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Calixarenes as Prototypes of Biochemical Receptors: a Quantum Chemical Investigation

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A series of functionalized "host" molecules (calixarenes, resorcinarenes, pyrogalloarenes) has been theoretically investigated using the modern quantum chemistry methods. Such medium size (100 to 500 atoms) species are known to form stable adducts with various neutral and charged "guest" molecules and thus, can be considered as simplified models for biochemical receptors, such as enzymes. An estimated thermodynamic stability of the corresponding adducts includes host-guest size consistency and an approximate quantum chemical description for the most important specific interactions (electrostatic and Van der Waals forces, hydrogen bonding). Some modern approaches (*Density functional theory methods with an implemented description of electron dispersion effects*, *Resolution of the Identity*, etc.) are analyzed as perspective instruments for the implementation in the biochemical area, for example, for searching new effective enzyme inhibitors. In order to solve the size problem, using of some tricks is still necessary to separate an active fragment of the enzyme for calculations.

[1] A.B. Rozhenko, W.W. Schoeller, M.C. Letzel, B. Decker, C. Agena, J. Mattay *Chem. Eur. J.* **12**, p. 8995.