22nd Iranian Inorganic Chemistry Conference,
23-25 August, 2023
University of Kurdistan

Cooperative effect between the chalcogen (Ch…N) and dihydrogen (H…H) bonds in the series of XHTe…NCH…HY (X=F, Cl, Br, I, H, Y=Li, Na, BeH, MgH) and FHCh…NCH…HNa (Ch=Te, Se, S) triads

Aboulfazl Soufi

Department of Chemistry, Faculty of Science, Arak Islamic AzadUniversity, , Arak, Iran

*E-mai: soufiaboalfazl@gmail.com

Focus on the bonds between molecules instead of bonds between atoms, results in the creation of large molecules with unusual structures and different physical and chemical properties, which are useful for various applications([1]). Such interactions lead to a tremendous increase in the variety of crystal architectures and thus properties to be discovered([2]).There are some well-known methodologies for evaluating the degree of cooperativity of noncovalent bonds, but herein we emphasize on our proposed methodology that evaluates the origin of the cooperativity of bonds. Cooperative energy of chalcogen and dihydrogen bonds in some ABC triad systems of the types XHTe…NCH…HY (X=F, Cl, Br, I, H, Y=Li, Na, BeH, MgH) and FHCh…NCH…HNa (Ch=Te, Se, S) were computed and compared at MP2/TZVPPD, BP86/TZVPPD, BP86-D3/TZVPPD, and BP86-D3/QZVP levels of theory. The cooperative energies were evaluated using two different equations/methods, on the basis of interaction energies versus stabilization energies of the triads and corresponding dyads. In addition, a number of good to excellent correlations were observed between the interaction, stabilization, and cooperative energies and change in Te…N and H…H bond lengths upon the formation of triads from the corresponding dyads. All resulting data showed that the strengths of chalcogen (Te…N) and dihydrogen (H…H) bonds increase in the order of H< I < Br < Cl < F, and Be < Mg < Li < Na, respectively. Thus, the shortest Te…N and H…H bond lengths and the largest values of interaction, stabilization, and cooperative energies were observed for FHTe…NCH…HNa triad. Then, the resulting data for the above triad were compared with those for FHSe…NCH…HNa and FHS…NCH…HNa triads. The data showed that the interaction, stabilization, and cooperativity energies decrease in the order of Te > Se > S. Also, it was shown that the more electronegative fluorine atom bonded to chalcogen atom would have no meaningful effect on the strengths of the Ch…N bond and its cooperativity with the H…H bond in present triad complexes, when F−Ch bond is not along Ch…N bond. Finally, the nature of both dihydrogen and chalcogen bonds and the origin of the cooperativity of bonds were evaluated by NBO and EDA analyses ([3]).

Keywords: Cooperativity, dihydrogen bonds, chalcogen bonds, Stabilization energies, Interaction energies.

References

[1] D. Braga and F. Grepioni, *Accounts of chemical research*, 2000, **33**, 601-608.
[2] G. R. Desiraju, *Journal of the Chemical Society, Dalton Transactions*, **2000**, 3745-3751
[3] Frenking G, Matthias Bickelhaupt F. **2014**:121-57.