Reinforcing chalcogen bonds through alkaline-earth bonds

Otilia Mó, a M. Merced Montero-Campillo, a Ibon Alkorta, b José Elguero b and Manuel Yáñez a

a Departamento de Química, Facultad de Ciencias, Universidad Autónoma de Madrid (28049 Cantoblanco, Madrid, Spain), b Instituto de Química Médica, IQM-CSIC (C/ Juan de la Cierva 3, 28006 Madrid, Spain).

mm.montero@uam.es

G4 calculations show that the strength of chalcogen interactions is dramatically enhanced by the presence of alkaline-earth bonds. Cooperativity between these two kinds of non-covalent interactions is studied exploring different complexes between chalcogen derivatives, alkaline-earth derivatives and N-bases. In terms of binding energies, chalcogen bonds in ternary complexes can be enhanced by one order of magnitude with respect to binary complexes. This is due to the interplay of all non-covalent interactions involved: the strong cooperativity between chalcogen and alkaline-earth bonds, and the appearance of secondary non-covalent interactions (hydrogen bonds). These results will be compared to other previous results from our group in cooperativity phenomena.

References