

## Thermodynamics of 6-amino -1-methyluracil

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### ABSTRACT

Computation of thermodynamic functions, viz. enthalpy, heat capacity, free energy function, and entropy for 6-amino -1-methyluracil have been carried out based on vibrational frequencies obtained from IR and Raman spectra, and the results are briefly discussed.

**Keywords-** Thermodynamics functions, 6-amino -1-methyluracil, Hartree-Fock, Density functional theory.

## I. INTRODUCTION

The spectral interpretation of N-heterocyclics such as pyrimidine, cytosine, thymine, uracil, and their derivatives are difficult because of their high complexity and low symmetry. Because these molecules are of considerable biological interest, detailed spectral investigations are important; as such, many workers[1-8] have studied the vibrational and electronic spectra of such molecules. The vibrational spectra of these compounds may provide some evidence about outstanding structural problems. One of these concerns is tautomerism in some molecules, which is possible with the involvement of functional groups like -OH, -NH<sub>2</sub>, and -SH and which may affect their function in metabolism. A full understanding of vibrational spectra of nucleic acid bases are of importance in biophysical research [9-11]. The position of substituents their tautomeric behavior, and the hydrogen bonding ability of the C-O bond in substituted uracils will have considerable biological relevance [12-14]. The studies of nucleic acid bases and their derivatives which contain uracil moieties have been carried out both experimentally and theoretically. The thermodynamic functions have also been computed and discussed.

## II. EXPERIMENTAL

The investigated compound was purchased from Tokyo chemical (TCI) India Pvt. Ltd with a stated purity of more than 99.9%, and was used as such to record the vibrational spectra without further purification. The FT-IR absorption spectrum of 6-amino-1,3-dimethyl was recorded in central Instrumentation Facility, Jamia Millia Islamia, New Delhi on Bruker, Tensor 37 range 4000-600cm<sup>-1</sup>. The Raman Spectrum was recorded in the range of 3500-100cm<sup>-1</sup> in the Centre for nanotechnology.

## III. COMPUTATIONAL DETAILS

In the present work after getting the data and spectrum recorded by experimentally by different spectrophotometer of the compound 6-amino -1-methyluracil the theoretical calculations were carried out. Density functional Theory (DFT) method was applied for these calculations. For making structure and visualize the geometry, the Gauss view molecular visualization program was run while for the calculations of vibrational, geometric, electronic and thermodynamic parameters Gaussian-09 program [15] set was employed. Three parameters that are combined with DFT by Lee, Yang and Parr (LYP) is electron correlation functional [16]. These three-hybrid functional group (B3) parameters by Becke's[17] were used for DFT

calculations make one single electron density functional method B3LYP. In this work two different theory HF and B3LYP with same basis sets, 6-31++ (d,p) are used for the titled compound. Basis sets are very important in these quantum calculations. After optimized the structure of the title compound using density functional theory, the bond length, dihedral angle and bond angle was calculated. Vibrational frequencies (IR and FT-Raman) were also calculated and obtained the spectrum of the 6-amino -1-methyluracil. Thermodynamic properties such as, Heat capacity, Entropy, Enthalpy rotational constant also calculated by the B3LYP/6-31. Variation of thermodynamics properties with temperature also determined.

#### IV. RESULTS AND DISCUSSION

The Structural diagram of the compound 6-amino-1-methyluracil is given in fig .1

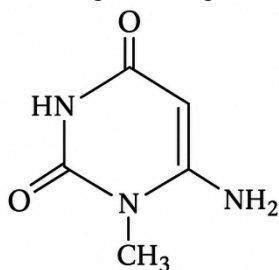


Fig. 1 Molecular Structure of 6-amino-1-methyluracil

##### Thermodynamic Function

The statistically computed thermodynamic functions, viz., enthalpy function, free energy function, entropy, and heat capacity with absolute temperature is shown in the Table 2 and Table 3 for 6,1-AMU, respectively. The variation of enthalpy function and heat capacity with absolute temperature is shown in Fig. 2, while the variation of free energy functions and entropy with absolute temperature is shown in Fig. 3.

All other angles were taken as  $120^\circ$  in the ring. The thermodynamic functions have been calculated at different temperatures between (200-1500) K using 24 fundamental frequencies. Assuming the  $-NH_2$  group as single mass atom and assuming the rigid rotor harmonic oscillator approximation. The calculations were performed for 1 mole of an ideal gas of 1 atmospheric pressure. The symmetry number for overall rotation as 2 and for internal rotation as 2. The principal moments of inertia were found to be 0.5881, 0.4120 and  $1.0001 \times 10^{-37}$  gm-cm<sup>2</sup> in this molecule.

Table 1

| Bond Length (Å) | Bond Angle (°)           |
|-----------------|--------------------------|
| $N_1C_2 = 1.40$ | $\angle N_1C_2N_3 = 118$ |
| $C_2N_3 = 1.35$ | $\angle N_3C_4C_5 = 122$ |
| $N_3C_4 = 1.36$ | $\angle C_5C_6N_1 = 118$ |

|                    |                             |
|--------------------|-----------------------------|
| $C_4C_5 = 1.45$    | $\angle C_6N_1C_2 = 124$    |
| $C_5C_6 = 1.35$    | $\angle N_1C_2O_8 = 120$    |
| $C_6N_1 = 1.36$    | $\angle C_2N_3C_4 = 118$    |
| $N_1C_7 = 1.48$    | $\angle O_2C_2N_3 = 122$    |
| $C_2O_8 = 1.23$    | $\angle N_3C_4O_9 = 118$    |
| $C_4O_9 = 1.25$    | $\angle O_4C_4C_5 = 120$    |
| $C_6N_{10} = 1.36$ | $\angle C_5C_6N_{10} = 122$ |
|                    | $\angle N_{10}C_6N_1 = 120$ |
|                    | $\angle C_6N_1C_7 = 120$    |
|                    | $\angle C_7N_1C_2 = 116$    |

The statistically computed thermodynamic functions viz. enthalpy function, free energy function, entropy and heat capacity function with absolute temperature are shown in Table 2 and Table 3 respectively. The variation of enthalpy function ( $H^\circ - E_0^\circ$ )/T and heat capacity  $C_p^\circ$  with absolute temperature have been shown graphically in Fig. 2 while that of free energy function ( $F^\circ - E_0^\circ$ )/T and entropy  $S^\circ$  in Fig. 3 which are in agreements with the trend reported in the literature.

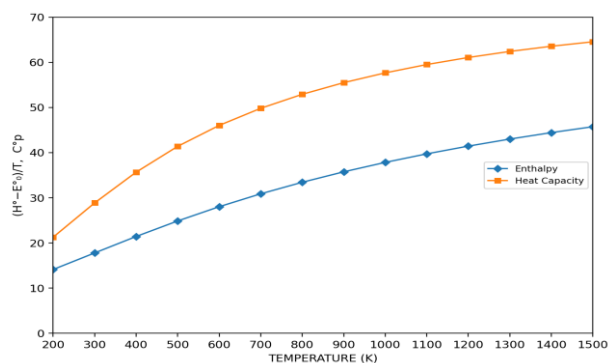


Fig. 2 Variation of enthalpy function ( $H^\circ - E_0^\circ$ )/T and heat capacity function ( $C_p^\circ$ ) at different temperatures of 6-amino -1-methyluracil using B3LYP/6-31++G(d,p)

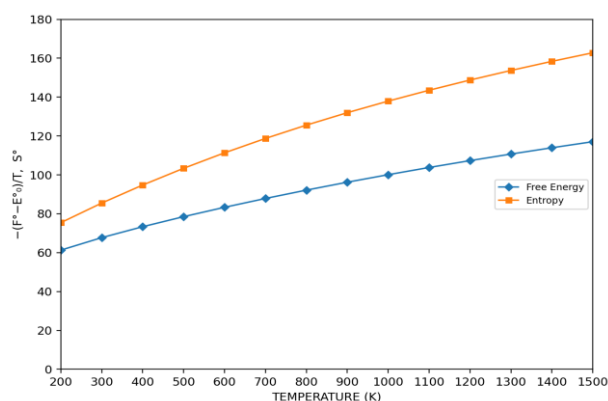


Fig. 3 Variation of free energy function ( $F^\circ - E_0^\circ$ )/T and entropy function at different temperatures of 6-amino -1-methyluracil using B3LYP/6-31++G

**Table 2: Thermodynamic properties enthalpy function ( $H^\circ - E_0^\circ$ )/T and heat capacity function ( $C_p^\circ$ ) of 6-amino -1-methyluracil at different temperatures of B3LYP/6-31++G(d, p)**

| TEMPERATURE (K) | ( $H^\circ - E_0^\circ$ )/T | $C_p^\circ$ |
|-----------------|-----------------------------|-------------|
| 200             | 14.83                       | 21.27       |
| 300             | 17.89                       | 28.82       |
| 400             | 21.24                       | 35.66       |
| 500             | 24.57                       | 41.33       |
| 600             | 28.23                       | 46.00       |
| 700             | 30.58                       | 49.81       |
| 800             | 33.14                       | 52.96       |
| 900             | 35.65                       | 55.42       |
| 1000            | 37.24                       | 57.66       |
| 1100            | 39.53                       | 59.50       |
| 1200            | 41.14                       | 61.06       |
| 1300            | 43.80                       | 62.40       |
| 1400            | 44.13                       | 63.55       |
| 1500            | 45.04                       | 64.54       |

Where ( $H^\circ - E_0^\circ$ ) - Enthalpy,  $C_p^\circ$  - Heat Capacity

**Table 3: Variation of free energy function ( $F^\circ - E_0^\circ$ )/T and entropy function at different temperatures of 6-amino -1-methyluracil using B3LYP/6-31++G(d,p)**

| TEMPERATURE (K) | -( $F^\circ - E_0^\circ$ )/T | $S^\circ$ |
|-----------------|------------------------------|-----------|
| 200             | 61.33                        | 75.82     |
| 300             | 67.70                        | 85.40     |
| 400             | 73.36                        | 94.46     |
| 500             | 78.42                        | 103.26    |
| 600             | 83.36                        | 111.43    |
| 700             | 87.88                        | 118.42    |
| 800             | 92.15                        | 125.78    |
| 900             | 96.28                        | 131.47    |
| 1000            | 100.49                       | 137.73    |
| 1100            | 103.59                       | 143.82    |
| 1200            | 107.42                       | 148.46    |
| 1300            | 110.50                       | 153.10    |
| 1400            | 113.24                       | 158.77    |
| 1500            | 117.05                       | 162.79    |

Where  $S^\circ$  = entropy  $F^\circ$  = free energy and  $E_0^\circ$  = zero-point energy

## V. CONCLUSION

For the computation of these properties' molecular weight, a moment of inertia, fundamental vibration frequencies, and temperature are needed. Using

Vibrational frequencies computed by DFT, these thermodynamics properties we calculated with the help of a computer program at different temperatures ranging from 100 - 1000 K. Variation of these properties with temperature are shown in Figure 3.2, and data are listed in Table3.2(b). It is seen that all the properties listed in table and shown in figure increased linearly with low-temperature range. After that curve become flatten and increases less rapidly. This is due to that at lower temperature range only the translation vibration part of the molecule takes part in motion. As the temperature increases, the other portion of molecular motion (Vibrational, Rotational) also makes a contribution in excitation. The entropy of the title molecule is the function of the measurement of disorderness. As the temperature rises the molecular motion increased and leads to an increase in entropy. This data can be used to calculate the other thermodynamics properties and predict the pathway of any related chemical reaction according to the law and relationship of thermodynamics in thermochemical field.

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