

S, Se and Te atoms as Anion Binding Sites

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Abstract:

The detection and quantification of anion species through the development of new anion chemosensors¹ is a relevant area of interest to the scientific community due to the important role that these species play in a large number of biological and medical systems.

In the last decades, non-covalent interactions like anion- π and halogen bonding have emerged as interesting alternatives to the hydrogen bonding to improve the anion recognition. More recently, the increase of the computational capacity has allowed to the theoretical chemists to find new non-covalent interactions of high interest based in the existence of the denominated σ -hole. Theoretical calculations obtained by some researchers show regions of positive charge density in the atoms of the oxygen group².

Chalcogen bonding³ (ChB) is defined as the interaction between a positively polarized chalcogen atom (S, Se or Te) and a Lewis-base (LB).

Motivated by these results, the purpose of this research is the synthesis and the anion binding study of a new family of receptors **1-3** bearing the 1-3-5-trifluorobenzene units as spacers and the thiophene, selenophene or telurophene as chalcogen bonding binding sites (Figure 1).

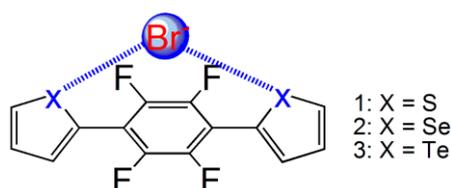


Figure 1. Structure of the receptors **1-3**.

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References

1. N. H. Evans, P. D. Beer. *Angew. Chemie – Int. Ed.* **2014**, 53, 2-41.
2. P. Politzer, J. S. Murray, C. Clark, G. Resnati. *Phys. Chem. Chem. Phys.* **2017**, 19, 32166-32178.
3. G. Rolf, G. Haberhauer, D. B. Werz, F. Rominger, C. Bleiholder. *Chem. Rev.* **2018**, 118, 2010-2041.