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Chalcogen bond: A computational study for better bond characterization towards novel applications in material and drug design

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*Noncovalent interactions play a vital role in the stabilization of drug-receptor complexes and biological macromolecules such as DNA and proteins. One of these noncovalent interactions is called chalcogen bond where chalcogen refers to Group VI atoms. This type of interaction is attributed to the existence of a positive region called sigma-hole on the chalcogen atom acting as an acceptor for electron density from a Lewis base[1]. Nature and other characteristics of chalcogen bond are still under debate[2]. In the current study, chalcogen bond properties were reinvestigated using our recent developed approach, called point-of-charge (PoC) model. The study was carried on two model (CX2 and H2X, where X=O, S and Se). The studied molecules were firstly optimized at MP2/6-311++G** level. Molecular electrostatic potential (MEP) for the studied molecules was generated at B3LYP/6-311++G** level. The quantum theory of atoms in molecules (QTAIM) was applied to characterize the nature of interactions. The stabilization energy of the molecules was calculated in the presence of a point-of-charge with a value of -0.1, -0.25, -0.5 and -1 a.u. 2D stabilization energy surface at a distance of 2.5 Å on X-axis was generated for the studied six molecules at MP2/aug-cc-PVTZ level. Furthermore, 1D stabilization energy curve with C-X···PoC distance ranging from 1.5 to 8 Å on X-axis, as well as C-X···PoC angel effect curve from 90° to 180°, were studied. All calculations were carried out using Gaussian09 software. According to the MEP and PoC results, we concluded that oxygen cannot form this type of interaction due to the absence of sigma-hole. Despite there is a significant attractive interaction in case of sulfur- and selenium-containing molecules. The results proved that the strength of interaction increases with increasing the atomic radius of the chalcogen atom. As well, stabilization energy increases with increasing Lewis base strength. Due to the highly importance role of sulfur interaction in drugs[3] and protein structures, the current study serves as a foundation for sulfa drugs research.*