

Type I C=S...S=C Interactions

Rahul Shukla¹, Deepak Chopra¹¹Department Of Chemistry, Indian Institute Of Science Education And Research Bhop, Bhopal, India

E-mail: rahulshukla@iiserb.ac.in

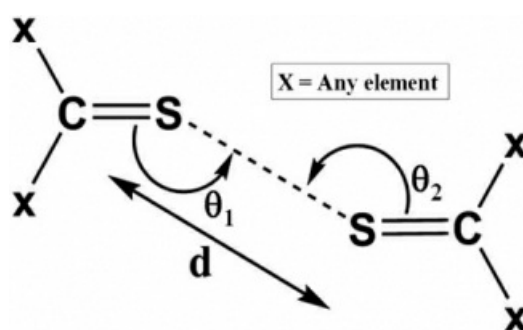
Depending on the electronic environment, chalcogen atoms (mainly S, Se, Te) can act as both acceptor and donor during the formation of a noncovalent interaction. This dual behavior of chalcogens can lead to the formation of highly stabilized chalcogen-chalcogen interactions [1]. Among the chalcogen-chalcogen interactions, S...S interactions has garnered immense attention due to several applications such as in organic conductors and nanotube formations. Role of S...S interactions in molecular structures has been explored both experimentally and computationally [2]. However, a closer look at the literature reveals that most studies on S...S is centered around sp³ hybridized sulfur atom with a negligible focus to sp² hybridized sulfur atom. A simple Cambridge Structural Database [2] search revealed that there are more than 1000 structures having sp² hybridized organic sulfur participating in the formation of C=S...S=C interactions. However, a systematic and detailed investigation of this interaction in crystal structures has not be explored previously.

In this study, we have analyzed the nature and characteristics of C=S...S=C chalcogen-chalcogen interactions by screening the Cambridge Structural Database. In addition to this, we have also performed a topological analysis and binding energy calculations on full scale dimers extracted from the Cambridge Structure Database in addition to analysing C=S...S=C interactions in (X₂CS)₂ model systems where X = -H, -NH₂, -OH, -F, -Cl by means of the electrostatic potential maps and energy decomposition analysis

[1] Bleiholder, C. et al. (2006). J. Am. Chem. Soc. 128, 2666-2674.

[2] Allen, F. H. (2002). Acta Crystallogr., Sect. B: Struct. Sci. B58, 380- 388.

[3] Shukla, R. et al. (2016). Cryst. Growth Des. 16, 6734-6742.



Keywords: [chalcogens](#), [C=S...S=C interactions](#), [Type I contact](#)