Theoretical study of chloride complexes with hybrid macrocycles

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Abstract
Anions show relevant roles in biological routes. The supramolecular chemistry investigates the chemical bonding between two or more molecules and/or ions. Herein, the nature of the bond between chloride anions and macrocycle receptors elaborated from (i) pyridines, (ii) pyrroles, (iii) borazines, (iv) triazines, and (v) 1,2,3-triazole rings are studied. The energy decomposition analysis (EDA) shows that the receptors that predominantly establish non-covalent interactions with the Cl-anions proportionate a preferable bond than the macrocycles that mostly form a covalent interaction with the Cl- anions. The substitution of pyridine by borazine rings in the macrocycles or the protonation of the receptors increases the interaction with the Cl-anions since there is an increase in the number of -BH or -NH groups available to establish hydrogen bonds with the Cl- anions. In addition, the pyridine → borazine substitution decreases the number of repulsive interactions. The substitution of pyrrole by 1,2,3-triazole rings does not relevantly favor the interaction with the Cl-anions. The substitution of pyridine by the triazine rings or the addition of electron-withdrawing groups (-OH, -F and -NO2) in the receptor structures increases the acidity of the cavity of the macrocycles and, therefore, favors the interaction with the Cl- anions. The addition of electron-donating groups (-NH2) to the receptor structure promotes the opposite effect. Accordingly, the present investigation brings relevant information for the design of new hybrid macrocycles with the potential for anionic recognition.

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