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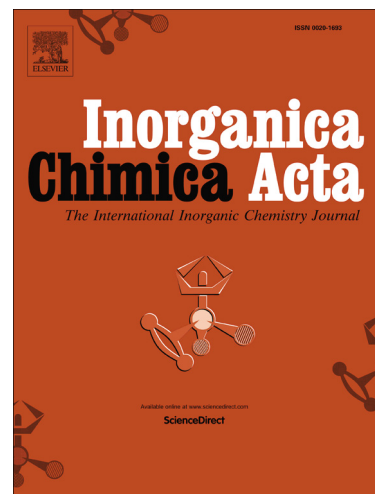
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Anion- π weak interactions in a heteroaromatic calixarene receptor. A theoretical Investigation.

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Abstract

The interactions between a series of differently shaped anions (NO_3^- , BF_4^- , PF_6^- , SCN^-) and a heteroaromatic calixarene receptor (tetraoxacalix[2]arene[2]triazine) have been investigated in acetonitrile solution by using density functional (wB97XD and B3LYP-D3 exchange-correlation functionals) and second-order Möller-Plesset perturbation levels of theory in order to strengthen the presence of anion- π interactions in condensed phase. From the computed binding energies, a considerable interaction has been found, whose magnitude seems to depend on the size of considered anions. The obtained geometrical structures well agree with the corresponding X-ray data, while the reproduction of the binding energies depends on the used level of theory.

Paper dedicated to Carlo Mealli special issue

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