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THERMODYNAMIC DATA FOR SELECTED GAS IMPURITIES IN THE PRIMARY COOLANT OF HIGH-TEMPERATURE GAS-COOLED REACTORS

by

R. C. Feber

ABSTRACT

The literature of thermodynamic data for selected fission-product species is reviewed and supplemented in support of complex chemical equilibrium calculations applied to fission-product distributions in the primary coolant of high-temperature gas-cooled reactors. Thermodynamic functions and heats and free energies of formation are calculated and tabulated to 3000 K for CsI (s,l,g), Cs₂I₂(g), CH₃I(g), COI₂(g), and CsH(g).

I. INTRODUCTION

The impurity content of the primary coolant of a high-temperature gas-cooled reactor (HTGR) has two important aspects. The first has to do with the interaction of the impurities with the graphite core and structural members and, of course, has been the subject of much experimental and calculational effort. The second aspect is the effect of a variable distribution among impurity species on the form in which fission products may be present in the primary coolant loop or under accident conditions. In this context, impurity species refer to those resulting from graphite-steam reaction. In addition, compound formation may be possible among fission-product species themselves; for example, between cesium and iodine.

The computer code QUIL has been used recently to solve complex chemical equilibrium distributions in HTGR environments.¹ The equilibrium distribution of cesium among its vapor species and a number of other impurity distributions were calculated for a range of normal and abnormal reactor coolant conditions. Many of the thermodynamic data required for these calculations were available in the JANAF tables,² but others were not. In this report we describe the sources and treatment of data that we found in the literature and which we used to compile the additional thermodynamic data that are tabulated. Because we decided to carry all tables to 3000 K, we extended the data from the literature to that temperature in two cases. Tables are given for CsI(s,l,g), Cs₂I₂(g), CH₃I(g), COI₂(g), and CsH(g). Behrens has recently recalculated thermodynamic data for Cs₂(g) on the basis of a new value for r_e .³

II. THERMODYNAMIC DATA FOR THE CESIUM-IODINE SYSTEM

A. Low-Temperature Heat Capacity of CsI(s)

The low-temperature heat capacity of CsI(s) has been measured at 54 points between 13.91 and 298.39 K (Ref. 4), at 189 points between 1.50 and 299.21 K (Ref. 5), and at 17 points between 2.13 and 10.00 K (Ref. 6). Table I shows thermodynamic quantities at 298.15 K calculated by the authors of Refs. 4-6 as well as our recalculation of their data by computer smoothing and numerical integration. From the last calculation of Table I we use $C_{p,298}^{\circ} = 12.590$ gibbs/mole and $S_{298}^{\circ} = 29.200$ gibbs/mole.

B. High-Temperature Heat Content of CsI(s,l)

Identical high-temperature heat content data (obtained with an ice calorimeter) between 369.3 and 1172.2 K are reported in Refs. 7 and 8, but these data are treated in different ways. The problem is that without constraints the heat content data do not extrapolate to near the origin (to zero at 273.15 K) nor do they give an extrapolated C_p° at room temperature that is close to the C_p° from low-temperature heat capacity measurements.

In both papers the heat content data for the solid are fitted to an equation of the form

$$H_f^{\circ} - H_{273}^{\circ} = a + bT + cT^2 + d/T.$$

In Ref. 8 the data are forced through the origin, from which fit $C_{p,298}^{\circ} = 11.899$ gibbs/mole. Also, in Ref. 8 the heat content data for the liquid are fitted to an equation of the form

$$H_f^{\circ} - H_{273}^{\circ} = a + bT + cT^2 \text{ (without constraints).}$$

From the two fits, at a melting point of 899 K, $C_p^{\circ}(s) = 16.015$ and $C_p^{\circ}(l) = 14.073$ gibbs/mole ($\Delta H_{\text{fusion}}^{\circ} = 6170$ cal/mole). It is unlikely that $C_{p,mp}^{\circ}(s)$ is greater than $C_{p,mp}^{\circ}(l)$.

In Ref. 7, the fit to the solid heat content data had the additional constraint that $C_{p,298}^{\circ} = 12.39$ gibbs/mole, which produces a minimum in the heat capacity-temperature curve between 273.15 and 370 K. The melting point is taken as 907 K and, although the same experimental data for the liquid heat content are fitted to an equation of the same form as in Ref. 8, the equations for the fits are not the same. From Ref. 7, $\Delta H_{\text{fusion}}^{\circ} = 5979$ cal/mole at 907 K.

On the assumption that the heat content data are not sufficiently precise to warrant a d/T term for the solid or a cT^2 term for the liquid, we recalculated a fit for the solid data to $H_f^{\circ} - H_{273}^{\circ} = a + bT + cT^2$ (without constraints) and for the liquid data to $H_f^{\circ} - H_{273}^{\circ} = a + bT$ (a constant heat capacity). The equation for the solid extrapolated to a respectable -49 cal/mole at 273.15 K, compared with -821 cal/mole if the d/T term was retained and an unconstrained fit was made.

With our fits, $C_{p,298}^{\circ}(s) = 12.140$ gibbs/mole; $C_{p,899}^{\circ}(s) = 15.793$ gibbs/mole; $C_{p,899}^{\circ}(l) = 16.448$ gibbs/mole; and $\Delta H_{\text{fusion}}^{\circ} = 5947$ cal/mol. We take $C_p^{\circ}(l)$ to be 16.45 gibbs/mole and use 5950 cal/mole for $\Delta H_{\text{fusion}}^{\circ}$ at a melting point of 899 K.⁹ We do not reference other measurements of the melting point, which range from 894-907 K.

From recent predictions of C_p° 's for a number of molten alkali metal halides using a model of the fused salts,¹⁰ $C_p^{\circ} \text{ CsCl}(l) = 16.4$ gibbs/mole and $C_p^{\circ} \text{ CsI}(l) = 14.8$ gibbs/mole. The heat of fusion of CsI has also been reported as 5640 ± 100 cal/mole¹¹ and 6580 ± 200 cal/mole.¹² According to the JANAF tables,² $C_p^{\circ} \text{ CsF}(l) = 17.7$ gibbs/mole and $C_p^{\circ} \text{ CsCl}(l) = 18.5$ gibbs/mole.

We join the low-temperature heat capacity data smoothly to our fit of the high-temperature heat content data of Refs. 7 and 8 and calculate the thermodynamic functions C_p° , S_T° , $-(F_T^\circ - H_{298}^\circ)/T$, and $H_T^\circ - H_{298}^\circ$ for CsI(s,l) given in Table II.

C. Heat of Formation of CsI(s)

In NBS Circular 500,⁹ $\Delta H_{f,298}^\circ \text{CsI(s)}$ was listed as -80.5 ± 2.5 kcal/mole. This value was later corrected^{13,14} to -83.9 kcal/mole to be consistent with a more recent $\overline{\Delta H}^\circ$ for Cs^+ . A still more recent value of -81.1 kcal/mole has been reported for $\Delta H_{f,298}^\circ \text{CsI(s)}$ from heat-of-solution measurements.¹⁵ This last quantity was in turn recalculated¹⁶ to -83.47 ± 0.3 kcal/mole using reference thermodynamic data for solutions from the NBS.¹⁷ We use the value of -83.9 kcal/mole because a more negative value is preferred, for reasons to be given later.

Table III contains values of ΔH_T° and ΔG_T° for CsI(s,l) as a function of temperature to 3000 K.

D. Thermodynamic Functions for CsI(g) and $\text{Cs}_2\text{I}_2(\text{g})$

Vibrational and rotational constants for CsI(g) available since 1950¹⁸ are given in Refs. 19-23. We used the constants for the $^1\Sigma$ ground state given in Ref. 23. Constants included in the calculations and their values in cm^{-1} are:

$$\begin{array}{ll} \omega_e = 119.178 & B_e = 2.36273 \times 10^{-2} \\ \omega_e x_e = 0.2505 & \alpha_e = 6.82625 \times 10^{-6} \\ \omega_e y_e = 0. & \gamma_e = 4.893 \times 10^{-8} \\ & D_e = 3.71464 \times 10^{-9} \end{array}$$

Our method of calculation was based on the approximation to level summation described by Mayer and Mayer.²⁴ Presumably, slightly more accurate functions could be calculated using direct summation of levels with cut-off of rotational and vibrational levels.^{25,26} The results of our calculations for CsI(g) are given in Table IV.

The thermodynamic functions for $\text{Cs}_2\text{I}_2(\text{g})$ given in Table V were calculated with the harmonic oscillator, rigid rotor approximation and the molecular parameters estimated in Ref. 27:

<u>Frequencies</u>	<u>Moments of Inertia</u>
$\nu_1 = 69 \text{ cm}^{-1}$	$I_A = 3088.3 \times 10^{-40} \text{ g cm}^2$
$\nu_2 = 58$	$I_B = 2359.3$
$\nu_3 = 69$	$I_C = 5447.6$
$\nu_4 = 33$	
$\nu_5 = 77$	$\sigma = 4$
$\nu_6 = 83$	

Molecular constants also have been estimated for a number of other alkali halide dimers.²⁸⁻³⁰

E. Heats of Formation of CsI(g) and $\text{Cs}_2\text{I}_2(\text{g})$

We need to know the value of $\Delta H_{f,298}^\circ$ for CsI(g) and for $\text{Cs}_2\text{I}_2(\text{g})$. The former value can be obtained from a Born-Haber cycle by adding $\Delta H_{f,298}^\circ \text{CsI(s)}$ and $\Delta H_{\text{subl},298}^\circ$ to the monomer (from

vapor pressure measurements corrected, if necessary, for the partial pressure of the dimer). The latter value can be obtained by knowing, in addition, the dissociation energy ($\text{Cs}_2\text{I}_2(\text{g}) \xrightarrow{\Delta H} 2 \text{Cs}(\text{g}) + 2 \text{I}(\text{g})$) or the heat of dimerization ($\text{Cs}_2\text{I}_2(\text{g}) \xrightarrow{\Delta H} 2 \text{CsI}(\text{g})$). There may also be other sources of information for $\Delta H_{f,298}^\circ \text{CsI}(\text{g})$ that do not depend on knowledge of the vapor pressure and that could therefore be used as a check. Because of experimental uncertainties, a completely unambiguous set of heats may not be achievable, but a reasonable, self-consistent set within those uncertainties should be.

1. Vapor Pressure of $\text{CsI}(\text{s}, \ell)$. Sources of vapor pressure data for CsI are given in Table VI. Literature on the amount of dimers (and, in some cases, trimers) in the vapors of the alkali halides is extensive. The general conclusion is that as the mass of the cation increases, the amount of polymeric species in the vapor decreases. Thus cesium halide vapors contain relatively small amounts of the dimer. In general, as the temperature increases, the proportion of dimer with respect to the monomer could increase or decrease, depending on the relative magnitudes of the heats of sublimation to the monomer and the dimer.

Pre-1961 literature for all alkali halides was worked into thermodynamic data by Brewer and Brackett,¹⁴ and data for many of the cesium halides (but not CsI) are also given in the JANAF tables.³

We calculated the heats of sublimation at 298.15 K for CsI from the data sources of Table VI, and results are given in Table VII. The possible presence of the dimer has been ignored for the moment, and the uncertainties are standard deviations.

With one exception, which derives from an equation for the data, all third-law heats are lower than second-law heats. Aside from systematic experimental errors, such a prevailing variation could be caused by too small a Δ (free-energy function) for the vaporization process, or by the presence of dimer in the vapor, or by a combination of effects.

Before looking further at the evidence for the presence of dimers in CsI vapors, we will mention two sources for $\Delta H_{f,298}^\circ \text{CsI}(\text{g})$ that do not depend on a Born-Haber cycle. From them we can calculate $\Delta H_{f,298}^\circ \text{CsI}(\text{s})$ by using a preliminary value from Table VII of 46.4 kcal/mole for $\Delta H_{\text{subl},298}^\circ \text{CsI}(\text{s})$ to the monomer. To show the reasonableness of the $\Delta H_{f,298}^\circ \text{CsI}(\text{s})$ value given in Sec. II-C, we will go through the exercise but will not make further use of data from these two sources. The effect of dimers in the vapor will be to increase $\Delta H_{\text{subl},298}^\circ \text{CsI}(\text{s})$ to the monomer by a few tenths of a kcal/mole at most.

From flame photometry measurements, Bulewicz, Phillips, and Sugden⁴¹ reported $D_0^\circ \text{CsI}(\text{g}) = 83.7 \pm 4$ kcal/mole, from which $\Delta H_{f,0}^\circ \text{CsI}(\text{g}) = -39.4$ kcal/mole, or $\Delta H_{f,298}^\circ \text{CsI}(\text{g}) = -40.3 \pm 4$ kcal/mole. Thus, $\Delta H_{f,298}^\circ \text{CsI}(\text{s}) = -86.7 \pm 4$ kcal/mole.

Berkowitz⁴² reported $D_0^\circ \text{CsI}(\text{g}) = 82.3 \pm 1$ kcal/mole from thresholds for photodissociative ionization, from which $\Delta H_{f,298}^\circ \text{CsI}(\text{g}) = -38.9 \pm 1$ kcal/mole and $\Delta H_{f,298}^\circ \text{CsI}(\text{s}) = -85.3 \pm 1$ kcal/mole.

Our selected value for the heat of formation of the solid is somewhat more positive than these last two values, but can be regarded as consistent with the assigned uncertainties.

2. Monomer-Dimer Equilibrium in CsI Vapor. Direct experimental evidence for the amount of dimer in CsI vapors is somewhat contradictory. Only the more pertinent references are cited here, including some on other cesium halides and some on theoretical or empirical predictions. It is convenient to refer not only to the percentage of dimer in the vapors, but also to express results or predictions in terms of a dimer dissociation energy (DDE), which is taken as the heat for the reaction $\text{Cs}_2\text{I}_2(\text{g}) = 2 \text{CsI}(\text{g})$. When necessary, thermodynamic functions in Tables IV and V are used to reduce the DDE to 298.15 K.

Miller and Kusch^{43,44} analyzed the velocity distribution of CsCl and CsBr molecules through an aperture from an isothermal enclosure (temperature range of 825-1017 K for CsCl and 828-965 K for CsBr). They found no substantial evidence for the presence of dimers for those particular halides, but from the experimental uncertainties they placed upper limits of 4 and 6%, respectively, on the percentage of dimer. Rothberg, Eisenstadt, and Kusch⁴⁵ later applied the same technique to molecules freely evaporating from the surface of single crystals of CsBr and CsI and reported $\leq 3\%$ dimer from CsBr (765-830 K) and $< 0.5\%$ dimer from CsI (757-772 K) (corresponding to $DDE_{298} < 32$ kcal/mole). Akishin and Rambidi⁴⁶ made an electron diffraction study of the structure of the cesium halides and concluded that their results were indirect confirmation of the data of Miller and Kusch,^{43,44} according to which no noticeable amounts of dimer were present in the vapors of the cesium halides.

Other direct experimental data of which we are aware suggest a greater amount of dimer in vapors over the cesium halides. For example, Datz, Smith, and Taylor⁴⁷ found the mole fraction of the dimer over CsCl to be about 0.2 at 1250 K, decreasing to about 0.1 at 1400 K. They had measured the vapor density as a function of temperature, and their data were used for the JANAF tables.²

From mass spectrometric measurements using a double effusion chamber as an ion source, Akishin, Gorokhov, and Sidorov⁴⁸ reported the DDE for CsI to be 31.2 ± 0.1 kcal/mole over the temperature range 755-862 K. With this quantity, $DDE_{298} = 32.1 \pm 0.1$ kcal/mole. A mass spectrometric study of Knudsen cell effusates over CsI (705-882 K) was also made by Winchell.⁴⁹ From his data, $DDE_{794} = 38 \pm 7$ kcal/mole and therefore $DDE_{298} = 38.9 \pm 7$ kcal/mole.

Murgulescu and Topor^{39,40} combined the results of quasi-static Rodebush-Dixon vapor pressure determinations with transpiration measurements to deduce the composition of CsI vapors (1276-1376 K). Over that range they reported the mole fraction of the dimer to be 0.29. From their equations for the partial pressures of the monomer and dimer, $DDE_{298} = 40.3 \pm 0.3$ kcal/mole (third-law calculation).

Thus, experimentally based values for DDE_{298} have ranged from 32.1 to 40.3 kcal/mole, if we neglect the even more discordant results of Kusch et al.⁴³⁻⁴⁵ A similar range of values has been proposed from theoretical or empirical considerations. Some of these latter values converted, if necessary, to DDE_{298} are given in Table VIII. We take DDE_{298} to be 35 kcal/mole.

3. Heats of Sublimation to the Monomer and to the Dimer. With $DDE_{298} = 35$ kcal/mole, we calculate heats of sublimation at 298.15 K to the monomer and dimer from the cited vapor pressure measurements. Results are given in Table IX.

The Knudsen cell data of Refs. 34, 35, and 38 could be corrected for the assumption that the gaseous species was monomeric. However, because of the relatively small amounts of dimer corresponding to the selected DDE and the relatively large disagreement between sets of vapor pressure data, the effect of such a correction would be trivial.

An average of all third-law values of $\Delta H_{\text{subl},298}^\circ$ to the monomer is almost identical with the third-law value in Ref. 32, which in turn has the best agreement between second- and third-law values. Therefore, we take that quantity to be 46.3 kcal/mole, and $\Delta H_{\text{subl},298}^\circ$ to the dimer becomes 57.6 kcal/mole. With $\Delta H_{f,298}^\circ \text{ CsI(s)} = -83.9$ kcal/mole, $\Delta H_{f,298}^\circ \text{ CsI(g)} = -37.6$ kcal/mole, and $\Delta H_{f,298}^\circ \text{ Cs}_2\text{I}_2(\text{g}) = -110.2$ kcal/mole. Table X is a tabulation of the pressures calculated with the adopted quantities.

Values of $\Delta H_{f,298}^\circ$ and $\Delta G_{f,298}^\circ$ for CsI(g) are given in Table XI, and Table XII contains the analogous data for Cs₂I₂(g).

4. **Polyiodides.** Thermodynamic data for the polyiodides, such as CsI_3 , CsI_4 , and Cs_2I_5 , are not included because these condensed phases were not important to the applications considered in this report. For example, the dissociation pressure of $\text{I}_2(\text{g})$ over CsI_3 at the melting point (487 K) is about 0.17 atm ($\text{CsI}_3(\text{l}) = \text{CsI}(\text{s}) + \text{I}_2(\text{g})$). Some relatively recent thermodynamic data for these compounds and references to earlier work can be found in Refs. 54 and 55.

III. THERMODYNAMIC DATA FOR METHYL IODIDE (CH_3I)

We have calculated ideal gas thermodynamic functions for methyl iodide from 298.15-3000 K using the harmonic oscillator, rigid rotor approximation. These functions were recently calculated to 1500 K by Kudchadker and Kudchadker.⁶⁶ Vibrational frequencies (in cm^{-1}) used in Ref. 56 and those used here are given in Table XIII, together with the references used in each tabulation.

In Ref. 56 and in our calculation, the moments of inertia ($I_A = 5.354 \times 10^{-40} \text{ g cm}^2$; $I_B = I_C = 110.92 \times 10^{-40} \text{ g cm}^2$) are calculated from the equilibrium ground-state rotational constants given by Matsuura and Overend,⁶⁹ and values for the moments are close to those calculated by Duncan.⁷⁰

Wagman et al.⁷¹ have recently recommended $\Delta H_f^\circ, 298 \text{ CH}_3\text{I}(\text{g}) = 3.1 \text{ kcal/mole}$. Other recommended values based on evaluations of data from the literature include 3.34 kcal/mole,⁷² $3.4 \pm 0.3 \text{ kcal/mole}$,⁷³ and $3.29 \pm 0.28 \text{ kcal/mole}$.⁵⁶ We use 3.30 kcal/mole.

Calculated values of C_p° , S° , $-(F^\circ - H_{298}^\circ)/T$, and $H^\circ - H_{298}^\circ$ are given in Table XIV, and values of ΔH_f° and ΔG_f° are given in Table XV.

IV. THERMODYNAMIC DATA FOR CARBONYL IODIDE (COI_2)

Molecular parameters have been estimated for gaseous carbonyl iodide and ideal gas thermodynamic functions calculated from 298.15-1500 K.⁷⁴ Although in Ref. 74 the authors also estimated the required $\Delta H_f^\circ, 298 \text{ COI}_2(\text{g}) = -6 \text{ kcal/mole}$, they did not calculate ΔG_f° as a function of temperature. Estimated molecular parameters for this C_{2v} molecule were:

Frequencies (cm^{-1})	Bond Lengths ($\text{\AA}$)
$\nu_1 = 1782$	C-I = 2.2
$\nu_2 = 332$	C=O = 1.1
$\nu_3 = 134$	
$\nu_4 = 532$	Bond Angle
$\nu_5 = 292$	(deg)
$\nu_6 = 439$	
	I-C-I = 112

We have used their estimates to calculate thermodynamic functions (Table XVI) and ΔH_f° and ΔG_f° (Table XVII) to 3000 K. All necessary auxiliary thermodynamic data are from the JANAF tables.³

V. THERMODYNAMIC DATA FOR CESIUM HYDRIDE (CsH)

Thermodynamic functions to 2000 K were calculated over 15 yr ago by Kelley,⁷⁶ using spectroscopic constants listed by Herzberg.¹⁸ Since Herzberg's compilation, spectroscopic constants for CsH have been reported by Bartky,⁷⁶ Ringstrom,⁷⁷ and Tam and Happer.⁷⁸ We use spectroscopic constants for the $^1\Sigma^+$ ground state as listed by Bartky⁷⁶ and calculate thermodynamic functions with a modification of the usual approximation to numerical summation of vibrational-rotational levels given by Mayer and Mayer:²⁴

$$\begin{aligned}\omega_e &= 891.29 \text{ cm}^{-1} & B_e &= 2.7085 \text{ cm}^{-1} \\ \omega_e x_e &= 12.794 & \alpha_e &= 5.70 \times 10^{-2} \\ & & D_e &= 1.00 \times 10^{-4}\end{aligned}$$

Two other relatively low-lying electronic states are known for CsH.^{76,77} Because the approximation using the Euler-Maclaurin summation formula²⁴ is not satisfactory for excited states of molecules having dissociation energies as low as that of CsH, these states were not included in the calculation. For such states it is preferable to perform a direct summation of vibrational-rotational states and take account of the cut-off of vibrational-rotational quantum numbers as limited by predissociation at the dissociation limit.^{25,26} The simplified procedure used here is considered satisfactory to 3000 K; i.e., if the excited electronic states are ignored, at that temperature the entropy and free-energy function (Table XVIII) are estimated to be low by about 1 and 0.1%, respectively.

The heat of formation of CsH(g) is based on spectroscopic dissociation energies and is somewhat uncertain. We have used $\Delta H_f^\circ,_{298} \text{ CsH(g)} = 27.8 \text{ kcal/mole}$, which is based on $D_0^\circ = 1.81 \text{ eV}$, as given by Ringstrom.⁷⁷ This is at the lower limit of a range of recommended values to 2.08 eV,⁷⁸ which would correspond to $\Delta H_f^\circ,_{298} = 21.6 \text{ kcal/mole}$. Values for ΔH_f° and ΔG_f° using the more positive heat of formation at 298.15 K are given in Table XIX.

We have not derived thermodynamic data for dimeric cesium hydride, although interatomic distances and a dimerization energy have been predicted.⁷⁹

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TABLE I
THERMODYNAMIC QUANTITIES CALCULATED FOR
THE CESIUM-IODINE SYSTEM AT 298.15 K

	$C_{p,298}^0$ (gibbs/mole)	S_{298}^0 (gibbs/mole)	$H_{298}^0 - H_0^0$ (cal/mole)
Ref. 4	12.62	29.41	3231.95
Ref. 5	12.571	29.127	3216.44
Recalculation	12.566	29.108	3216.36
Recalculation of Refs. 5 and 6	12.566	29.117	3216.43
Recalculation of all data	12.591	29.192	3221.31

TABLE II
HIGH-TEMPERATURE THERMODYNAMIC FUNCTIONS
FOR CESIUM IODIDE (s,l)

<u>Temp.</u> <u>(K)</u>	<u>C_p^o</u> <u>(gibbs/mole)</u>	<u>S_T^o</u> <u>(gibbs/mole)</u>	<u>-(F_T^o - H₂₉₈^o)/T</u> <u>(gibbs/mole)</u>	<u>H_T^o - H₂₉₈^o</u> <u>(kcal/mole)</u>
298.15(s)	12.590	29.200	29.200	0.000
300.00	12.595	29.278	29.200	0.023
325.00	12.675	30.287	29.245	0.339
350.00	12.750	31.231	29.354	0.657
375.00	12.830	32.114	29.509	0.977
400.00	12.915	32.942	29.698	1.298
425.00	13.010	33.730	29.912	1.623
450.00	13.120	34.477	30.145	1.949
475.00	13.235	35.187	30.391	2.278
500.00	13.367	35.871	30.649	2.611
550.00	13.671	37.159	31.183	3.287
600.00	13.975	38.360	31.731	3.978
700.00	14.583	40.563	32.840	5.406
800.00	15.191	42.549	33.931	6.895
899.00	15.793	44.354	34.980	8.428
899.00(l)	16.450	50.973	34.980	14.378
900.00	16.450	50.991	34.997	14.394
1000.00	16.450	52.724	36.685	16.039
1100.00	16.450	54.292	38.215	17.684
1200.00	16.450	55.723	39.616	19.329
1300.00	16.450	57.040	40.906	20.974
1400.00	16.450	58.259	42.103	22.619
1500.00	16.450	59.394	43.218	24.264
1600.00	16.450	60.456	44.263	25.909
1700.00	16.450	61.453	45.245	27.554
1800.00	16.450	62.393	46.172	29.199
1900.00	16.450	63.283	47.049	30.844
2000.00	16.450	64.127	47.882	32.489
2100.00	16.450	64.929	48.675	34.134
2200.00	16.450	65.694	49.431	35.779
2300.00	16.450	66.426	50.154	37.424
2400.00	16.450	67.126	50.847	39.069
2500.00	16.450	67.797	51.512	40.714
2600.00	16.450	68.442	52.150	42.359
2700.00	16.450	69.063	52.765	44.004
2800.00	16.450	69.662	53.358	45.649
2900.00	16.450	70.239	53.930	47.294
3000.00	16.450	70.796	54.483	48.939

$$H_{298}^o - H_0^o = 3.221 \text{ kcal/mole}$$

TABLE III
THERMODYNAMICS OF FORMATION OF CESIUM IODIDE (s,l)

<u>Temp.</u> <u>(K)</u>	<u>ΔH_f°</u> <u>(kcal/mole)</u>	<u>ΔG_f°</u> <u>(kcal/mole)</u>
298.15(s)	-83.900	-82.400
300.00	-83.903	-82.391
400.00	-86.476	-81.633
500.00	-91.673	-79.930
600.00	-91.497	-77.596
700.00	-91.258	-75.298
800.00	-90.960	-73.038
899.00	-90.606	-70.841
899.00(l)	-84.657	-70.841
900.00	-84.652	-70.823
1000.00	-100.280	-68.490
1100.00	-99.585	-65.345
1200.00	-98.891	-62.263
1300.00	-98.198	-59.238
1400.00	-97.507	-56.269
1500.00	-96.815	-53.347
1600.00	-96.126	-50.472
1700.00	-95.439	-47.639
1800.00	-94.755	-44.848
1900.00	-94.073	-42.092
2000.00	-93.396	-39.375
2100.00	-92.725	-36.689
2200.00	-92.061	-34.037
2300.00	-91.402	-31.413
2400.00	-90.754	-28.820
2500.00	-90.117	-26.254
2600.00	-89.490	-23.710
2700.00	-88.878	-21.190
2800.00	-88.282	-18.695
2900.00	-87.702	-16.220
3000.00	-87.142	-13.766

TABLE IV

IDEAL GAS THERMODYNAMIC FUNCTIONS OF MONOMERIC CESIUM IODIDE (g)

Temp. (K)	C_p° (gibbs/mole)	S_T° (gibbs/mole)	$-(F_T^\circ - H_{298}^\circ)/T$ (gibbs/mole)	$H_T^\circ - H_{298}^\circ$ (kcal/mole)
0.00	0.000	0.000	Infinite	-2.521
100.00	8.540	56.157	73.656	-1.750
200.00	8.866	62.208	66.583	-0.875
298.15	8.951	65.767	65.767	0.000
300.00	8.952	65.822	65.767	0.017
400.00	8.998	68.404	66.119	0.914
500.00	9.031	70.416	66.784	1.816
600.00	9.061	72.065	67.531	2.720
700.00	9.089	73.464	68.281	3.628
800.00	9.116	74.679	69.007	4.538
900.00	9.143	75.755	69.698	5.451
1000.00	9.170	76.719	70.353	6.367
1100.00	9.198	77.595	70.972	7.285
1200.00	9.226	78.396	71.558	8.206
1300.00	9.254	79.136	72.112	9.130
1400.00	9.283	79.823	72.639	10.057
1500.00	9.313	80.464	73.139	10.987
1600.00	9.343	81.066	73.616	11.920
1700.00	9.374	81.633	74.071	12.856
1800.00	9.405	82.170	74.507	13.795
1900.00	9.437	82.680	74.923	14.737
2000.00	9.470	83.164	75.323	15.682
2100.00	9.503	83.627	75.708	16.631
2200.00	9.537	84.070	76.078	17.583
2300.00	9.571	84.495	76.435	18.538
2400.00	9.606	84.903	76.779	19.497
2500.00	9.642	85.296	77.112	20.459
2600.00	9.679	85.675	77.434	21.426
2700.00	9.715	86.041	77.746	22.395
2800.00	9.753	86.395	78.049	23.369
2900.00	9.791	86.738	78.342	24.346
3000.00	9.830	87.070	78.628	25.327

TABLE V

IDEAL GAS THERMODYNAMIC FUNCTIONS OF DIMERIC CESIUM IODIDE (g)

Temp. (K)	C_p° (gibbs/mole)	S_T° (gibbs/mole)	$-(F_T^\circ - H_{298}^\circ)/T$ (gibbs/mole)	$H_T^\circ - H_{298}^\circ$ (kcal/mole)
0.00	0.000	0.000	Infinite	-5.400
100.00	19.001	81.207	119.987	-3.878
200.00	19.645	94.647	104.325	-1.935
298.15	19.769	102.519	102.519	0.000
300.00	19.778	102.642	102.520	0.037
400.00	19.814	108.336	103.296	2.016
500.00	19.835	112.760	104.763	3.999
600.00	19.846	116.377	106.406	5.983
700.00	19.853	119.437	108.055	7.968
800.00	19.857	122.089	109.647	9.953
900.00	19.860	124.428	111.162	11.939
1000.00	19.862	126.520	112.595	13.925
1100.00	19.864	128.413	113.948	15.912
1200.00	19.865	130.142	115.227	17.898
1300.00	19.866	131.732	116.436	19.885
1400.00	19.867	133.204	117.582	21.871
1500.00	19.868	134.575	118.669	23.858
1600.00	19.868	135.857	119.704	25.845
1700.00	19.868	137.062	120.690	27.832
1800.00	19.869	138.197	121.631	29.819
1900.00	19.869	139.272	122.532	31.805
2000.00	19.869	140.291	123.395	33.792
2100.00	19.870	141.260	124.222	35.779
2200.00	19.870	142.184	125.018	37.766
2300.00	19.870	143.068	125.784	39.753
2400.00	19.870	143.913	126.522	41.740
2500.00	19.870	144.725	127.234	43.727
2600.00	19.870	145.504	127.921	45.714
2700.00	19.870	146.254	128.587	47.701
2800.00	19.870	146.976	129.231	49.688
2900.00	19.871	147.674	129.855	51.675
3000.00	19.871	148.347	130.460	53.662

TABLE VI

VAPOR PRESSURE DATA FOR CESIUM IODIDE

Ref.	Method	Temp. Range (K)	No. Points
31	Boiling point	1325-1553	9
32	Boiling point	1296-1553	5
33	Absolute manometer ^a	767-847	15
34	Knudsen cell	696-894	51
35	Knudsen cell	671-876	22
36	Quasi-static ^b	1156-1374	12
37	Knudsen cell	c	c
38	Knudsen cell	650-850	d

^aForce exerted by beam of CsI(g) on aluminum vane attached to quartz fiber (electromagnetic balance).

^bRodebush-Dixon method; additional data given as equations in Refs. 39 and 40.

^cTemperature range unstated, but apparently above and below the melting point; vapor pressures not given, but stated to be 20% below those of Ref. 35.

^dData represented by equation.

TABLE VII
CALCULATED HEATS OF SUBLIMATION
FOR CESIUM IODIDE AT 298.15 K

Ref.	$\Delta H_{\text{subl},298}^{\circ}$ CsI to Monomer Alone (kcal/mole)	
	Third Law	Second Law
31	46.683 ± 0.632	59.547
32	46.248 ± 0.190	48.518
33	46.958 ± 0.062	48.235
34	46.602 ± 0.655	49.251 ^a
	(47.215 ± 0.165)	48.949 ^a
	(46.012 ± 0.322)	49.107 ^a
35	45.951 ± 0.193	48.042
36	46.158 ± 0.048	46.908
38	44.965	46.974

^aApparently, data were not reproducible and depended on the experimental sequence for some unspecified reason. The data can be broken into two parts, and calculated heats from the two subsets are enclosed in parentheses.

TABLE VIII
DDE₂₉₈ VALUES CALCULATED FROM THEORETICAL OR EMPIRICAL PREDICTIONS

DDE ₂₉₈ (kcal/mole)	Reference	Source of Calculation
35	Polyachenok ³⁶	From an electrostatic model
33.2	Brewer and Brackett ¹⁴	From the authors' estimate of DDE ₁₀₀₀ = 32 kcal/mole
39.3	Milne and Cubicciotti ¹¹	Based on the authors' calculation of monomer and dimer energies, which in turn was based on a model suggested by Pauling. The authors have also calculated energies of the gaseous trimers ²²
32.3	Blander ⁴³	From a dimensional analysis of the statistical-mechanical equations for the association of ionic molecules in the vapor
31.5	Datz et al. ⁴⁷	An extrapolation of the authors' plot of the DDE's of the alkali halide dimers vs the reciprocal of the anion-cation distance in the dimers
32	Bauer et al. ³⁰	An extrapolation of a graphical correlation similar to that in Ref. 47.

TABLE IX
HEATS OF SUBLIMATION FOR CESIUM IODIDE
AT 298.15 K WITH $DDE_{298} = 35$ kcal/mole

Ref.	$\Delta H_{\text{subl},298}^{\circ}$ (kcal/mole)			
	To Monomer		To Dimer	
	Third Law	Second Law	Third Law	Second Law
31	46.855 $\pm$ 0.593	58.793	58.710 $\pm$ 1.186	82.587
32	46.463 $\pm$ 0.167	48.400	57.872 $\pm$ 0.335	61.799
33	46.986 $\pm$ 0.058	48.046	58.972 $\pm$ 0.116	61.093
34	46.641 $\pm$ 0.631	49.229	58.282 $\pm$ 1.263	63.458
	(47.239 $\pm$ 0.158)	48.784	59.478 $\pm$ 0.316	62.567) ^a
	(45.066 $\pm$ 0.288)	48.875	57.131 $\pm$ 0.577	62.751) ^a
35	45.994 $\pm$ 0.171	47.752	56.987 $\pm$ 0.341	60.505
36	46.325 $\pm$ 0.035	46.793	57.650 $\pm$ 0.070	58.586
38	45.029	46.589	55.058	58.177

^aSee footnote to Table VII.

TABLE X
CALCULATED PARTIAL PRESSURES OF MONOMERIC
AND DIMERIC CESIUM IODIDE

Temp. (K)	P_{monomer} (atm)	P_{dimer} (atm)	P_{total} (atm)	$\frac{100X}{P_{\text{dimer}}/P_{\text{monomer}}}$ (atm)
300	1.83×10^{-26}	4.80×10^{-33}	1.83×10^{-26}	2.62×10^{-6}
400	4.60×10^{-18}	1.33×10^{-22}	4.60×10^{-18}	2.89×10^{-8}
500	4.56×10^{-13}	2.10×10^{-16}	4.56×10^{-13}	0.0460
600	9.11×10^{-10}	2.54×10^{-12}	9.13×10^{-10}	0.279
700	1.95×10^{-7}	1.90×10^{-9}	1.97×10^{-7}	0.974
800	1.04×10^{-6}	2.49×10^{-7}	1.06×10^{-6}	2.39
900	2.19×10^{-4}	1.02×10^{-6}	2.29×10^{-4}	4.67
1000	1.74×10^{-3}	9.64×10^{-6}	1.83×10^{-3}	5.56
1100	9.12×10^{-3}	5.69×10^{-4}	9.69×10^{-3}	6.24
1200	3.54×10^{-2}	2.38×10^{-3}	3.78×10^{-2}	6.73
1300	0.109	7.65×10^{-3}	0.116	7.04
1400	0.279	2.01×10^{-2}	0.299	7.19
1500	0.621	4.49×10^{-2}	0.666	7.23
1600	1.23	8.84×10^{-2}	1.32	7.17
1700	2.23	0.157	2.38	7.04
1800	3.72	0.256	3.98	6.86
1900	5.84	0.388	6.22	6.65
2000	8.67	0.555	9.22	6.40

TABLE XI

THERMODYNAMICS OF FORMATION OF MONOMERIC CESIUM IODIDE (g)

<u>Temp. (K)</u>	<u>ΔH_f° (kcal/mole)</u>	<u>ΔG_f° (kcal/mole)</u>
298.15	-37.600	-47.003
300.00	-37.609	-47.061
400.00	-40.560	-49.902
500.00	-46.168	-51.697
600.00	-46.455	-52.776
700.00	-46.736	-53.807
800.00	-47.017	-54.798
900.00	-47.295	-55.754
1000.00	-63.652	-55.858
1100.00	-63.684	-55.077
1200.00	-63.714	-54.294
1300.00	-63.742	-53.506
1400.00	-63.769	-52.719
1500.00	-63.792	-51.929
1600.00	-63.815	-51.137
1700.00	-63.837	-50.343
1800.00	-63.859	-49.551
1900.00	-63.880	-48.753
2000.00	-63.903	-47.959
2100.00	-63.928	-47.158
2200.00	-63.956	-46.361
2300.00	-63.988	-45.559
2400.00	-64.026	-44.757
2500.00	-64.070	-43.954
2600.00	-64.123	-43.148
2700.00	-64.187	-42.339
2800.00	-64.262	-41.530
2900.00	-64.350	-40.715
3000.00	-64.454	-39.901

TABLE XII
THERMODYNAMICS OF FORMATION OF DIMERIC CESIUM IODIDE (g)

<u>Temp.</u> <u>(K)</u>	<u>ΔH_f°</u> <u>(kcal/mole)</u>	<u>ΔG_f°</u> <u>(kcal/mole)</u>
298.15	-110.200	-120.355
300.00	-110.215	-120.418
400.00	-115.932	-123.226
500.00	-126.970	-123.991
600.00	-127.367	-123.358
700.00	-127.761	-122.659
800.00	-128.157	-121.903
900.00	-128.553	-121.098
1000.00	-161.114	-118.605
1100.00	-161.026	-114.359
1200.00	-160.943	-110.121
1300.00	-160.859	-105.888
1400.00	-160.781	-101.664
1500.00	-160.701	-97.444
1600.00	-160.626	-93.229
1700.00	-160.555	-89.018
1800.00	-160.489	-84.815
1900.00	-160.429	-80.609
2000.00	-160.379	-76.412
2100.00	-160.339	-72.209
2200.00	-160.313	-68.017
2300.00	-160.300	-63.821
2400.00	-160.306	-59.627
2500.00	-160.334	-55.433
2600.00	-160.385	-51.237
2700.00	-160.464	-47.034
2800.00	-160.574	-42.832
2900.00	-160.716	-38.625
3000.00	-160.900	-34.414

TABLE XIII
VIBRATIONAL FREQUENCIES OF METHYL IODIDE^a

<u>Frequencies</u>	<u>Degeneracy</u>	<u>Ref. 56^a</u>	<u>This Calculation^a</u>
ν_1	1	2933 (58)	2971.3 (63)
ν_2	1	1252 (58)	1250.8 (59)
ν_3	1	533 (58, 59)	533.2 (59)
ν_4	2	3060 (58, 60, 62)	3060.1 (62, 64)
ν_5	2	1436 (61)	1434.7 (65, 66, 67)
ν_6	2	882 (59, 60)	882.7 (68)

^aNumbers in parentheses indicate the references that pertain to the given frequency. The frequencies used in Ref. 56 had been recommended in the review by Shimanouchi.⁶⁷

TABLE XIV

IDEAL GAS THERMODYNAMIC FUNCTIONS OF METHYL IODIDE

Temp. (K)	C_p° (gibbs/mole)	S_T° (gibbs/mole)	$-(F_T^\circ - H_{298}^\circ)/T$ (gibbs/mole)	$H_T^\circ - H_{298}^\circ$ (kcal/mole)
0.00	0.000	0.000	Infinite	-2.585
100.00	8.005	51.012	68.905	-1.789
200.00	8.923	56.780	61.540	-0.952
298.15	10.536	60.631	60.631	0.000
300.00	10.569	60.697	60.631	0.019
400.00	12.333	63.981	61.067	1.165
500.00	13.917	66.907	61.948	2.480
600.00	15.274	69.568	62.999	3.941
700.00	16.444	72.012	64.115	5.528
800.00	17.465	74.276	65.245	7.225
900.00	18.364	76.386	66.367	9.017
1000.00	19.155	78.363	67.469	10.894
1100.00	19.852	80.222	68.545	12.845
1200.00	20.464	81.976	69.591	14.862
1300.00	21.001	83.636	70.609	16.936
1400.00	21.473	85.210	71.596	19.060
1500.00	21.886	86.706	72.554	21.228
1600.00	22.249	88.130	73.483	23.435
1700.00	22.569	89.489	74.385	25.677
1800.00	22.852	90.787	75.260	27.948
1900.00	23.102	92.029	76.110	30.246
2000.00	23.324	93.220	76.936	32.567
2100.00	23.521	94.363	77.739	34.910
2200.00	23.697	95.461	78.520	37.271
2300.00	23.855	96.518	79.280	39.649
2400.00	23.997	97.537	80.019	42.042
2500.00	24.125	98.519	80.740	44.448
2600.00	24.240	99.467	81.442	46.866
2700.00	24.345	100.384	82.127	49.295
2800.00	24.439	101.271	82.795	51.735
2900.00	24.526	102.130	83.447	54.183
3000.00	24.604	102.963	84.083	56.640

TABLE XV
THERMODYNAMICS OF FORMATION OF METHYL IODIDE

<u>Temp.</u> <u>(K)</u>	<u>ΔH_f°</u> <u>(kcal/mole)</u>	<u>ΔG_f°</u> <u>(kcal/mole)</u>
298.15	3.300	3.723
300.00	3.284	3.726
400.00	0.557	4.063
500.00	-5.258	5.505
600.00	-5.673	7.698
700.00	-6.013	9.953
800.00	-6.285	12.253
900.00	-6.500	14.584
1000.00	-6.658	16.935
1100.00	-6.773	19.302
1200.00	-6.848	21.674
1300.00	-6.893	24.054
1400.00	-6.912	26.437
1500.00	-6.913	28.818
1600.00	-6.900	31.200
1700.00	-6.871	33.580
1800.00	-6.833	35.958
1900.00	-6.785	38.333
2000.00	-6.731	40.706
2100.00	-6.673	43.078
2200.00	-6.612	45.448
2300.00	-6.547	47.810
2400.00	-6.482	50.175
2500.00	-6.418	52.532
2600.00	-6.352	54.889
2700.00	-6.289	57.242
2800.00	-6.225	59.597
2900.00	-6.164	61.946
3000.00	-6.105	64.291

TABLE XVI

IDEAL GAS THERMODYNAMIC FUNCTIONS OF CARBONYL IODIDE

Temp. (K)	C_p° (gibbs/mole)	S° (gibbs/mole)	$-(F^\circ - H_{298}^\circ)/T$ (gibbs/mole)	$H^\circ - H_{298}^\circ$ (kcal/mole)
0.00	0.000	0.000	Infinite	-3.600
100.00	10.549	63.616	90.775	-2.716
200.00	14.025	72.098	79.457	-1.472
298.15	15.760	78.063	78.063	0.000
300.00	15.782	78.160	78.063	0.029
400.00	16.712	82.839	78.695	1.658
500.00	17.325	86.638	79.915	3.361
600.00	17.784	89.839	81.310	5.118
700.00	18.142	92.609	82.730	6.915
800.00	18.426	95.051	84.121	8.744
900.00	18.652	97.234	85.459	10.598
1000.00	18.834	99.209	86.737	12.473
1100.00	18.980	101.012	87.954	14.364
1200.00	19.100	102.668	89.112	16.268
1300.00	19.198	104.201	90.214	18.183
1400.00	19.279	105.627	91.265	20.107
1500.00	19.347	106.959	92.267	22.038
1600.00	19.404	108.210	93.225	23.976
1700.00	19.453	109.388	94.141	25.919
1800.00	19.495	110.501	95.020	27.866
1900.00	19.531	111.556	95.862	29.818
2000.00	19.562	112.558	96.672	31.772
2100.00	19.589	113.514	97.452	33.730
2200.00	19.613	114.425	98.203	35.690
2300.00	19.634	115.298	98.927	37.652
2400.00	19.652	116.134	99.627	39.617
2500.00	19.669	116.936	100.303	41.583
2600.00	19.683	117.708	100.958	43.550
2700.00	19.697	118.451	101.592	45.519
2800.00	19.708	119.168	102.207	47.490
2900.00	19.719	119.859	102.804	49.461
3000.00	19.729	120.528	102.384	51.433

TABLE XVII
THERMODYNAMICS OF FORMATION OF CARBONYL IODIDE

<u>Temp.</u> <u>(K)</u>	<u>ΔH_f°</u> <u>(kcal/mole)</u>	<u>ΔG_f°</u> <u>(kcal/mole)</u>
298.15	-6.000	-13.288
300.00	-6.005	-13.333
400.00	-10.150	-15.597
500.00	-20.654	-15.962
600.00	-20.550	-15.035
700.00	-20.466	-14.122
800.00	-20.396	-13.222
900.00	-20.340	-12.328
1000.00	-20.289	-11.441
1100.00	-20.248	-10.558
1200.00	-20.213	-9.679
1300.00	-20.184	-8.801
1400.00	-20.160	-7.926
1500.00	-20.142	-7.054
1600.00	-20.126	-6.181
1700.00	-20.114	-5.309
1800.00	-20.108	-4.440
1900.00	-20.104	-3.568
2000.00	-20.105	-2.698
2100.00	-20.108	-1.828
2200.00	-20.118	-0.956
2300.00	-20.130	-0.088
2400.00	-20.146	0.786
2500.00	-20.167	1.660
2600.00	-20.193	2.532
2700.00	-20.223	3.407
2800.00	-20.255	4.282
2900.00	-20.294	5.158
3000.00	-20.338	6.035

TABLE XVIII

IDEAL GAS THERMODYNAMIC FUNCTIONS OF CESIUM HYDRIDE

Temp. (K)	C_p° (gibbs/mole)	S_T° (gibbs/mole)	$-(F_T^\circ - H_{298}^\circ)/T$ (gibbs/mole)	$H_T^\circ - H_{298}^\circ$ (kcal/mole)
0.00	0.000	0.000	Infinite	-2.114
100.00	6.964	43.625	57.832	-1.421
200.00	7.127	48.482	52.078	-0.719
298.15	7.542	51.402	51.402	0.000
300.00	7.551	51.449	51.402	0.014
400.00	7.959	53.679	51.703	0.790
500.00	8.265	55.490	52.285	1.602
600.00	8.486	57.017	52.950	2.440
700.00	8.649	58.338	53.627	3.297
800.00	8.774	59.502	54.290	4.169
900.00	8.873	60.541	54.928	5.051
1000.00	8.954	61.480	55.537	5.943
1100.00	9.024	61.337	56.117	6.842
1200.00	9.086	63.125	56.669	7.747
1300.00	9.142	63.854	57.194	8.659
1400.00	9.194	64.534	57.694	9.576
1500.00	9.242	65.170	58.171	10.498
1600.00	9.289	65.768	58.628	11.424
1700.00	9.334	66.332	59.064	12.355
1800.00	9.377	66.867	59.483	13.291
1900.00	9.420	67.375	59.885	14.231
2000.00	9.463	67.859	60.272	15.175
2100.00	9.505	68.322	60.644	16.123
2200.00	9.547	68.765	61.003	17.076
2300.00	9.588	69.190	61.350	18.033
2400.00	9.630	69.599	61.685	18.994
2500.00	9.673	69.993	62.010	19.959
2600.00	9.715	70.374	62.324	20.928
2700.00	9.758	70.741	62.629	21.902
2800.00	9.801	71.097	62.925	22.880
2900.00	9.844	71.441	63.213	23.862
3000.00	9.888	71.776	63.493	24.848

TABLE XIX
THERMODYNAMICS OF FORMATION OF CESIUM HYDRIDE

Temp. (K)	ΔH_f° (kcal/mole)	ΔG_f° (kcal/mole)
298.15	27.835	23.229
300.00	27.828	23.201
400.00	26.996	21.873
500.00	26.709	20.627
600.00	26.445	19.434
700.00	26.222	18.282
800.00	26.000	17.163
900.00	25.787	16.072
1000.00	9.499	15.825
1100.00	9.539	16.455
1200.00	9.581	17.082
1300.00	9.623	17.705
1400.00	9.665	18.326
1500.00	9.707	18.943
1600.00	9.745	19.557
1700.00	9.782	20.171
1800.00	9.818	20.779
1900.00	9.851	21.388
2000.00	9.880	21.993
2100.00	9.902	22.600
2200.00	9.920	23.202
2300.00	9.933	23.808
2400.00	9.937	24.410
2500.00	9.930	25.012
2600.00	9.914	25.617
2700.00	9.886	26.223
2800.00	9.845	26.827
2900.00	9.789	27.435
3000.00	9.716	28.045