Halogen-halogen interaction in light of many-body approach.

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The many-body theory was applied in order to estimate the character of interaction in quadruple complex consisting of four bromomethane molecules. The scheme of such system is shown in the Figure.

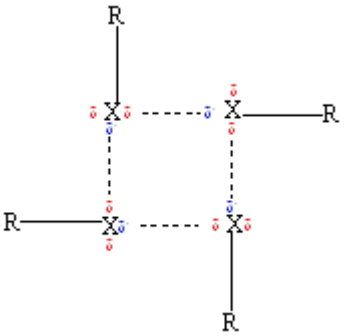

Figure. The scheme of the structural motif that occurs in the system under investigation.

The tetrameric complex used as a model system was found in the crystal structure in which the halogen bonds were stabilizing the solid state structure.[1] Decomposition of interaction energy[2] on two-, three- and four-body terms allowed to conclude that the individual halogen bonds very weakly cooperate forming the complex. The non-additive contribution to interaction energy is negative, but of very small value in respect to total interaction energy (less than 0.01%), indicating very weak cooperativity of halogen bridges. Moreover, a few Basis Set Superposition Error (BSSE)[3] schemes (namely: SSFC,[4] PAFC,[4] and VMFC[5]) were applied in order to study the influence of BSSE on the interaction energy and its terms. Both structural and energetic consequences of complexation were investigated. The importance of the chemistry model used in calculations was also studied.

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