

## CHEMICAL THERMODYNAMICS AND THERMOCHEMISTRY

# Thermodynamic Parameters of Scandium Trifluoride and Triiodide in the Condensed State

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**Abstract**—The thermodynamic properties of new classes of compounds, particularly scandium trihalides  $\text{ScF}_3$ ,  $\text{ScCl}_3$ ,  $\text{ScBr}_3$ , and  $\text{ScI}_3$ , are added to the IVTANTHERMO software package. A critical analysis and processing of the entire array of primary data available in the literature is performed. An equation approximating the temperature dependence of heat capacity in the temperature range  $298.15 - T_m$  (K) is derived for each crystalline scandium trihalide. The resulting equations  $C_p^\circ(T)$  for the solid state and the data for the liquid phase are used to calculate the thermodynamic functions of entropy, the reduced Gibbs free energies, and the enthalpy increments. Both the experimental data available in literature and the missing estimated thermodynamic data are used in calculations. The error of the recommended values is estimated in all cases. In the first part of this work, we describe the thermodynamic properties of  $\text{ScF}_3$  and  $\text{ScI}_3$  used as the reference data for calculating the thermodynamic functions of  $\text{ScCl}_3$  and  $\text{ScBr}_3$ , for which experimental data are either very scarce or missing altogether. The resulting data are added to the database of the IVTANTHERMO software package.

**Keywords:** scandium trifluoride  $\text{ScF}_3$ , scandium trifluoride  $\text{ScCl}_3$ , scandium tribromide  $\text{ScBr}_3$ , scandium triiodide  $\text{ScI}_3$ , thermodynamic properties.

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## INTRODUCTION

Scandium and its derivatives began to be of interest for researchers as microelectronics, space engineering, and other cutting-edge fields of engineering developed. Early studies and publications were devoted to geochemistry, technologies for the extraction of metallic scandium, and analytical chemistry and its applications. The long list of references in [1] focused on the unique properties of scandium and its derivatives, particularly complex oxides, halides, organic derivatives, and so on. Scandium halides are used in the electrical engineering industry. The studies of Speros et al. [2] and Minaev and Zyuzin [3] enabled the design and development of mercury-free general lighting service lamps and special light bulbs. Scandium halides, particularly  $\text{ScBr}_3$  and  $\text{ScI}_3$ , are used as filler components in mercury-free metal halide lamps. Technical effects of this invention include improved environmental safety of lamp production, service, and storage. Anhydrous  $\text{ScF}_3$  and  $\text{ScCl}_3$  purified from oxygen are used as initial compounds in the production of metallic scandium.

Data on the temperature dependence of the heat capacity and enthalpy over a broad range of temperatures, phase transition enthalpies, and enthalpies of formation are needed to calculate tables of the ther-

modynamic functions of a certain compound in crystalline and liquid states. The information on the thermodynamic properties of scandium trihalides required for solving a number of fundamental and engineering problems is far from complete, since the great strength of the Sc–F bond increases the stability of fluoride compounds [1]. Hence, scandium trifluoride  $\text{ScF}_3$  is likely to result from interaction between scandium and fluorine. The strength of the Sc–Hal bond is significantly lower for scandium derivatives obtained via reactions with other halogens (Cl, Br, I) and decreases in the series  $\text{Cl} \rightarrow \text{Br} \rightarrow \text{I}$ . Compounds  $\text{ScCl}_3$ ,  $\text{ScBr}_3$ , and  $\text{ScI}_3$  are easily hydrolyzed, yielding various hydroxy and oxo compounds. When heated in air, all scandium halides are eventually converted into  $\text{Sc}_2\text{O}_3$ . The increased volatility of scandium trihalides is also noteworthy; like bond strength, the sublimation enthalpies decline in the series  $\text{ScF}_3 \rightarrow \text{ScCl}_3 \rightarrow \text{ScBr}_3 \rightarrow \text{ScI}_3$ . The synthesis of scandium halides and investigations of their properties thus require special safety measures that impede studies. Thermodynamic parameters of these compounds are estimated if no experimental data are available.

There are neither experimental data on the low-temperature heat capacity of  $\text{ScF}_3$ ,  $\text{ScCl}_3$ , and  $\text{ScBr}_3$ ,

**Table 1.** Thermodynamic properties of ScF<sub>3</sub> (cr, l)

<i>T</i> , K	$C_p^\circ(T)$ , J K <sup>-1</sup> mol <sup>-1</sup>	$\Phi^\circ(T)$ , J K <sup>-1</sup> mol <sup>-1</sup>	$S^\circ(T)$ , J K <sup>-1</sup> mol <sup>-1</sup>	$H^\circ(T) - H^\circ(0)$ , kJ mol <sup>-1</sup>
298.15	83.500	43.044	90.000	14.000
300	83.705	43.335	90.517	14.155
400	91.041	58.392	115.747	22.942
500	94.593	72.000	136.485	32.242
600	96.657	84.240	153.928	41.813
700	98.017	95.293	168.936	51.550
800	99.003	105.337	182.092	61.404
900	99.771	114.528	193.799	71.344
1000	100.404	122.991	204.345	81.354
1100	100.949	130.830	213.940	91.422
1200	101.433	138.127	222.745	101.541
1300	101.875	144.953	230.882	111.707
1400	102.286	151.364	238.447	121.915
1500	102.674	157.408	245.517	132.163
1600	103.045	163.125	252.156	142.450
1700	103.403	168.547	258.413	152.772
1800	103.750	173.706	264.334	163.130
1825	103.835	174.957	265.765	165.725
1825	120.000	174.957	300.083	228.355
1900	120.000	179.992	304.916	237.355
2000	120.000	186.394	311.071	249.355
2100	120.000	192.471	316.926	261.355
2200	120.000	198.256	322.508	273.354
2300	120.000	203.775	327.842	285.354
2400	120.000	209.052	332.950	297.354
2500	120.000	214.106	337.848	309.354

When preparing the reference book *Thermodynamic Properties of Individual Substances*, edited by Academician Glushko [32], and the IVTANTHERMO software package based on it, it was decided to present the values of thermodynamic functions with an accuracy of three digits after the decimal point. The number of these digits is usually higher than the accuracy of the reference data, since the changes between the reference and interpolated values as functions of temperature must be kept smooth so there is strict agreement between the values calculated using different thermodynamic cycles.

nor data on the high-temperature heat capacity or enthalpy of ScBr<sub>3</sub> in the literature. Dworkin and Bredig [4] measured the enthalpy increments of ScCl<sub>3</sub> (cr, l) in the temperature range of 468–1273 K. Spedding et al. [5] measured the enthalpy increments of ScF<sub>3</sub> (cr, l) at 400–1900 K. All of the required thermodynamic data are available only for scandium triiodide ScI<sub>3</sub>. O'Hare et al. [6] measured the low-temperature heat capacity of ScI<sub>3</sub> in the range of 7 to 346 K and its enthalpy increments in the temperature range of 350–

1325 K, allowing them to calculate the thermodynamic functions of crystalline and liquid ScI<sub>3</sub>. The results from processing all of the experimental data available in the literature and thermodynamic functions calculated using these findings were used in this work as reference data to estimate the missing parameters for ScF<sub>3</sub>, ScCl<sub>3</sub>, and ScBr<sub>3</sub>. It should be noted that in the series ScF<sub>3</sub>–ScCl<sub>3</sub>–ScBr<sub>3</sub>–ScI<sub>3</sub>, trihalides ScF<sub>3</sub> and ScI<sub>3</sub> determine the limits for the thermodynamic functions of isostructural compounds ScCl<sub>3</sub> and ScBr<sub>3</sub> being estimated, giving grounds for dividing our results into two parts.

#### *Thermodynamic Parameters of ScF<sub>3</sub> (cr, l)*

Table 1 lists the thermochemical properties of crystalline and liquid scandium trifluoride in the standard state at 298.15–2500 K. The cubic modification was considered to be the standard state of ScF<sub>3</sub>(cr) at 0–1825 K [5, 7].

There are no experimental data in the literature for the low-temperature heat capacity of ScF<sub>3</sub> at  $T \leq 298.15$  K. The value  $C_p^\circ(298.15 \text{ K}) = 83.5 \text{ J K}^{-1} \text{ mol}^{-1}$  was obtained by Spedding et al. [5], who measured the enthalpy increments of a high-purity ScF<sub>3</sub> sample in the temperature range of 400–1900 K. Entropy increments in the Latimer system [8] were used to calculate standard entropy  $S^\circ(298.15 \text{ K}) = 90 \text{ J K}^{-1} \text{ mol}^{-1}$ . Barin et al. [9] and Kubaschewski and Alcock [10] seem to have used the same additive method: the  $S^\circ(298.15 \text{ K})$  value they estimated was also  $90 \text{ J K}^{-1} \text{ mol}^{-1}$ . Based on EDS data, Rezhukhina et al. [11] found that entropy of ScF<sub>3</sub>(cr) at 298.15 K is  $92 \pm 8 \text{ J K}^{-1} \text{ mol}^{-1}$ . Note that high-precision measurements of low-temperature heat capacity for YF<sub>3</sub> according to Flotov et al. [12] yielded  $S^\circ(298.15 \text{ K}) = 88.7 \text{ J K}^{-1} \text{ mol}^{-1}$ . The  $S^\circ(298.15 \text{ K})$  values given in [5, 7, 13–16] were estimated using a variety of approximation techniques and came to  $70.6\text{--}100.4 \text{ J K}^{-1} \text{ mol}^{-1}$  with a data spread of  $30 \text{ J K}^{-1} \text{ mol}^{-1}$ . The value  $H^\circ(298.15 \text{ K}) - H^\circ(0) = 14 \text{ kJ mol}^{-1}$  taken for ScF<sub>3</sub> was estimated via comparative calculation using the corresponding values derived from reliable experimental data on low-temperature heat capacity of YF<sub>3</sub> ( $14.910 \text{ kJ mol}^{-1}$ ) [12], LaF<sub>3</sub> ( $16.717 \text{ kJ mol}^{-1}$ ) [17], CeF<sub>3</sub> ( $17.729 \text{ kJ mol}^{-1}$ ) [18], PrF<sub>3</sub> ( $17.946 \text{ kJ mol}^{-1}$ ) [19], NdF<sub>3</sub> ( $17.360 \text{ kJ mol}^{-1}$ ) [20], GdF<sub>3</sub> ( $15.804 \text{ kJ mol}^{-1}$ ) [12], DyF<sub>3</sub> ( $16.785 \text{ kJ mol}^{-1}$ ) [21], and ErF<sub>3</sub> ( $17.040 \text{ kJ mol}^{-1}$ ) [21].

Based on the data in [5] and the estimates made in this work, the standard thermodynamic values at 298.15 K are thus

$$C_p^\circ(298.15 \text{ K}) = 83.5 \pm 1.0 \text{ J K}^{-1} \text{ mol}^{-1},$$

$$S^\circ(298.15 \text{ K}) = 90 \pm 7 \text{ J K}^{-1} \text{ mol}^{-1},$$

$$H^\circ(298.15 \text{ K}) - H^\circ(0) = 14 \pm 1 \text{ kJ mol}^{-1}.$$

We obtained the equation for the heat capacity of  $\text{ScF}_3(\text{cr})$  in the 298.15–1825 K temperature range derived from the results of measurements of relative enthalpies by Spedding et al. [5] ( $\text{J K}^{-1} \text{ mol}^{-1}$ ):

$$C_p^\circ(T) = 98.923 + 2.930 \times 10^{-3}T - 14.487 \times 10^{-5}T^{-2}. \quad (1)$$

The measurements in [5] were performed by drop-calorimetry using a  $\text{ScF}_3$  sample thoroughly purified by vacuum sublimation. The error in measuring enthalpy increments was 1%. It should be noted that in addition to calorimetric measurements, Spedding et al. [5] conducted a DTA study of the same sample and did not detect the phase (polymorphic) transition reported by Komissarova and Pokrovskii in [22] ( $T_{\text{tr}} = 1623 \text{ K}$ ) and Ippolitov and Maklachkov [23] ( $T_{\text{tr}} = 1748 \text{ K}$ ). Petzel et al. [24] studied the  $\text{Sc}_2\text{O}_3$ – $\text{ScF}_3$  system via DTA and X-ray diffraction analysis at 1400–1840 K and detected no phase transitions in  $\text{ScF}_3$  either.

In an inert atmosphere,  $\text{ScF}_3$  melts without decomposition. The melting point ( $1825 \pm 5 \text{ K}$ ) and enthalpy of fusion ( $62.63 \pm 2.00 \text{ kJ mol}^{-1}$ ) were taken from the data in [5]. The results of [23] ( $1823 \pm 20 \text{ K}$ ) and [24] ( $1822 \pm 30 \text{ K}$ ) show good agreement with the  $T_{\text{m}}$  value. The values 1803 and 1788 K were obtained in [22] and [25], respectively. As was mentioned in [22, 23], the experiment was complicated by the thermal instability of  $\text{ScF}_3$  in air, which was manifested as the weight loss of the sample at temperatures above 673 K. A heat capacity of  $\text{ScF}_3(\text{l})$  ( $120 \pm 10 \text{ J K}^{-1} \text{ mol}^{-1}$ ) was estimated in this work with allowance for the experimental data on the heat capacity of liquid trifluorides of yttrium, lanthanum, and a number of other lanthanides obtained by Spedding et al. [5, 26]. These measurements were performed for the well-tested samples over a quite wide range of temperatures. The only exception was  $\text{ScF}_3(\text{l})$ , for which the enthalpy was measured only at one temperature and a constant heat capacity value of  $88.87 \text{ J K}^{-1} \text{ mol}^{-1}$  was assumed, considerably lower than that of crystalline  $\text{ScF}_3$  in the melting point [5].

The standard enthalpy of formation of crystalline  $\text{ScF}_3$  at 298.15 K is assumed to be  $\Delta_f H^\circ(\text{ScF}_3, \text{cr}, 298.15 \text{ K}) = -1629 \pm 8 \text{ kJ mol}^{-1}$ . This value was taken from the study by Hubbard et al. (Argonne National Laboratory, United States), who measured the enthalpy of combustion of metallic scandium in fluorine in a calorimetric bomb. This work was conducted using high-purity and thoroughly characterized samples. It has yet to be published, but its data are available in a brief ANL report [27]. Considering the high quality of research in the field of fluorine calorimetry conducted at this laboratory, however, preference should be given to the results obtained by Hubbard et al. using

direct calorimetry. This method is the only one possible in thermochemical studies of a number of fluorides, since the extremely high reactivity of fluorine allows us to conduct thermochemical studies of a greater number of compounds that cannot be investigated via other reactions due to their inertness. The data obtained in [27] have been confirmed by findings of Skelton and Patterson [28] who used EMF to investigate the equilibrium of the reaction  $3\text{Ni}(\text{cr}) + 2\text{ScF}_3(\text{cr}) = 3\text{NiF}_2(\text{cr}) + 2\text{Sc}(\text{cr})$  in the temperature range of 928–1121 K. These findings were used to calculate the enthalpy of the reaction  $\Delta_r H^\circ(298.15 \text{ K}) = -1292 \pm 12 \text{ kJ mol}^{-1}$  (Third Law), and the value  $\Delta_f H^\circ(\text{ScF}_3, \text{cr}, 298.15 \text{ K}) = -1632 \pm 8 \text{ kJ mol}^{-1}$  was obtained. Rezhukhina et al. [11] studied the equilibrium of the reaction  $2\text{Sc}(\text{cr}) + 3\text{MgF}_2(\text{cr}) = 2\text{ScF}_3(\text{cr}) + 3\text{Mg}(\text{cr})$  in the temperature range of 720–1120 K by means of EMF. The enthalpy of formation  $\Delta_f H^\circ(\text{ScF}_3, \text{cr}, 298.15 \text{ K}) = -1648.9 \pm 8.4 \text{ kJ mol}^{-1}$  calculated using these data differed notably from the one used in this work.

The errors in the  $\Phi^\circ(T)$  values at 298.15, 500, 1000, 1500, 2000, and 2500 K (Table 1) are estimated at 4, 5, 6, 7, 8, and 12  $\text{J K}^{-1} \text{ mol}^{-1}$ , respectively. The reduced Gibbs free energy  $\Phi^\circ(T)$  was calculated using the formula  $\Phi^\circ(T) = S^\circ(T) - [H^\circ(T) - H^\circ(0)]/T$ .

The thermodynamic functions of  $\text{ScF}_3(\text{cr}, \text{l})$  in the temperature range of 298–2000 K were listed in the reference works of Pankratz [29], Knacke et al. [30], and Barin [31]. The discrepancies between the data obtained in this study and the reference books listed above were due to differences in entropy estimates. The value  $S^\circ(298.15 \text{ K}) = 97.906 \text{ J K}^{-1} \text{ mol}^{-1}$  borrowed from [7] was used for standard entropy in [29–31]. This value resulted from combining the  $S^\circ(298.15 \text{ K})$  value estimated in [15] and the results from EMF measurements performed in [11]. The calculations in [7] were based on an erroneous assertion that the standard entropy in [15] was determined calorimetrically. The value taken for the heat capacity of liquid  $\text{ScF}_3$  [29–31] was derived from the results of a single measurement of enthalpy in [5] and was obviously underestimated. It should be noted that no estimates of the  $H^\circ(298.15 \text{ K}) - H^\circ(0)$  value are available in the reference literature [29–31].

#### *Thermodynamic Parameters of $\text{ScI}_3(\text{cr}, \text{l})$*

The thermodynamic properties of crystalline and liquid scandium triiodide in the standard state at 298.15–2000 K are listed in Table 2. The rhombohedral modification ( $\text{FeCl}_3$ -type structure) is assumed to be the standard state of crystalline  $\text{ScI}_3$  in the temperature range of 0–1225 K [6].

At  $T \leq 298.15 \text{ K}$ , the thermodynamic functions of  $\text{ScI}_3$  were calculated using the results from high-precision measurements of the heat capacity in the tem-

**Table 2.** Thermodynamic properties of  $\text{ScI}_3$  (cr, l)

$T, \text{K}$	$C_p^\circ(T),$ $\text{J K}^{-1} \text{mol}^{-1}$	$\Phi^\circ(T),$ $\text{J K}^{-1} \text{mol}^{-1}$	$S^\circ(T),$ $\text{J K}^{-1} \text{mol}^{-1}$	$H^\circ(T) -$ $H^\circ(0),$ $\text{kJ mol}^{-1}$
100	79.360	39.359	85.879	4.652
200	94.870	79.175	146.900	13.545
298.15	98.950	108.229	185.660	23.086
300	99.015	108.709	186.272	23.269
400	102.066	131.870	215.196	33.330
500	104.352	150.915	238.229	43.657
600	106.090	167.111	257.415	54.183
700	107.496	181.215	273.877	64.864
800	108.786	193.718	288.316	75.678
900	110.175	204.958	301.207	86.624
1000	111.881	215.176	312.900	97.724
1100	114.119	224.556	323.663	109.018
1200	117.105	233.238	333.715	120.572
1225	117.994	235.313	336.138	123.511
1225	146.000	235.313	401.444	203.511
1300	146.000	245.150	410.120	214.461
1400	146.000	257.325	420.940	229.061
1500	146.000	268.572	431.013	243.661
1600	146.000	279.022	440.435	258.261
1700	146.000	288.780	449.287	272.861
1800	146.000	297.931	457.632	287.461
1900	146.000	306.546	465.526	302.061
2000	146.000	314.684	473.014	316.661

perature range of 7–346 K [6]. The measurements were performed using an adiabatic calorimeter with an error of 5% at 6 K, 1% at 14 K, and 0.2% above 25 K. Neutron activation analysis showed that the  $\text{ScI}_3$  sample used in [6] contained  $0.082 \pm 0.010$  wt % oxygen. Mass spectrometry revealed that it contained negligible amounts of Si, Cl, Mg, and K impurities (in total, 0.001%). Below 9 K, the  $C_p^\circ(T)$  function for  $\text{ScI}_3$  strictly obeyed the Debye cubic equation. According to [6], the following values were obtained at 6 K by extrapolating the heat capacity to 0 K:  $S^\circ(6 \text{ K}) = 0.313 \text{ J K}^{-1} \text{mol}^{-1}$  and  $H^\circ(6 \text{ K}) - H^\circ(0) = 1.408 \text{ J mol}^{-1}$ .

The standard thermodynamic parameters at 298.15 K adopted on the basis of [6] were

$$C_p^\circ(298.15 \text{ K}) = 98.95 \pm 0.20 \text{ J K}^{-1} \text{mol}^{-1}$$

$$S^\circ(298.15 \text{ K}) = 185.66 \pm 0.40 \text{ J K}^{-1} \text{mol}^{-1},$$

$$H^\circ(298.15 \text{ K}) - H^\circ(0) = 23.086 \pm 0.050 \text{ kJ mol}^{-1}.$$

Equation (2), derived from the results of measuring enthalpy increments at 350–1225 K [6], was used at

$T > 298.15 \text{ K}$  for the heat capacity of  $\text{ScI}_3(\text{cr})$  in the temperature range of 298.15–1225 K:

$$C_p^\circ(T) = 83.115 + 74.193 \times 10^{-3} T - 81.446 \times 10^{-6} T^2 + 36.019 \times 10^{-9} T^3 (\text{J K}^{-1} \text{mol}^{-1}). \quad (2)$$

The drop-calorimetric system was used for the enthalpy increments measurements [6] with the sample described above. This equation describes the experimental data with a root-mean-square deviation of  $\pm 0.18\%$ . The enthalpy increments deviated substantially from linearity as the melting temperature was approached. This is why O'Hare et al. [6] reported enthalpy increments for temperatures between 1175 K and  $T_m$  that were obtained by extrapolating the results from measurements at lower temperatures. It should be mentioned that a similar phenomenon was observed by Dworkin and Bredig [4], who measured the enthalpy increments of  $\text{ScCl}_3$ . They explained the abnormally rapid increase in enthalpy near  $T_m$  by the pre-melting of  $\text{ScCl}_3$ . It should also be noted that  $\text{ScCl}_3$  and  $\text{ScI}_3$  sublime noticeably as the temperature rises.

The melting point of  $\text{ScI}_3$  ( $1225 \pm 3 \text{ K}$ ) was taken from the measurements for the certified test sample in [6]. The same value (1225 K) is found in Gmelin's reference book [33] with a cite to a thesis paper that is not available for us. The value  $T_m = 1218 \pm 8 \text{ K}$ , determined by Fischer et al. [34] for a less pure  $\text{ScI}_3$  sample, agrees fairly well with this value of the melting point. The fusion enthalpy ( $80 \pm 1 \text{ kJ mol}^{-1}$ ) was calculated as the difference between the enthalpies of the liquid and crystalline phases of  $\text{ScI}_3$  at the melting point. O'Hare et al. [6] gave the linear equation  $C_p^\circ(T) = 697.909 - 433.438 \times 10^{-3} T (\text{J K}^{-1} \text{mol}^{-1})$  for the heat capacity of liquid  $\text{ScI}_3$  in the temperature range of 1225–1325 K. According to this equation, the heat capacity of  $\text{ScI}_3(\text{l})$  falls from  $166.95 \text{ J K}^{-1} \text{mol}^{-1}$  at  $T_m = 1225 \text{ K}$  to  $123.60 \text{ J K}^{-1} \text{mol}^{-1}$  at 1325 K. It is difficult to find a physical explanation for this, so the mean value  $C_p^\circ(\text{ScI}_3, \text{l}) = 146 \pm 10 \text{ J K}^{-1} \text{mol}^{-1}$ , calculated on the basis of six measurements of enthalpy in the temperature range of 1231–1325 K [6], was used in this work for the heat capacity of liquid  $\text{ScI}_3$ . This heat capacity of  $\text{ScI}_3$  melt agrees with those of other liquid scandium trihalides.

According to O'Hare et al. [6], the standard enthalpy of formation of crystalline  $\text{ScI}_3$  at 298.15 K  $\Delta_f H^\circ(\text{ScI}_3, \text{cr}, 298.15 \text{ K})$  was assumed to be equal to  $-568.74 \pm 0.98 \text{ kJ mol}^{-1}$ . This value was based on high-precision calorimetric measurements of the enthalpy of dissolution of high-purity samples of metallic scandium in a mixture of solutions of hydroiodic  $\text{HI}(\text{sol})$  and hydrochloric  $\text{HCl}(\text{sol})$  acids, and of the enthalpy of dissolution of  $\text{ScI}_3$  in hydrochloric acid solutions  $\text{HCl}(\text{sol})$ . Based on their own high-tempera-

ture studies, Hirayama et al. [35] calculated the standard enthalpy of formation of  $\text{ScI}_3(\text{cr})$ :  $-552 \pm 29 \text{ kJ mol}^{-1}$ . In [36–38], the value  $\Delta_f H^\circ(\text{ScI}_3, \text{cr}, 298.15 \text{ K})$  was estimated using a variety of approximation methods, yielding the values  $-523$ ,  $-498$ , and  $-474.5 \text{ kJ mol}^{-1}$ , respectively. These estimates are characterized by considerable dispersion ( $\sim 50 \text{ kJ mol}^{-1}$ ) and differ notably from the experimental values in [6].

The errors of the  $\Phi^\circ(T)$  values at 298.15, 500, 1000, 1500, and 2000 K (Table 2) were estimated at 0.3, 0.7, 1, 3, and  $8 \text{ J K}^{-1} \text{ mol}^{-1}$ , respectively.

The thermodynamic functions of  $\text{ScI}_3(\text{cr}, \text{l})$  have yet to be published in any reference book.

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