CONCLUSION

Geometry of CDMABA conformation was optimized using HF and DFT employing 6-311++G(d,p) basis sets and also compared with XRD data. Significant differences are not obtained and therefore, geometry optimized by DFT is used for further investigation. A comparison of the scaled wavenumbers calculated using HF and DFT methods with the experimental wavenumbers from Raman and IR spectra revealed that DFT results have better agreement than HF probably because DFT includes some of the effects of electron correlation. A detailed normal coordinate analysis of all the normal modes along with PED very clearly indicates the composition of each normal mode in terms of internal coordinates. Any discrepancies between the observed and the calculated wavenumbers may be attributed to the fact that the calculations have been actually performed on single (or isolated) molecule in the gaseous state. Thus some reasonable deviations from the experimental values seem to be justified. The natural bond orbital analysis (NBO) giving information on the intramolecular bonding, interactions among bonds and delocalization of unpaired electrons has been made. The electrostatic potential surface, which serves as a useful quantity to explain hydrogen bonding, reactivity and structure–activity relationship of molecules, mapped with isodensity surface has been obtained. To the best of our knowledge this is the first study where a complete vibrational assignments with PED are reported along with NBO and ESP studies.