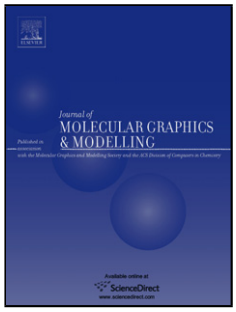

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Revealing Halogen bonding Interactions with Anomeric Systems: An *ab initio* Quantum Chemical Studies

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Abstract: A computational study has been performed using MP2 and CCSD(T) methods on a series of O···X (X = Br, Cl and I) halogen bonds to evaluate the strength and characteristic of such highly directional noncovalent interactions. The study has been carried out on a series of dimeric complexes formed between interhalogen compounds (such as BrF, BrCl and BrI) and oxygen containing electron donor molecule. The existence and consequences of the anomeric effect of the electron donor molecule has also been investigated through an exploration of halogen bonding interactions in this halogen bonded complexes. The *ab initio* quantum chemical calculations have been employed to study both the nature and directionality of the halogen molecules towards the sp^3 oxygen atom in anomeric systems. The presence of anomeric $n_O \rightarrow \sigma^*_{C\text{-}N}$ interaction involves a dominant role for the availability of the axial and equatorial lone pairs of donor O atom to participate with interhalogen compounds in the halogen-bonded complexes. The energy difference between the axial and equatorial conformers with interhalogen compounds reaches up to 4.60 kJ/mol, which however depends upon the interacting halogen atoms and its attaching atoms. The energy decomposition analysis further suggests that the total halogen bond interaction energies are mainly contributed by the attractive electrostatic and dispersion components. The role of substituents attached with the halogen atoms has also been evaluated in this study. With the increase of halogen atom