On the recognition of chloride, bromide and nitrate anions by anthracene-squaramide conjugated compounds: a computational perspective

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Abstract

Anion recognition is widely used in several biological fields. Squaramide derived compounds appear as potential structures to recognize anions. Here, the bond mechanisms between the chloride (Cl-), bromide (Br-) and nitrate (NO3-) anions and anthracene-squaramide conjugated compounds are elucidated considering the influence of the: (i) number, (ii) nature, and (iii) position of the substituents: trifluoromethyl (-CF3) and nitro (-NO2). Energy decomposition analysis (EDA) shows that the interactions between Cl-, Br- and NO3- and anthracene-squaramide have an attractive interaction energy supported predominantly by electrostatic energy followed by orbital contribution. Molecular electrostatic potential (MEP) surfaces imply electrostatic interactions between Cl-, Br- and the oxygen atom from NO3- and the hydrogen atoms from N-H and C-H bonds present in the squaramide structure, and an aryl group, respectively. Cl- interacts with the receptors more strongly than Br-. The NO3- recognition is less attractive than those presented by Cl- and Br-, in agreement with the hardness-softness features of these anions. Importantly, one and, mostly, two group substitutions, -H -> -CF3 or -NO2, favor the recognition of Cl-, Br- and NO3- due to the increase of the polarization in the receptor-NHMIDLINE HORIZONTAL ELLIPSISanion interaction. The -NO2 group promotes a larger effect relative to the -CF3 ligand. The -NO2 ligand positioned at the largest distance conceivable to the benzene-NH group promotes the lowest interference in the N-HMIDLINE HORIZONTAL ELLIPSISCl- interaction. These results provide information to design receptors with a larger capability to recognize anions.

Palabras clave

KeyWords Plus:MOLECULAR-ORBITAL METHODS; DRINKING-WATER; BASIS-SETS; NONCOVALENT INTERACTIONS; HYDROGEN-BOND; COMBINATION; CHEMISTRY; ELEMENTS; VALENCE; BINDING

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