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# Thermodynamic Properties of Gaseous Silicon Monotelluride and the Bond Dissociation Enthalpy $D_m^\circ(\text{SiTe})$ at $T \rightarrow 0$

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Statistical-thermodynamic calculations have been combined with the results of high-temperature Knudsen-effusion studies of the vaporization of  $\text{Si}_2\text{Te}_3$  to calculate the thermodynamic properties of  $\text{SiTe}(\text{g})$  from  $T \rightarrow 0$  to  $T = 2000$  K. The dissociation enthalpy  $D_m^\circ(\text{SiTe}, T \rightarrow 0)$  is  $(448 \pm 8)$   $\text{kJ}\cdot\text{mol}^{-1}$ ; its value is discussed vis-à-vis the other silicon monochalcogenides.

Key words: Silicon monotelluride; thermodynamic properties; enthalpy of formation; Gibbs free energy of formation; entropy; enthalpy; heat capacity; dissociation enthalpy.

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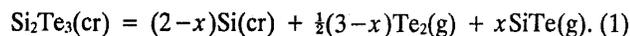
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## 1. Introduction

For efficient technological applications of  $\text{Si}_2\text{Te}_3$  (see Ref. 1, for example) it is desirable to understand the thermodynamics of its behavior not only at low temperatures, the topic with which our recently described measurements<sup>1</sup> of the standard molar enthalpy of formation  $\Delta_f H_m^\circ$  at  $T = 298.15$  K were mostly concerned, but also at high temperatures. According to Exsteen *et al.*,<sup>2</sup> vaporization of  $\text{Si}_2\text{Te}_3$  occurs as follows (no value of  $x$  was given):



Thus, in addition to the well-established thermodynamic functions of  $\text{Si}(\text{cr})$ <sup>3</sup> and  $\text{Te}_2(\text{g})$ ,<sup>4</sup> the same quantities, with comparable accuracy, are also required for  $\text{SiTe}(\text{g})$ . At present, those are available only in approximate form, at just a few temperatures, computed on the basis of estimated spectroscopic constants. Thanks to a recent extensive rotational analysis by Gopal and coworkers<sup>5</sup> of the  $A^1\Pi-X^1\Sigma^+$  band system of the emission spectrum of  $\text{Si}^{130}\text{Te}$ , the missing spectroscopic information has become available and it is now possible, by means of the well-known formulae of statistical mechanics, to cal-

culate the thermodynamic properties of  $\text{SiTe}(\text{g})$  as a function of temperature with the desired high level of reliability.

## 2. Calculations

Because Gopal *et al.*<sup>5</sup> determined spectroscopic constants for  $\text{Si}^{130}\text{Te}$  only, their results were modified by us to refer to  $\text{SiTe}$  formed from  $\text{Te}$  of normal isotopic composition, the material encountered in everyday chemical reactions. We used the formulae given by Herzberg,<sup>6</sup> and first calculated the factor  $\rho = \mu(\text{Si}^{130}\text{Te}) = 0.99839$ , where  $\mu$  denotes the reduced mass of the molecule on the basis of the molar masses of the elements:  $28.0855$   $\text{g}\cdot\text{mol}^{-1}$  for  $\text{Si}$ ,<sup>7</sup>  $127.60$   $\text{g}\cdot\text{mol}^{-1}$  for  $\text{Te}$  of normal isotopic composition,<sup>7</sup> and  $129.9062$   $\text{g}\cdot\text{mol}^{-1}$  for  $^{130}\text{Te}$ .<sup>8</sup> The following relations from Herzberg<sup>6</sup> were adopted in the present study:  $\omega_e(\text{SiTe}) = \omega_e(\text{Si}^{130}\text{Te})/\rho$ ;  $\omega_{x_e}(\text{SiTe}) = \omega_{x_e}(\text{Si}^{130}\text{Te})/\rho^2$ ;  $B_e(\text{SiTe}) = B_e(\text{Si}^{130}\text{Te})/\rho^2$ ;  $\alpha_e(\text{SiTe}) = \alpha_e(\text{Si}^{130}\text{Te})/\rho^3$ ; and  $D_e(\text{SiTe}) = D_e(\text{Si}^{130}\text{Te})/\rho^4$ . The resulting adjusted spectroscopic constants (the Gopal *et al.* values for  $\text{Si}^{130}\text{Te}$  are in parentheses) were:  $\omega_e = 481.44$   $\text{cm}^{-1}$  ( $480.66$   $\text{cm}^{-1}$ );  $\omega_{x_e} = 1.3471$   $\text{cm}^{-1}$  ( $1.3428$   $\text{cm}^{-1}$ );  $B_e = 0.14212$   $\text{cm}^{-1}$  ( $0.141661$   $\text{cm}^{-1}$ );  $\alpha_e = 0.5353\cdot 10^{-3}$  ( $0.5327\cdot 10^{-3}$ ); and  $D_e = 0.49\cdot 10^{-7}$  ( $0.49\cdot 10^{-7}$ ). The symmetry number and the ground-state degeneracy of  $\text{SiTe}$  were each taken to be 1. Values of the physical constants are those recommended by CODATA,<sup>9</sup> with  $R = 8.31451$   $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ .

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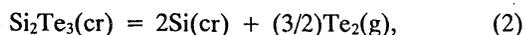
### 3. Results

Table 1 gives the thermodynamic functions computed with the JANAF program<sup>3</sup> by treating SiTe(g) as an anharmonic oscillator, non-rigid rotor. A state sum program was used in which the contributions to the thermal functions of all vibration-rotation levels up to the dissociation limit ( $\approx 37450 \text{ cm}^{-1}$ ) were included, as was done in the JANAF<sup>3</sup> tables for such molecules as H<sub>2</sub>, D<sub>2</sub>, HD, and N<sub>2</sub>. Exploratory calculations showed that at  $T \leq 2000 \text{ K}$  the effect on the results was negligible when the lowest excited state ( $^1\Pi$ ) was included. Therefore, the quantities in Table 1 were determined solely on the basis of the ground ( $^1\Sigma^+$ ) electronic state. Also included in the table are values of the standard molar enthalpy of formation,  $\Delta_f H_m^\circ(T)$ , and the standard Gibbs free energy of formation,  $\Delta_f G_m^\circ(T)$ . Those quantities have as their bases  $\Delta_f H_m^\circ(298.15 \text{ K})$ , the derivation of which will be discussed in the next section. Thermodynamic functions  $X$  in columns 2 through 5 of Table 1 are believed to be uncertain by no more than  $\pm 0.002 X$ , and both  $\Delta_f H_m^\circ/10^3 \cdot \text{R} \cdot \text{K}$  and  $\Delta_f G_m^\circ/10^3 \cdot \text{R} \cdot \text{K}$  are estimated to be uncertain by approximately  $\pm 0.2$ .

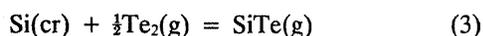
### 4. Discussion

There are differences between the quantities in columns 2 to 5 of Table 1 and those reported by previous investigators, none of whom had access to detailed spectroscopic information on SiTe. Brebrick's<sup>10</sup> values, which he listed at five temperatures only, are quite close to ours and tend to deviate from them by approximately one per cent. This seems to be due, almost entirely, to his use of  $r_e = 0.251 \text{ nm}$ , somewhat greater than the  $r_e = 0.22697 \text{ nm}$  implicit in the measurements of Gopal *et al.* There is similar disagreement with the results of Kelley and King,<sup>11</sup> calculated on the basis of an estimated moment of inertia.

Unlike the conflicting partial pressures,  $p(\text{Te}_2)$ , reported by Exsteen *et al.*<sup>2</sup> and Brebrick<sup>10</sup> for the dissociation of Si<sub>2</sub>Te<sub>3</sub> according to:



their results for  $p(\text{SiTe})$  in the reaction:



are in good agreement. For temperatures between 775 K and 950 K, Exsteen *et al.* gave the relation:

$$\lg[p(\text{SiTe})/0.1 \text{ MPa}] = -(12.1 \pm 0.3) \cdot 10^3 \cdot (K/T) + (8.3 \pm 0.4), \quad (4)$$

and Brebrick, for  $873 \leq (T/K) \leq 1213$ , reported:

$$\lg[p(\text{SiTe})/0.1 \text{ MPa}] = -12.31 \cdot 10^3 \cdot (K/T) + 8.176. \quad (5)$$

The dimensionless constant on the right-hand side of Eq. (5) has been modified by us to take into account the new thermodynamic functions for SiTe(g) and the most up-to-date values<sup>4</sup> for Te<sub>2</sub>(g). Exsteen *et al.* and Brebrick did not list experimental pressures at individual tempera-

tures. Accordingly, we have calculated the molar enthalpy change  $\Delta_f H_m^\circ < T >$  and the molar Gibbs free energy change  $\Delta_f G_m^\circ < T >$  of reaction (3) from Eqs. (4) and (5) at the mean temperature  $< T >$  of each investigation, and used the second- and third-law methods to deduce the enthalpy of the reaction at  $T = 298.15 \text{ K}$ . Auxiliary thermodynamic quantities were taken from Ref. 4 for Te<sub>2</sub>(g); from Ref. 3 for Si(cr); and from Table 1 for SiTe(g).

Results are summarized in Table 2. The mean of the four derived  $\Delta_f H_m^\circ$ s, weighted as the inverse of the squares of the uncertainties, is  $< \Delta_f H_m^\circ > = (124.9 \pm 1.6) \text{ kJ} \cdot \text{mol}^{-1}$ . At the bottom of Table 2 is a Hess cycle that leads to  $D_m^\circ(\text{SiTe})$ , the standard molar dissociation enthalpy of SiTe( $^1\Sigma^+$ ) at  $T \rightarrow 0$ , where the Si(g) and Te(g) products are each taken to be in their  $^3P_2$  ground-state configurations.

In his assessment of the thermochemistry of SiTe, Mills<sup>12</sup> listed  $D_m^\circ$ s that ranged from  $540 \text{ kJ} \cdot \text{mol}^{-1}$  to  $430 \text{ kJ} \cdot \text{mol}^{-1}$ , the higher values from extrapolations of spectroscopic information, and the lower, which he favored, from the vaporization studies we have just analyzed. Lakshminarayana and Gopal<sup>13</sup> discussed  $D_m^\circ(\text{SiTe})$ . In summary, they gave  $550 \text{ kJ} \cdot \text{mol}^{-1}$  (the linear Birge-Sponer extrapolation of  $\omega_0$ ) as the upper limit; estimated  $479 \text{ kJ} \cdot \text{mol}^{-1}$  by comparing  $D_m^\circ(\text{Si-X})$  for  $X = \text{O}, \text{S}, \text{Se},$  and  $\text{Te}$ ; and regarded Huber and Herzberg's<sup>14</sup> selection of the thermochemical value of  $443 \text{ kJ} \cdot \text{mol}^{-1}$  as "somewhat low."

As we have seen, second- and third-law treatments of the results of studies<sup>2,10</sup> of the high-temperature vaporization of Si<sub>2</sub>Te<sub>3</sub> yield four values of  $\Delta_f H_m^\circ(\text{SiTe}, \text{g}, 298.15 \text{ K})$  that are in excellent agreement. Those, in turn, lead to  $D_m^\circ(\text{SiTe})$  that is close to Huber and Herzberg's<sup>14</sup> choice. It is clear that  $D_m^\circ(\text{SiTe})$  from thermochemistry is now known with an accuracy of at least  $\pm 10 \text{ kJ} \cdot \text{mol}^{-1}$ . Any diminution of the uncertainty attached to  $\Delta_f H_m^\circ(\text{Si}, \text{g})$ , surprisingly large at  $\pm 8 \text{ kJ} \cdot \text{mol}^{-1}$ ,<sup>3</sup> will help define  $D_m^\circ(\text{SiTe})$  even more precisely.

In an earlier publication,<sup>15</sup> we observed that  $D_m^\circ(\text{GeX})$ , with  $X = \text{S}, \text{Se},$  or  $\text{Te}$ , decreased almost linearly from GeS to GeTe. A comparable trend should occur for  $D_m^\circ(\text{SiX})$  because of the similarity in bonding. Gurvich *et al.*<sup>16</sup> selected  $D_m^\circ(\text{SiS}) = (613.7 \pm 2.4) \text{ kJ} \cdot \text{mol}^{-1}$  on the basis of a very short extrapolation of vibrational levels of the  $E^1\Sigma^+$  electronic state, reported<sup>17</sup> up to  $50670 \text{ cm}^{-1}$ , and this value is believed to be reliable. In the case of the selenium analog, the situation is somewhat different. Mills<sup>12</sup> recommended  $D_m^\circ(\text{SiSe}) = (484 \pm 21) \text{ kJ} \cdot \text{mol}^{-1}$  on the basis of thermochemical measurements and in preference to the spectroscopic value of  $\approx 525 \text{ kJ} \cdot \text{mol}^{-1}$  from the studies of Vago and Barrow<sup>18</sup> as assessed by Gaydon.<sup>19</sup> Subsequently, Huber and Herzberg<sup>14</sup> extrapolated the same vibrational levels of the  $E^1\Sigma^+$  state and obtained  $D_m^\circ(\text{SiSe}) = 544 \text{ kJ} \cdot \text{mol}^{-1}$ . In light of the values of  $D_m^\circ(\text{GeX})$ , the spectroscopic  $D_m^\circ(\text{SiSe})$  appears to be more reasonable than the thermochemical result, even though it incorporates a  $90 \text{ kJ} \cdot \text{mol}^{-1}$  extrapolation. Knudsen-effusion studies of the high-temperature vaporization

of silicon selenide to SiSe(g) could help resolve the discrepancy. It has been shown<sup>20</sup> that SiSe(cr) cannot be prepared, but an investigation of the high-temperature dissociation of the diselenide [SiSe<sub>2</sub>(cr) + Si(cr) = 2SiSe(g)] has been reported.<sup>21</sup> Results from that study can be used to derive a value of  $\Delta_f H_m^\circ(\text{SiSe, g})$  and, thus,  $D_m^\circ(\text{SiSe})$ , but a reliable value of  $\Delta_f H_m^\circ(\text{SiSe}_2, \text{cr}, 298.15 \text{ K})$ , hitherto unavailable, is required. Preliminary measurements<sup>22</sup> of that quantity in progress at this laboratory are in harmony with  $D_m^\circ(\text{SiSe}) \approx (534 \pm 10) \text{ kJ}\cdot\text{mol}^{-1}$ , and thus tend to support the spectroscopic value. If that  $D_m^\circ$  is corroborated, then the progression of  $D_m^\circ(\text{SiX})$  for  $X = \text{S, Se, Te}$  will indeed be approximately linear, in parallel with  $D_m^\circ(\text{GeX})$ .

From Table 2, we take  $\Delta_f H_m^\circ(298.15 \text{ K}) = (124.9 \pm 1.6) \text{ kJ}\cdot\text{mol}^{-1}$  for reaction (3) and combine it with  $\frac{1}{2}\Delta_f H_m^\circ$

$(\text{Te}_2, \text{g}) = (81.6 \pm 0.3) \text{ kJ}\cdot\text{mol}^{-1}$  to yield  $\Delta_f H_m^\circ(\text{SiTe, g}, 298.15 \text{ K}) = (206.5 \pm 1.6) \text{ kJ}\cdot\text{mol}^{-1}$  for:



This value for the standard molar enthalpy of formation of SiTe(g) agrees within the combined uncertainties with Mills's<sup>12</sup> selection,  $(220 \pm 13) \text{ kJ}\cdot\text{mol}^{-1}$ , but is more precise because we have taken a weighted mean for  $\Delta_f H_m^\circ$  of reaction (3).

We wish to call attention to  $\Delta_f H_m^\circ$  and  $\Delta_f G_m^\circ$  in Table 1. Both quantities refer to reaction (3); thus, *the thermochemical reference state of tellurium is arbitrarily taken to be Te<sub>2</sub>(g) throughout the entire temperature range of the table.*

TABLE 1. Thermodynamic properties of SiTe(g);  $R = 8.31451 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ ,  $p^\circ = 0.1 \text{ MPa}$ ,  $T' = 298.15 \text{ K}^a$

| $T$<br>K          | $\frac{C_{p,m}^\circ}{R}$ | $\frac{\Delta_f H_m^\circ}{10^3 \cdot R \cdot K}$ | $\frac{(\Delta_f S_m^\circ - \Delta_f H_m^\circ/T)}{R}$ | $\frac{\Delta_f S_m^\circ}{R}$ | $\frac{\Delta_f H_m^\circ}{10^3 \cdot R \cdot K}$ | $\frac{\Delta_f G_m^\circ}{10^3 \cdot R \cdot K}$ |
|-------------------|---------------------------|---|---|--------------------------------|---|---|
| 0                 | 0                         | -1.119  | $\infty$  | 0                              | 14.89   | 14.89   |
| 100               | 3.548                     | -0.769  | 32.822  | 25.135                         | 15.03   | 13.89   |
| 200               | 3.904                     | -0.397  | 29.683  | 27.699                         | 15.06   | 12.74   |
| 298.15            | 4.153                     | 0.000   | 29.310  | 29.310                         | 15.02   | 11.59   |
| 300               | 4.156                     | 0.008   | 29.310  | 29.336                         | 15.02   | 11.58   |
| 400               | 4.286                     | 0.430   | 29.475  | 30.551                         | 14.96   | 10.44   |
| 600               | 4.397                     | 1.301   | 30.146  | 32.314                         | 14.81   | 8.20  |
| 800               | 4.440                     | 2.185   | 30.854  | 33.585                         | 14.59   | 6.04  |
| 1000              | 4.461                     | 3.075   | 31.503  | 34.579                         | 14.34   | 3.93  |
| 1200              | 4.472                     | 3.969   | 32.086  | 35.393                         | 14.05   | 2.87  |
| 1400              | 4.480                     | 4.864   | 32.609  | 36.083                         | 13.75   | -0.14   |
| 1600 <sup>b</sup> | 4.485                     | 5.761   | 33.081  | 36.682                         | 13.43   | -2.09   |
| 1800              | 4.488                     | 6.658   | 33.511  | 37.210                         | 7.08  | -3.62   |
| 2000              | 4.490                     | 7.556   | 33.905  | 37.683                         | 6.81  | -4.77   |

<sup>a</sup>Note that  $\Delta_f H_m^\circ$  and  $\Delta_f G_m^\circ$  both refer to the formation reaction:  $\text{Si}(\text{cr or l}) + \frac{1}{2}\text{Te}_2(\text{g}) = \text{SiTe}(\text{g})$ , as explained in the text.

<sup>b</sup>There is a transition at  $T = 1685 \text{ K}$ , the melting temperature of Si.

TABLE 2. Enthalpy of the reaction:  $\text{Si}(\text{cr}) + \frac{1}{2}\text{Te}_2(\text{g}) = \text{SiTe}(\text{g})$  at  $T' = 298.15 \text{ K}$  and  $p^\circ = 0.1 \text{ MPa}$ , and derivation of  $D_m^\circ(\text{SiTe})$ 

| Reference  | Second law<br>$\Delta_r H_m^\circ / (\text{kJ}\cdot\text{mol}^{-1})$                                 | Third law<br>$\Delta_r H_m^\circ / (\text{kJ}\cdot\text{mol}^{-1})$ |
|--|--|---|
| Exsteen <i>et al.</i> <sup>2</sup>   | 120.1 ± 3.0  | 127.4 ± 4.5   |
| Brebrick <sup>10</sup>   | 124.6 ± 2.5  | 132.4 ± 4.0   |
| $\langle \Delta_r H_m^\circ \rangle = (124.9 \pm 1.6) \text{ kJ}\cdot\text{mol}^{-1 \text{ a}}$                        |  |   |
| $\text{SiTe}(\text{g}, T') = \text{Si}(\text{cr}, T') + \frac{1}{2}\text{Te}_2(\text{g}, T')$                          | $\Delta_r H_m^\circ = -(124.9 \pm 1.6) \text{ kJ}\cdot\text{mol}^{-1 \text{ a}}$                     |   |
| $\frac{1}{2}\text{Te}_2(\text{g}, T') = \text{Te}(\text{g}, T')$   | $\Delta_r H_m^\circ = (127.9 \pm 0.5) \text{ kJ}\cdot\text{mol}^{-1 \text{ b}}$                      |   |
| $\text{Si}(\text{cr}, T') = \text{Si}(\text{g}, T')$   | $\Delta_r H_m^\circ = (450 \pm 8) \text{ kJ}\cdot\text{mol}^{-1 \text{ c}}$                          |   |
| $\text{Te}(\text{g}, T') = \text{Te}(\text{g}, T \rightarrow 0)$   | $\Delta_r H_m^\circ = -(6.2 \pm 0.2) \text{ kJ}\cdot\text{mol}^{-1 \text{ b}}$                       |   |
| $\text{Si}(\text{g}, T') = \text{Si}(\text{g}, T \rightarrow 0)$   | $\Delta_r H_m^\circ = -(7.6 \pm 0.3) \text{ kJ}\cdot\text{mol}^{-1 \text{ c}}$                       |   |
| $\text{SiTe}(\text{g}, T \rightarrow 0) = \text{SiTe}(\text{g}, T')$   | $\Delta_r H_m^\circ = (9.3 \pm 0.3) \text{ kJ}\cdot\text{mol}^{-1 \text{ d}}$                        |   |
| $\text{SiTe}(\text{g}, T \rightarrow 0) = \text{Si}(\text{g}, T \rightarrow 0) + \text{Te}(\text{g}, T \rightarrow 0)$ | $\Delta_r H_m^\circ = D_m^\circ(\text{SiTe}) = (448 \pm 8) \text{ kJ}\cdot\text{mol}^{-1 \text{ e}}$ |   |

<sup>a</sup>Weighted mean of the four values at the top of the table, as discussed in text.

<sup>b</sup>Reference 4.

<sup>c</sup>Reference 3.

<sup>d</sup>Table 1.

<sup>e</sup>For the dissociation of  $\text{SiTe}({}^1\Sigma)$  to  $\text{Si}({}^3\text{P})$  and  $\text{Te}({}^3\text{P})$ .

## 5. Acknowledgment

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