variation of the thermodynamic properties of COS for (A) molar entropy and (B) molar-reduced Gibbs free energy.

![Figure 1](image)

Figure 2. Schematic diagram of the vibration modes of the COS molecule.

![Figure 2](image)
\[ b = \frac{\delta_1}{\nu_{\text{max}} + 1 + \delta_2} - \frac{\nu_{\text{max}} + 1 + \delta_2}{2} \delta_1 = \frac{\mu_{\text{OS}} D_e}{\hbar \alpha^2 q} (e^{2\mu_{\text{OS}} q} - q^2) \]
\[ \delta_2 = \frac{1}{2} (1 \pm \sqrt{1 + \frac{8 \mu_{\text{OS}} D_e (e^{2\mu_{\text{OS}} q} + q^2)^2}{\hbar^2 \alpha^2 q^2}}) \quad \text{and} \quad \hbar = \frac{k}{2\pi} \]

Here, the Planck constant, \( \mu_{\text{OS}} \) represents the reduced mass of oxygen and sulfur atoms, \( r_{\text{CS}} = r_{\text{CO}} + r_{\text{CS}} \) \( r_{\text{CS}} \) represents the C–O bond length, \( r_{\text{CS}} \) represents the C–S bond length, and \( q \) is a dimensionless adjustable parameter. The \( \pm \) signs are taken as the plus and minus for \( q < 0 \) and \( q > 0 \), respectively. The parameter \( \alpha \) is given by
\[ \alpha = \pi c \nu_{\text{CS}} \sqrt{\frac{2 \mu_{\text{OS}} D_e}{\hbar^2 \alpha^2 q^2}} \left( 1 - \frac{\ln(1 + \ln(1 + \alpha))}{2 + \ln(1 + \alpha)} \right) \]

Here, \( \nu_{\text{CS}} \) is the Planck constant, \( \mu_{\text{CS}} \) represents the reduced mass of oxygen and sulfur atoms, \( r_{\text{CS}} = r_{\text{CO}} + r_{\text{CS}} \) \( r_{\text{CS}} \) represents the C–O bond length, \( r_{\text{CS}} \) represents the C–S bond length, \( g \) is a dimensionless adjustable parameter. The \( \pm \) signs are taken as the plus and minus for \( q < 0 \) and \( q > 0 \), respectively. The parameter \( \alpha \) is given by
\[ \alpha = \pi c \nu_{\text{CS}} \sqrt{\frac{2 \mu_{\text{OS}} D_e}{\hbar^2 \alpha^2 q^2}} \left( 1 - \frac{\ln(1 + \ln(1 + \alpha))}{2 + \ln(1 + \alpha)} \right) \]

Here, \( [x] \) stands for the greatest integer, which is less than \( x \) for noninteger \( x \).

We attribute the antisymmetric stretching vibration and bending vibrations of the COS molecule to harmonic vibrations. The corresponding vibrational partition function can be represented by
\[ Q_{\text{HO}}^{v} = \frac{e^{\Theta_{\text{v}}/2T}}{e^{\Theta_{0}/T} - 1} \]

where \( \Theta_{v} = \hbar \omega_{v}/k \), \( \omega_{v} \) stands for the equilibrium frequency.

The basic thermodynamic formula employed in deriving analytical representations of the entropy and Gibbs free energy of COS are the following thermodynamic relationships
\[ S = k \ln Q + \frac{k T}{\partial Q}(\ln Q) \]
\[ G = H - TS = k T \left( \frac{\partial Q}{\partial V} \right)_T - k T \ln Q \]

From eqs 1, 3, and 4, we can obtain the molar vibrational entropy and Gibbs free energy subject to the contributions of the symmetric stretching vibration of COS and represent them as follows, respectively.
\[ S_{\text{v}}^{\alpha + \beta} = R \ln \left( \frac{e^{\Theta_{v}^\alpha/T}}{e^{\Theta_{0}/T} - 1} - \ln(1 - e^{\Theta_{v}^\alpha/T}) \right) + 2 R \left( \frac{\Theta_{v}^\beta/T}{e^{\Theta_{0}/T} - 1} - \ln(1 - e^{\Theta_{v}^\beta/T}) \right) \]

where \( \Theta_{v}^\alpha = \hbar \omega_{v}/k \) and \( \Theta_{v}^\beta = \hbar \omega_{v}/k \); here, \( \omega_{v} \) and \( \omega_{v} \) stand for the antisymmetric stretching vibration and bending vibration frequencies of COS, respectively.

The molar entropies subject to contributions of translation and rotation of COS can be represented by
\[ S^{\prime} = R \left( \frac{5}{2} + \ln \left( \frac{2 m_{\text{CO}} k T}{k^2} \right)^{3/2} \right) \]
where \( \Theta = \frac{k}{x_{\text{e}} R_{\text{c}}}, m_{\text{COS}} \) refers to the mass of the COS molecule, \( I_{\text{COS}} \) represents the rotational inertia of the COS molecule, and \( P \) represents the gas pressure. Referring to the literature, the molar Gibbs free energy values subject to contributions of translation and rotation of COS can be written as follows, respectively

\[
G' = -RT \ln \left( \frac{\left( 2\pi m_{\text{COS}} \right)^{3/2} (kT)^{3/2}}{h^3} \right)
\]

\[
G' = -RT \ln \left( \frac{T}{\Theta_1} \left( 1 + \frac{1}{3} \frac{\Theta_3}{T} + \frac{1}{15} \left( \frac{\Theta_3}{T} \right)^2 + \frac{4}{315} \left( \frac{\Theta_3}{T} \right)^3 \right) \right)
\]

With the help of eqs 5–12, we obtain analytical representations of the total molar entropy and Gibbs free energy of COS as follows, respectively

\[
S = S' + S_v + S_{v_l} + S_{v_{l+bv}}
\]

\[
G = G' + G_v + G_{v_l} + G_{v_{l+bv}}
\]

Because there are only six basic molecular constants involved in our calculation models, including \( D_a, T_{\text{eCOS}}, T_{\text{eCO}}, T_{\text{eSO}}, \omega_{\text{eCOS}} \) and \( \omega_{\text{eSO}} \), predictions of the molar entropy and Gibbs free energy of COS would become direct and simple through the proposed analytical representations and budget of atmospheric carbonyl sulfide (COS) and some similarities to CO2. J. Geophys. Res. 2007, 112, D9302.

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