H17	-	0.291	0.402	0.274
H18	-	0.434	0.274	0.421

Thermodynamic Properties

Few calculated thermo dynamical parameters such as the Zero Point Vibration Energies (ZPVE) the molar capacity at constant volume, the entropy and dipole moment are listed in table in the previous section. The variations in the ZPVES (Zero Point Vibration Energies) seem to be insignificant. Changes in the total entropy and the molar capacity at constant volume of thymine and thymine-water at DFT method B3LYP, X3LYP and B3PW91 method with 6-311++g (d,p) basis set are also marginal only.

CONCLUSION

The optimized geometries of thymine and three isomers of thymine-water complexes have been calculated employing *Ab initio* method MP2 and DFT method B3LYP, X3LYP and B3PW91 method with 6-311++G (d,p) basis set using Gaussian 09 program. Most of the geometrical parameters for thymine-water complexes remain the same as thymine except for the geometry of the site of the water bonded atom. Structural parameters of the optimized geometries, total energies and the APT charges of the thymine-water complex have been discussed in detail. From this analysis, it is noted that the theoretically calculated optimized bond lengths are comparatively larger than the experimental values because the theoretical calculations refer to isolated molecules in the gas phase while it is in the solid state for experimental results. We show that addition of water molecules in thymine, the strength of the binding energy decreases *i.e.* stability increases. The optimized bond length and bond angles are in agreement with the corresponding experimental results.

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