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Title: Competition between hydrogen bond , halogen bond and chalcogen bond in complexes of N-methylidenemethanamine(C_2H_5N)with HYX (Y=O, S and X=F, Cl, Br and I).

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An ab initio study of the complexes formed by N-methylidenemethanamine(C_2H_5N)with HYX (Y=O, S and X=F, Cl, Br and I) has been carried out at the MP2/aug-cc-PVDZ computational level. Interaction of HOX with N-methylidenemethanamine (C_2H_5N) lead to both hydrogen bond (C_2H_5N -HB) as well as halogen bond (C_2H_5N -XB) complexes Meanwhile Interaction of HSX with N-methylidenemethanamine (C_2H_5N) lead to hydrogen bond (C_2H_5N -HB) , halogen bond (C_2H_5N -XB) and chalcogen bond(C_2H_5N -YB) complexes The interaction strength and properties in all complexes are analysed with atoms in molecules (AIM) and natural bond orbital (NBO) theories.

Calculations were performed using the Gaussian 09 system of codes. The geometries of the isolated HYX(Y=O, S and X=F, Cl, Br and I) and C_2H_5N molecules as well as HYX- C_2H_5N complexes were fully optimized at the MP2 level of theory [1] with the aug-cc-pVDZ basis set for all atoms, except iodine, for which the DGDZVP[2] was used. Harmonic vibrational frequency calculations certified the structures as minima and provide the evaluation of the zero point energy (ZPE). The counterpoise procedure was used to correct the interaction energy for the basis set superposition error[3]. The AIM2000 package and AIMAll[4] were used to obtain bond properties; and to plot molecular graphs. The natural bond orbital (NBO) method has been used to evaluate the interaction of occupied and empty orbitals with the NBO package supplied with Gaussian 09.

Keywords: Hydrogen bond, halogen bond, chalcogen bond, blue shift, N-methylidene methanamine.

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