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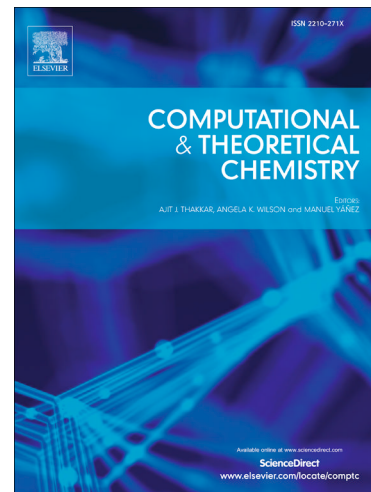
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DFT and Conceptual-DFT Assessment on Selective Tertiary Amine Functionalized Calix[4]arene-anion Interaction

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Abstract

In this paper, previously reported selectivity of a tetraamine-substituted calix[4]arene receptor (CX4) towards four biologically and environmentally relevant anions has been tried to be supported by two separate computational studies, of which the former is based on thermodynamical approach and the second is on the calculation of reactivity descriptor from conceptual-density functional theory (CDFT). The use of CDFT descriptor for computational interpretation of receptor-anion selectivity phenomenon has been first time suggested. Moreover, thermodynamical approach used here had utilized mostly in receptor-cation selectivity studies in the literature and related studies for receptor-anion interaction is extremely rare. The two methodologies have successfully supported the trends of CX4-anion interactions observed in the experimental studies previously reported.

Keywords: Calix[4]arene, DFT, Conceptual-DFT, anion recognition, reactivity descriptors, interaction energies

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