

Thermodynamic Functions of 2, 6- Di-bromo-phenol using spectroscopic data

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Abstract

Considering O-H group as a point mass, the vibrational spectrum of 2, 6 dibromo Phenol was analyzed and all the normal modes of vibrations were identified by assuming C_{2v} symmetry for the molecule with Z- axis passing through Cring–O bond and y axis perpendicular to the molecule.

Normal coordinate analysis was performed to compute the thermo dynamical functions using statistical methods. Variations of thermodynamic functions with temperature were plotted and trend discussed.

1. Introduction

Thermodynamic functions may be described as the application of statistical mechanics. The contribution of the vibration energy to the total energy possessed by molecule can be calculated using the vibration frequencies. But the direct experimental measurement of vibration contribution of thermodynamic parameters viz. enthalpy ($H_0 - E_0^0$)/T, heat capacity C_p^0 , free energy - ($F_0 - E_0^0$)/T and entropy function of this compound 2-6- dibromophenol (Fig. 1), has been computed by using standard expressions and taking X-axis to pass through the para position and Y-axis perpendicular to molecular plane as given in equations(1-4). Total energy of a molecule is divided into translational, vibration, rotational and electronic. The energy, E is then

$$E = \varepsilon_{tr} + \varepsilon_{rot} + \varepsilon_{vib} + \varepsilon_{elect} \quad (1)$$

And since the partition function, Q is related to energy by an exponential function equation, the total partition function will be:

$$Q = Q_{tr} \cdot Q_{rot} \cdot Q_{vib} \cdot Q_{elect} \quad (2)$$

Where,

$$Q_{tr} = \left(\frac{1}{h^3} \right) \left(\frac{2\pi mkT}{N} \right)^{3/2} \frac{RT}{P} \quad (3)$$

Where m is the molecular weight and P is the pressure and

$$Q_{vib} = \left(1 - e^{-\frac{v_1 h c}{kT}} \right)^{-d_1} \left(1 - e^{-\frac{v_2 h c}{kT}} \right)^{-d_2} \quad (4)$$

Where v_1, v_2, \dots are vibrational frequencies in wave number, while d_1, d_2, d_3, \dots being the degrees of degeneracy of vibrations.

Once the vibration frequencies of a molecule are obtained from the vibration spectra, it is possible to predict with great precision, the values of thermodynamic functions [1] such as heat capacity, enthalpy function, entropy and Gibb's free. Once the vibration frequencies of a molecule are obtained from the vibration spectra, it is possible to predict with great precision, the values of thermodynamic functions [1] such as heat capacity, enthalpy function, entropy and Gibb's free

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energy etc. Direct experimental measurement of these quantities is usually difficult and tedious and sometimes impossible so this calculation is of great practical importance. Moreover, the values calculated from spectroscopic data are more accurate than those determined by direct thermal measurements.

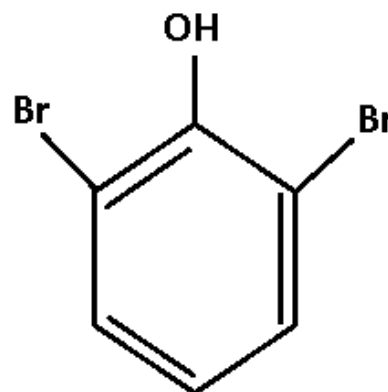


Fig. 1: Structural Diagram of 2, 6- Dibromophenol

2. Results & Discussion

Thermodynamic function have been calculated at different temperature between 200-1500K by using (3n-6) fundamental frequencies [2-6] for the said compounds and assuming rigid rotator harmonic oscillator approximation. Statistically computed thermodynamic functions viz. enthalpy, free energy, heat capacity and entropy with absolute temperature are given in Table 1. The variations of thermodynamic parameters with absolute temperature in different compounds are shown in figure 2 and figure 3 are in good agreement with the trend reported in literature [7-11].

All the thermodynamic parameters are plotted as function of temperature. It was found that all the thermodynamic parameters rise more rapidly in the low temperature range and less rapidly in the high temperature range.

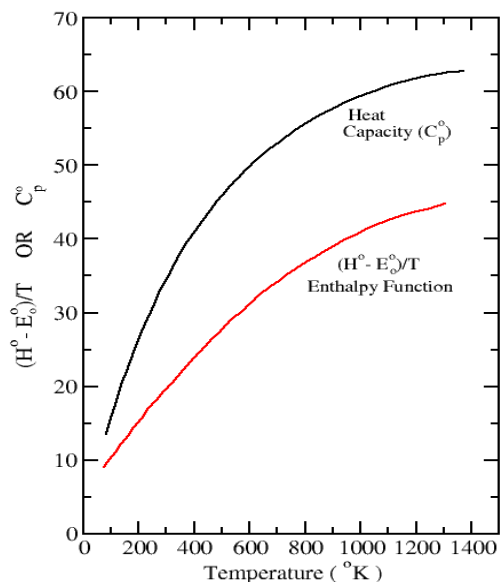


Fig. 2: Variation of enthalpy function and heat capacity with absolute temperature

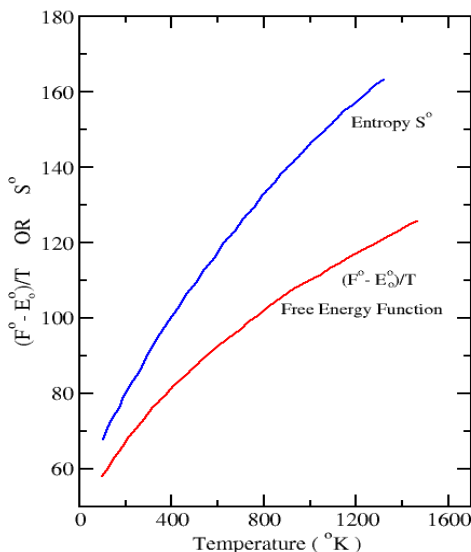


Fig. 3: Variation of free energy function and entropy as a function of temperature

Table 1: Thermodynamic functions in (Cal-mole/0K) of 2, 6- Dibromophenol

Temperature (0K)	(H0-E₀°)/T	-(F0-E₀°)/T	S	Cp°
100	8.736	58.052	66.892	13.297
200	12.880	66.688	79.999	21.571
273.15	16.013	71.847	86.919	27.568
298.15	17.066	73.455	89.426	29.538
300	17.144	73.573	89.621	29.679
400	21.173	79.657	99.507	36.630
500	24.848	85.237	108.312	42.241
600	28.128	90.448	116.792	46.642
700	31.031	95.295	124.350	50.108
800	33.595	99.875	131.495	52.886
900	35.868	104.196	138.094	55.153

1000	37.894	108.298	143.835	57.034
1100	39.708	112.198	149.417	58.612
1200	41.340	115.937	154.749	59.948
1300	42.797	119.415	159.754	61.087
1400	44.157	122.786	166.366	62.065
1500	45.380	126.012	169.315	62.909

3. Conclusions

This study shows its great biological importance and thermodynamic parameters will be used as an important tool in the field of research.

It is apparent from the graph that all the thermodynamic functions increases rapidly as temperature increases from lower value but increase slowly above 1000 OK. The trend is in accordance with experimental values reported in literature.

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