

MS31-2-2 Chalcogen Bond in Bioactive Compounds

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G. Resnati¹, A. Pizzi¹, K. Konidaris¹, A. Daolio¹, J. S. Murray², P. Politzer²

¹Politecnico di Milano - Milan (Italy), ²University of New Orleans - New Orleans (United States)

Abstract

The Chalcogen Bond (ChB) is the attractive interaction wherein elements of group 16 of the periodic table act as electrophiles [1]. The interaction is receiving major attention thanks to the role and applications in the structure and functions of molecular materials and compounds of biological and pharmacological relevance [2]. For instance, thiazole and benzo[d]thiazole derivatives are used in many drugs and in vivo imaging agents [3] and in this communication we will present the crystal structures of some N-alkyl thiazolium and benzo[d]thiazolium compounds of biopharmacological interest. Among others, we will report the structure of thiamine monophosphate, a vitamin B1 coenzyme. In these crystal structures the sulfur atom is chalcogen bonded with different nucleophiles, as proven by the geometric features of the interactions. The ability of the thiazolium and benzothiazolium moieties to form ChBs is confirmed by analyses of the Cambridge Crystallographic Database (CSD) and computational studies.

References

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