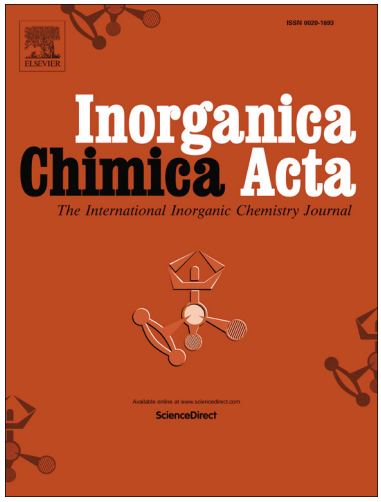


Research paper

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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 depends 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.



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