CAS-SCF COMPUTATIONS ON JAHN-TELLER, RENNER-TELLER AND SECOND ORDER JAHN-TELLER SYSTEMS

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The information that can be obtained from ab initio CAS-SCF computations on Jahn-Teller, Renner-Teller and second order Jahn-Teller systems will be presented in order to stimulate discussion of how this information can be used to rationalize experimental data. Several examples will be presented for each potential surface topology.
The D_{5h} Jahn-Teller crossing and associated C_{2v} minima and saddle points were optimised for the cyclopentadienyl radical at the CASSCF / cc-pVDZ level of theory. The C_{2v} structures were characterised by computing analytic force constants. Zero point energies calculated for all C_5H_4D and C_5HD_4 isomers of the C_{2v} minima suggest an alternative interpretation of the experimentally observed degeneracy resolution. For the benzene radical cation, the Jahn-Teller topology has also been mapped out. Finally, the use of symmetry in characterising the second order Jahn-Teller effect will also be discussed for D_{2h} pentalene and D_{8h} cyclooctatetraene.