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Spectroscopic Evaluation of Thermodynamic Parameters for Aluminum Based Diatomic Gas Molecules

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Abstract

On account of the high accuracy with which spectroscopic data are obtained, thermodynamic parameters estimated from these data are more reliable than those obtained by direct thermal measurements. Spectroscopic data of aluminum based diatomic gas molecules (AlO, AlH, AlD, AlF, AlC) and partition function theory have been used to evaluate the thermodynamical parameters in the temperature range 100 – 3000 ^{0}K. Equilibrium constants for astrophysically important chemical process have been calculated using partition function theory. It is noticed that for AlC the heat capacity decreases exponentially after the critical temperature 1200 ^{0}K.

Keywords: *Diatomic molecule; partition function; entropy; equilibrium constant.*

1. Introduction

If we can assume chemical equilibrium, then the abundance of a molecule is determined independent of its formation mechanism, and therefore the most important factor determining the thermodynamical stability of the molecule is the dissociation energy. The molecules in stellar atmospheres can be reasonably well understood on the basis of chemical equilibrium theory [1]. Thermodynamical parameters (such as free energy, enthalpy, entropy and heat capacity etc.) of diatomic molecules calculated experimentally are not accurate and sometimes such measurement is not possible. These properties have been useful in the fabrication of smart devices using intelligent materials [2,3]. These parameters have also been used in medical field [4]. Spectroscopic evaluation of thermodynamical parameters was first suggested by Tolman [5] using prior probability. Sauval and Tatum [6] have used the spectroscopic properties of high temperature data set to evaluate the polynomial expressions of partition functions and equilibrium constants for 300 molecules of astrophysical interest. Cardelino et al [7] have reported molecular thermodynamical parameters for indium compound. Hildenbrand and Lau [8] have determined the dissociation energies of copper and silver mono halides and nickel mono fluorides using thermodynamical parameters from the method of quantum chemical calculation. Most recently thermo dynamical parameters of tin chalcogenide [9] and platinum diatomic molecule [10] have been reported by statistical thermodynamics method using spectroscopy constants.

Thermodynamical data can be used for the estimation of equilibrium constants of various astro-chemical reactions. The thermodynamical study of metallic hydrides and deuterides is of astrophysical importance. Viswanathan et al [11] have identified the CrH and CrD molecular lines in sunspot umbral spectrum. Pavlenko et al [12] have reported equilibrium studies of MgH, MgD, CrH and CrD molecules. These studies are used for the deuterium test. Aluminum Monoxide (AlO) is an important gas phase combustion intermediate of aluminum with oxygen containing oxidizers, such as H_2O, CO_2, and O_2. Typically, it is seen in emission and absorption during combustion of aluminum particles at temperatures greater than 2300 ^{0}K. Swings [13] has reported the occurrence of AlO bands in stellar sources. Aluminum, the 12th most abundant element in space, is the most refractive of the 20 leading elements in the Periodic Table [14]. This high degree of refractivity translates into substantial interstellar depletions of gas-phase aluminum; in diffuse clouds, for example, 90%–99% of this element is found to be depleted into grains [15]. Despite the propensity of aluminum to condense, the element exhibits significant gas phase chemistry in carbon-rich circumstellar environments. Gas-phase thermodynamic equilibrium chemistry is the likely formation mechanism for the detection of AlO in VY CMa [16]. Also the detection of AlO is an evidence of an active gas-phase refractory chemistry in oxygen-rich envelopes. To the best of our knowledge, there has been no report so far in the literature on the thermo dynamical parameters of Al based diatomic molecules. Hence we have evaluated thermo dynamical parameters of AlO, AlH, AlD, AlF and AlC molecules by partition function theory, using the spectroscopic constants. The molecular constants used in this study were collected form the literature and are listed in Table 1. The astro-chemical reactions are also described in the following section and their equilibrium constants are listed in the respective table.

2. Partition Function and Thermodynamic Parameters

In the case of thermochemical non-equilibrium gas, multiple temperatures are defined to describe the partitioning of energy across the internal modes. For example, translational, rotational, vibrational, and electronic energy modes for the mixture or for each species may be used. The various states of each energy mode are assumed to be in equilibrium at the characteristic temperature. Each mode is described by its own energy conservation equation which includes terms coupling to the

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other energy modes. Usually, separate internal modes for each species are not defined because the energy modes are assumed to be strongly coupled between species. Therefore the total internal energy of a diatomic molecule is given by

$$E_T = E_{rot} + E_{vib} + E_{ele} + E_{tran} \tag{1}$$

To evaluate the partition function, it is necessary to know all the structural data (such as rotational, vibrational, electronic and translational) of each molecule. Therefore the total partition function of a molecular system can be expressed as:

$$Z_T = Z_{rot} \times Z_{vib} \times Z_{ele} \times Z_{tran} \tag{2}$$

In calculating the thermal parameters for high temperatures, the low-lying electronic states of the molecule should be considered. The different multiplet components of the lowest electronic states can be taken into account by calculating the electronic partition function Z_{ele} in “Eq. (2)”. This is not possible for electronic states that have different rotational and vibrational constants from the ground state. Rather an additional term corresponding to all the rotational and vibrational levels of the excited electronic state has to be added to the partition function for the ground state including the non-rigidity, anharmonicity and stretching effect. Thus the total partition function can be expressed as:

$$Z_T = Z_{tran} Z_{vr} \tag{3}$$

The translational partition function is given by

$$\frac{Z_{tran}}{N} = \left(\frac{2\pi mkT}{h^2}\right)^{3/2} \frac{kT}{P_0} \tag{4}$$

where *m, N, k, h, T* and $P_0 (= 1.01325 \times 10^5 \, \mathrm{Nm^{-2} atm^{-1}})$ represent the mass of the molecule, total number of molecules, Boltzmann’s constant, Planck’s constant, absolute temperature in Kelvin and standard state of one atmospheric pressure respectively. The translational part can always be separated and its contribution to the thermodynamical parameters can be calculated using following relations

Free energy $F_{tran} = -\frac{3}{2} RT \ln m - \frac{5}{2} RT \ln T + 6.697 RT$ (5)

Enthalpy $H_{tran} = \frac{5}{2} RT$ (6)

Entropy $S_{tran} = \frac{5}{2} R + \frac{F_{tran}}{T}$ (7)

Heat capacity at constant pressure $C_{P_{tran}} = \frac{5}{2} R$ (8)

For diatomic species the internal partition function includes vibrational and rotational energies,

$$Z_{vr} = \frac{1}{\sigma} \sum_{v=0}^{v_{\max}} \sum_{J=0}^{J_{\max}} g(v,J) e^{-\frac{E(v,J)}{kT}} \tag{9}$$

where *v* and *J* are the vibrational and rotational quantum numbers respectively and σ is the symmetry number.

The total internal energy of diatomic molecule is given by

$$\begin{aligned} E(v,J) = (\omega_e (v + 1/2) - \omega_e x_e (v + 1/2)^2 + B_e J(J+1) - \\ D_e J^2 (J+1)^2 - \alpha_e (v + 1/2) J(J+1)) \end{aligned} \tag{10}$$

which is useful for values v and J that significantly contribute to thermodynamic properties. Neglecting the zero point vibrational energy [17], an equation equivalent to “Eq. (6)” that gives the energy above the ground state (v = 0, J = 0) can be written as follows,

$$\begin{aligned} E(v,J) = \omega_0 v - \omega_0 x_0 v(v-1) + J(J+1) \\ [B_0 - D_e J(J+1) - \alpha_e v] \end{aligned} \tag{11}$$

where $B_0 = B_e - \frac{\alpha_e}{2}$;

$\omega_0 = \omega_e - 2\omega_e x_e$; $\omega_0 x_0 = \omega_e x_e$

Further substitution for simplification,

$$u = \frac{hc\omega_0}{kT} \,; \; y = \frac{hcB_0}{kT} \,; \; \beta = \frac{D_e}{B_0} \,; \; \delta = \frac{\alpha_e}{B_0}$$

and $D_e = \frac{4B_e^3}{\omega_e^2}$ gives:

$$\begin{aligned} E(v,J) = uv(1 - x(v-1) + J(J+1)y \\ [1 - \beta J(J+1) - v\delta] \end{aligned} \tag{12}$$

Then the vibration rotation partition function “Eq. (5)” can be simplified as

$$Z_{vr} = \frac{1}{\sigma y (1 - e^{-u})} \left[1 + \frac{2\beta}{y} + \frac{\delta}{e^u - 1} + \frac{2xu}{(e^u - 1)^2} + \frac{y}{3} + \frac{y^2}{15} \right] \tag{13}$$

here σ is the symmetry number and its value is 1 for hetronuclear molecule and 2 for homonuclear molecule and x is called the multiplicity of the electronic ground state of the molecule. Thus the vibration rotation contribution to the thermodynamical parameters can be calculated using following relations.

Free energy $F_{vr} = -RT \ln Z_{vr}$ (14)

Enthalpy $H_{vr} = RT^2 \frac{\partial}{\partial T} (\ln Z_{vr})$ (15)

Entropy $S_{vr} = R[(1 + \ln Z_{vr})] + RT \left[\frac{\partial}{\partial T} (\ln Z_{vr}) \right]$ (16)

Heat capacity at constant pressure

$$C_{P_{vr}} = RT \frac{\partial}{\partial T} (\ln Z_{vr}) \tag{17}$$

The sum of the translational and vibrational-rotational contributions gives the final value of the thermodynamical parameters.

3. Equilibrium Constants

Computations of chemical equilibria have been used directly for interpretations of observed molecular features in red giant stars [18] and also it can be used for the deuterium test. In general the chemical process involving the two reactants and two products is represented by

$$A + B \Leftrightarrow C + D \tag{18}$$

Then the equilibrium constant K is given by

$$K = \frac{Z(C)Z(D)}{Z(A)Z(B)} \times e^{-\left(\frac{\Delta E}{kT}\right)} \tag{19}$$

Here ΔE is the difference between zero point energies of the diatomic molecules of relative abundance. Z is the total partition functions which can be factorized into the internal and translational components.

We have calculated the equilibrium constants for the following three reactions of astrophysical interest in the temperature range 100 – 3000 K.

$$AlH + HD \Leftrightarrow AlD + H_2 \tag{20}$$

$$AlD + HD \Leftrightarrow AlH + D_2 \tag{21}$$

$$AlH + OD \Leftrightarrow AlD + OH \tag{22}$$

Almost in all the astrophysical sources, hydrogen and deuterium are primarily found in their molecular form. It is worth to study the chemical processes involving diatomic metallic hydrides and deuterides when found present in the astrophysical sources. The equilibrium constants are listed in Table 4. The equilibrium constants indicate that at low temperatures the formation of the deuterides are strongly favoured over the hydrides, but at high temperatures the hydrides become weakly favoured. It is worth noting that in cool dwarfs hydrogen and deuterium are primarily found in their molecular forms, H_2, HD and D_2 [12]. In a complete chemical equilibrium calculation the partition functions and dissociation energies of H_2, HD and D_2 will have an effect upon the abundances of the molecules of interest.

4. Results and Discussions

The estimated thermodynamical parameters are listed in Table 2 to 6. Results of the study show that free energy, enthalpy and entropy increase with increase in the temperature. Heat capacity also increases with temperature except for Aluminum Carbide (AlC). In AlC, heat capacity (C_P) increases up to critical temperature 1200 ^{0}K and then decreases. This is may be due to interaction of the molecule to its metastable state and to spin reorientation because of high multiplicity in ground state. A similar phenomenon is found in polyatomic molecules which involves hindered rotation [17]. Also this may be due to formation of ions of the molecule at such high temperature. Similar behavior is noticed in SiC at 2300 ^{0}K and in CrC at 1900 ^{0}K, the graphical representation of such variations is shown in "Fig. 1". In general it is noticed that all the diatomic carbides, having high ground state multiplicity exhibit such phenomena. Increase in entropy of the molecules shows that the disorder of the system is high at high temperatures. The equilibrium constant of the astrophysically important reaction in the temperature range 100 – 3000 ^{0}K are listed in the Table 7. Graphical representation of equilibrium constant versus temperature is shown in "Fig. 2". The study shows that the change in equilibrium constant goes on decreasing and becomes almost constant after a certain temperature. At low temperatures only translational part of motion gives its contribution but as temperature increases rotational, vibrational and electronic motions are excited. Enthalpy represents the thermal energy of any system and depends on internal energy, pressure and volume. Therefore the internal energy of an ideal gas depends only on its temperature. Molecules are said to be in thermal motion as a result of their being at a particular temperature, and their thermal motion increases with increased temperature. Therefore the molecules in a system at high temperature are highly distributed either in terms of their locations or in terms of occupation of their possible internal modes of energy states, such as rotation and vibration. The free energy is expressed in terms representing the translation and internal degrees of freedom. Internal energy and entropy are functions of temperature and hence increase with temperature.

5. Conclusions

Due to the involvement of spectroscopic data the estimated thermodynamic parameters are highly accurate; such measurement is not possible experimentally at high temperature. The equilibrium constant for the astrochemical processes is applicable to the deuterium test. Since silicon carbide is thought to be an important component of the dust shells surrounding the carbon rich stars [19,20]. The observation of SiC in the dust shell of carbon stars suggests that the metal carbides such as FeC [21], AlC, CrC and all diatomic carbides having high ground state multiplicity may be present as well. These data may be useful for chemical and electronic industries where the performance of the devices is affected by the thermodynamic parameters.

References

[1] H. N. Russell, Molecules in the Sun and Stars, *Astrophys. J.*, *79*, 317-342, 1934.

[2] K. Sadeghipour, R. Solamon, S. Neogi, Development of a novel electrochemically active membrane and 'smart' material based vibration sensor/damper, *Smart. Mater. Struct.*, *1*, 172-179, 1992.

[3] P. Kotzian, P. Brazdilova, K. Kalcher, K. Handlir, K. Vytras, Oxides of platinum metal group as potential catalysts in carbonaceous amperometric biosensors based on oxidases, *Sens. Actuators B. Chem.*, *124*, 297-302, 2006.

[4] D. R. Chialvo, Physiology: Unhealthy surprises, *Nature*, *419*, 263-264, 2002.

[5] R. C. Tolman, Rotational Specific Heat and Half Quantum Numbers, *Phys. Rev.*, *22*, 470-478, 1923.

[6] A. J. Sauval, J. B. Tatum, A Set of Partition Functions and Equilibrium Constants for 300 Diatomic Molecules of Astrophysical Interest, *Astrophys. J. Sup. Ser.*, *56*, 193-209, 1984.

[7] B. H. Cardelino, C. E. Moore, C. A. Cardelinp, D. O. Frazier, K. J. Bechmann, Theoretical Study of Indium Compounds of Interest for Organometallic Chemical Vapour Deposition. *J. Phys. Chem. A*, *105*, 849-868, 2001.

[8] D. L. Hildenbrand, K. H. Lau, Dissociation energies of the Cu and Ag monohalides and of Ni monofluoride, *J. Phys. Chem. A*, *110*, 11886-11889, 2006.

[9] Pavitra Tandon., K. N. Uttam, Estimation of thermodynamics quantities of tin chalcogenides from spectroscopic data, *Indian J. Pure and App. Phys.*, *47*, 725-729, 2009.

[10] Pavitra Tandon., K. N. Uttam, Thermodynamic properties of Platimum Diatomics: Properties of PtH, PtC, PtN, and PtO calculated from spectroscopic data, *Platinum Metal Review*, *53*,123-134, 2009.

[11] B. Viswanathan, R. Shanmugavel, S. P. Bagare, N. Rajamanickam, P. Sriramachandran, Identification of CrH and CrD Molecular Lines in the Sunspot Umbral Spectrum, *Solar Phys.*, *257*,261-269, 2009.

[12] Ya. V. Pavlenko, G. J. Harris, J. Tennyson, H. R. A. Jones, J. M. Brown, C. Hill, L. A. Yakovina, The electronic bands of CrD, CrH, MgD and MgH: application to the `deuterium test', *Mon. Not. Rom. Astrom. Soc.*, *386*, 1338-1346, 2008.

[13] P. Swings, Spectroscopic problems of astronomical interest, *J. Opt. Soc. Amer.*, *41*, 153-165, 1951.

[14] K. Lodders, Solar system abundances and condensation temperatures of the elements, *Astrophys. J.*, 5*91*, 1220-1247, 2003.

[15] B. E. Turner, A molecular line survey of Sagittarius B2 and Orion-KL from 70 to 115 GHz. II - Analysis of the data, *Astophys. J. Sup. Ser.*, *76*, 617-686, 1991.

[16] E. D. Tenenbaum, L. M. Ziurys, Millimeter Detection of AlO (X 2Σ+): Metal Oxide Chemistry in the Envelope of VY Canis Majoris, *Astrophys. J.*, *694*, L59-L63, 2009.

[17] J. Bevan Ott, Juliana Boerio–Goates, *Chemical Thermodynamics: Principles and Applications*, Elsevier Academic Press, San Diego, California, USA, 2000.

[18] J. M. Scalo, Studies of evolved stars. II. On the interpretation of the CN/C$_2$ and CO/C$_2$ ratios in cool carbon stars, *Astrophys. J.*, *184*, 801-813, 1973.

[19] A.T. Barrett, On the microwave detection of interstellar CH$_4$, SiH$_4$, and GeH$_4$. *Astrophys. J.*, *220*, L81-L85, 1978.

[20] D. M. Goldhaber, A. L. Betz, Silane in IRC +10216, *Astrophys. J.*, 279, L55-L58, 1984.

[21] M. D. Allen, T. C. Pesch, S. Ziury, The Pure Rotational Spectrum of FeC ($X\,^3\Delta_i$), *Astrophys. J.*, *472*, L57-L60, 1996.

[22] W. Szajana, M. Zachwieja, Emission spectroscopy of the A$^1\Pi$ - X$^1\Sigma^+$ system of AlH, *Eur. Phys. J. D*, *55*, 549-555, 2009.

[23] J. B. White, M. Dulick, P. F. Bernath, High resolution infrared emission spectra of AlH and AlD, J. Chem. Phys., 99, 8371-8378, 1993.

[24] R. B. Christopher, A. T. Mickelle, The electronic emission spectrum of aluminum carbide, *J. Mol. Spectrosc*, *258*, 42-49, 2009.

[25] M. D. Saksena, M. N. Deo, K. Sunanda, S. H. Behere, C. T. Londe, Fourier transform spectral study of B$^2\Sigma^+$ - X$^2\Sigma^+$ system of AlO, *J. Mol. Spectrosc.*, *247*, 47-56, 2008.

[26] R. F. Barrow, I. Kopp, C. Malmberg, The Electronic Spectrum of Gaseous AIF, *Physica Scripta*, *10*, 86-102, 1974.

[27] R. A. Durie, G. Herzberg, Forbidden transitions in diatomic molecules. V. The rotation-vibration spectrum of the hydrogen-deuteride (HD) molecule, *Can. J. Phys.*, *38*, 806-818, 1960.

[28] A.R. W. McKellar, W. Goetz, D. A. Ramsay, The rotation-vibration spectrum of HD - Wavelength and intensity measurements of the 3-0, 4-0, 5-0, and 6-0 electric dipole bands, *Astrophys. J.*, *207*, 663-670, 1976.

[29] M. Mizushima, Molecular Parameters of OH Free Radical, *Phys. Rev. A: Gen. Phys.*, *5*, 143-157, 1972.

[30] G. C. Dousmanis, T. M. Sanders, C. H. Townes, Microwave Spectra of the Free Radicals OH and OD, *Phys. Rev.*, *100*, 1735-1754, 1955.

[31] G. Herzberg, *Spectra of diatomic molecules*, 2nd *Ed.*, New York, Nastrand Reinhold, 1950.

[32] P. J. Brannon, C. H. Church, C. W. Peters, Electric field induced spectra of molecular hydrogen, deuterium and deuterium hydride, *J. Mol. Spectrosc.*, *27*, 44-54, 1968.

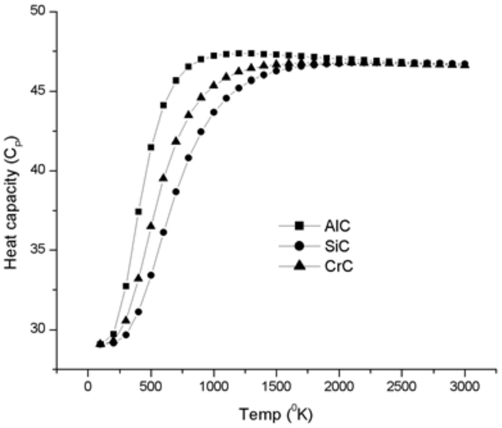

Fig. 1. Temperature versus Heat Capacity at constant Pressure.

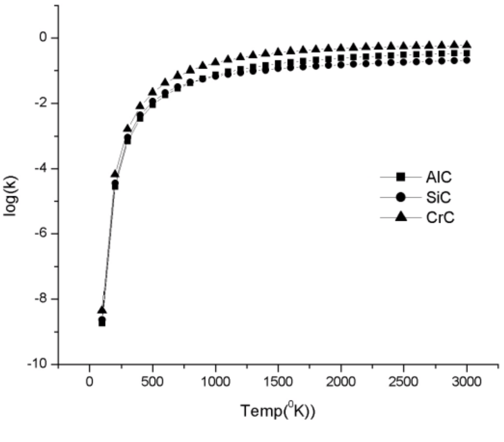

Fig. 2. Temperature versus logarithmic value of equilibrium constant.

Table 1. Spectroscopic Constants of Gas Phase Diatomic Molecules.

Mol.	*x*	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})	B_e (cm^{-1})	α_e (cm^{-1})	*MW (amu)*	*Ref.*
AlH	1	1682.374	29.051	6.393	0.187	27.989	[22]
AlD	1	1211.774	15.064	3.318	0.069	28.995	[23]
AlC	4	654.893	4.347	0.531	0.005	38.992	[24]
AlO	2	979.524	7.036	0.641	0.005	42.980	[25]
AlF	1	802.260	4.770	0.552	0.004	4.598	[26]
HD	1	3813.100	91.650	45.655	1.986	3.022	[27] [28]
OH	2	3737.760	84.881	18.910	0.724	17.007	[29]
OD	2	2720.240	44.055	10.020	0.275	18.013	[30]
H_2	1	4401.210	121.330	60.853	3.062	2.015	[31]
D_2	1	3115.500	61.820	30.443	1.078	4.028	[32]

Table 2. Calculated Thermodynamic Properties of AlO Molecule

$T(^0K)$	*F*	*H*	*S*	C_p
100	-12.589	2.908	163.28	29.078
200	-29.211	5.830	183.522	29.151
300	-47.383	8.880	195.856	29.600
400	-66.638	12.296	205.65	30.74
500	-86.819	16.264	214.48	32.528
600	-107.852	20.783	222.706	34.639
700	-129.676	25.717	230.304	36.738
800	-152.226	30.891	237.211	38.614
900	-175.432	36.166	243.424	40.185
1000	-199.227	41.452	248.993	41.452
1100	-223.549	46.698	253.994	42.453
1200	-248.347	51.883	258.506	43.236
1300	-273.574	57.002	262.603	43.847
1400	-299.193	62.055	266.349	44.325
1500	-325.171	67.050	269.795	44.700
1600	-351.480	71.993	272.985	44.995
1700	-378.097	76.890	275.954	45.229
1800	-405.002	81.748	278.731	45.415
1900	-432.175	86.572	281.339	45.564
2000	-459.602	91.368	283.799	45.684
2100	-487.267	96.139	286.127	45.780
2200	-515.160	100.888	288.336	45.858
2300	-543.268	105.619	290.439	45.921
2400	-571.582	110.335	292.446	45.973
2500	-600.092	115.036	294.366	46.014
2600	-628.790	119.726	296.205	46.048
2700	-657.667	124.404	297.971	46.076
2800	-686.718	129.074	299.669	46.098
2900	-715.936	133.735	301.305	46.116
3000	-745.315	138.389	302.882	46.130

Table 3. Calculated Thermodynamic Properties of AlH Molecule.

$T(^0K)$	*F*	*H*	*S*	C_p
100	-10.182	2.977	138.991	28.859
200	-24.375	5.891	159.185	28.997
300	-40.094	8.814	171.036	29.077
400	-56.812	11.785	179.578	29.234
500	-74.291	14.860	186.434	29.538
600	-92.404	18.095	192.327	30.006
700	-111.073	21.529	197.616	30.626
800	-130.250	25.183	202.493	31.365
900	-149.899	29.058	207.054	32.186
1000	-169.990	33.140	211.353	33.049
1100	-190.499	37.405	215.417	33.922
1200	-211.403	41.828	219.264	34.780
1300	-232.682	46.379	222.906	35.606
1400	-254.315	51.033	226.355	36.387
1500	-276.284	55.766	229.620	37.117
1600	-298.570	60.559	232.713	37.792
1700	-321.158	65.395	235.645	38.414
1800	-344.031	70.260	238.426	38.983
1900	-367.176	75.144	241.066	39.502
2000	-390.577	80.039	243.577	39.974
2100	-414.224	84.938	245.967	40.403
2200	-438.104	89.837	248.246	40.794
2300	-462.207	94.732	250.422	41.148
2400	-486.523	99.620	252.502	41.470
2500	-511.042	104.499	254.494	41.763
2600	-535.756	109.369	256.404	42.030
2700	-560.657	114.229	258.238	42.273
2800	-585.738	119.078	260.002	42.495
2900	-610.993	123.916	261.700	42.698
3000	-636.413	128.743	263.336	42.884

Table 4. Calculated Thermodynamic Properties of AlD Molecule.

$T(^0K)$	*F*	*H*	*S*	C_p
100	-10.756	2.989	144.851	28.98
200	-25.535	5.905	165.06	29.071
300	-41.847	8.871	177.073	29.267
400	-59.187	11.989	186.027	29.744
500	-77.342	15.353	193.522	30.523
600	-96.202	19.014	200.189	31.539
700	-115.698	22.975	206.288	32.691
800	-135.781	27.201	211.928	33.887
900	-156.407	31.644	217.159	35.058
1000	-177.537	36.251	222.012	36.16
1100	-199.135	40.978	226.516	37.169
1200	-221.167	45.784	230.697	38.077
1300	-243.602	50.641	234.585	38.884
1400	-266.412	55.526	238.205	39.596
1500	-289.572	60.424	241.584	40.222
1600	-313.059	65.325	244.747	40.771
1700	-336.852	70.22	247.715	41.252
1800	-360.933	75.105	250.507	41.674
1900	-385.285	79.977	253.142	42.045
2000	-409.894	84.836	255.634	42.372
2100	-434.745	89.679	257.997	42.661
2200	-459.826	94.508	260.243	42.917
2300	-485.127	99.322	262.383	43.144
2400	-510.637	104.121	264.426	43.346
2500	-536.346	108.908	266.38	43.527
2600	-562.247	113.681	268.252	43.688
2700	-588.331	118.443	270.049	43.834
2800	-614.592	123.193	271.776	43.965
2900	-641.022	127.933	273.44	44.084
3000	-667.615	132.664	275.044	44.191

Table 5. Calculated Thermodynamic Properties of AlC Molecule.

$T(^0K)$	*F*	*H*	*S*	*C_p*
100	-12.632	3.000	163.731	29.092
200	-29.320	6.035	184.634	29.720
300	-47.737	9.908	200.162	32.722
400	-67.668	15.053	214.889	37.404
500	-88.989	20.827	227.763	41.471
600	-111.477	26.571	238.242	44.133
700	-134.908	32.065	246.716	45.677
800	-159.109	37.314	253.729	46.528
900	-183.956	42.377	259.694	46.984
1000	-209.359	47.308	264.890	47.217
1100	-235.252	52.147	269.503	47.323
1200	-261.582	56.921	273.657	47.358
1300	-288.308	61.649	277.442	47.352
1400	-315.397	66.343	280.920	47.323
1500	-342.821	71.012	284.142	47.281
1600	-370.555	75.663	287.144	47.232
1700	-398.580	80.299	289.955	47.181
1800	-426.878	84.925	292.598	47.130
1900	-455.432	89.542	295.095	47.079
2000	-484.229	94.151	297.459	47.030
2100	-513.257	98.756	299.705	46.983
2200	-542.504	103.355	301.845	46.938
2300	-571.960	107.951	303.888	46.896
2400	-601.616	112.544	305.843	46.855
2500	-631.463	117.135	307.717	46.817
2600	-661.494	121.723	309.516	46.781
2700	-691.701	126.309	311.247	46.747
2800	-722.078	130.894	312.915	46.715
2900	-752.619	135.478	314.523	46.685
3000	-783.318	140.06	316.077	46.656

Table 6. Calculated Thermodynamic Properties of AlF Molecule.

$T(^0K)$	*F*	*H*	*S*	*C_p*
100	-12.805	3.000	165.445	29.084
200	-29.648	5.945	185.823	29.269
300	-48.070	9.108	198.603	30.056
400	-67.624	12.674	208.83	31.457
500	-88.13	16.681	217.755	33.18
600	-109.48	21.054	225.719	34.938
700	-131.584	25.681	232.848	36.557
800	-154.362	30.462	239.23	37.964
900	-177.745	35.325	244.957	39.149
1000	-201.671	40.222	250.117	40.131
1100	-226.089	45.124	254.789	40.939
1200	-250.953	50.017	259.046	41.605
1300	-276.224	54.891	262.948	42.154
1400	-301.869	59.744	266.544	42.609
1500	-327.861	64.574	269.877	42.988
1600	-354.174	69.382	272.98	43.307
1700	-380.787	74.170	275.883	43.576
1800	-407.682	78.940	278.609	43.805
1900	-434.841	83.692	281.178	44.000
2000	-462.25	88.429	283.608	44.169
2100	-489.895	93.152	285.913	44.315
2200	-517.766	97.863	288.104	44.442
2300	-545.85	102.562	290.193	44.553
2400	-574.138	107.252	292.189	44.65
2500	-602.622	111.933	294.1	44.737
2600	-631.293	116.606	295.933	44.813
2700	-660.143	121.271	297.693	44.881
2800	-689.166	125.930	299.388	44.942
2900	-718.356	130.583	301.021	44.997
3000	-747.706	135.231	302.596	45.047

Note: In Tables 1 – 6,
T – Temperature (^0K)
F - Free energy (KJ/mole)
H - Enthalpy (KJ/mole),
S - Entropy (KJ/mole)
C_P - Heat capacity (J/^0K mole)

Table 7. Equilibrium Constants of Reactions.

$T(^0K)$	*[a]*	*[b]*	*[c]*
100	1.87E-09	2.29E-09	4.33E-09
200	2.79E-05	3.60E-05	6.55E-05
300	6.88E-04	9.01E-04	1.62E-03
400	3.45E-03	4.47E-03	8.15E-03
500	9.18E-03	1.15E-02	2.17E-02
600	1.79E-02	2.14E-02	4.24E-02
700	2.92E-02	3.28E-02	6.91E-02
800	4.27E-02	4.47E-02	1.01E-01
900	5.79E-02	5.64E-02	1.36E-01
1000	7.43E-02	6.77E-02	1.73E-01
1100	9.16E-02	7.81E-02	2.11E-01
1200	1.09E-01	8.79E-02	2.49E-01
1300	1.27E-01	9.70E-02	2.86E-01
1400	1.45E-01	1.05E-01	3.20E-01
1500	1.63E-01	1.14E-01	3.53E-01
1600	1.80E-01	1.21E-01	3.83E-01
1700	1.96E-01	1.28E-01	4.10E-01
1800	2.12E-01	1.36E-01	4.35E-01
1900	2.27E-01	1.42E-01	4.57E-01
2000	2.41E-01	1.49E-01	4.76E-01
2100	2.55E-01	1.55E-01	4.93E-01
2200	2.67E-01	1.62E-01	5.09E-01
2300	2.79E-01	1.68E-01	5.23E-01
2400	2.90E-01	1.74E-01	5.35E-01
2500	3.00E-01	1.79E-01	5.46E-01
2600	3.10E-01	1.85E-01	5.57E-01
2700	3.19E-01	1.90E-01	5.66E-01
2800	3.28E-01	1.96E-01	5.75E-01
2900	3.36E-01	2.01E-01	5.83E-01
3000	3.43E-01	2.06E-01	5.90E-01

Note: In Table 7,
T – Temperature (^0K)
[a] - $AlH + HD \Leftrightarrow AlD + H_2$
[b] - $AlD + HD \Leftrightarrow AlH + D_2$
[c] - $AlH + OD \Leftrightarrow AlD + OH$