

VIBRATION-ROTATION-TUNNELING STATES OF THE BENZENE DIMER: AN AB INITIO STUDY

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An improved intermolecular potential surface for the benzene dimer has been constructed from interaction energies computed by symmetry-adapted perturbation theory with the inclusion of third-order contributions. The potential was used in calculations of vibration-rotation-tunneling levels of the dimer by a method appropriate for large amplitude intermolecular motions and tunneling between multiple equivalent minima in the potential. The resulting levels were analyzed using the permutation-inversion full cluster tunneling group G_{576} and a chain of subgroups that starts from the molecular symmetry group $C_s(M)$ of the rigid dimer at its equilibrium C_s geometry and leads to G_{576} if all possible intermolecular tunneling mechanisms are feasible.