AB INITIO CALCULATION OF NUCLEAR QUADRUPOLE COUPLING CONSTANTS IN VAN DER WAALS COMPLEXES

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Nuclear quadrupole coupling constants available from high-resolution microwave work can yield important information about the structure and the bonding of weakly bound atomic and molecular clusters. The change of these constants in the complex relative to the free molecules or atoms is determined by the electrostatic interaction between the fragments of the cluster, changes in the molecular geometry on complexation, and cluster dynamics (large amplitude motions). The goal of the present study is to investigate whether *ab initio* calculations can reproduce the experimentally observed nuclear quadrupole splittings for this kind of molecular systems and to clarify the importance of the factors mentioned above. For this purpose we have performed calculations using coupled cluster techniques on a number of model systems including rare gas dimers and trimers and complexes of Cl_2.