The Singlet−Triplet Gap in Trimethylenmethane and the Ring-Opening of Methylenecyclopropane: A Multireference Brillouin−Wigner Coupled Cluster Study

Abstract

We performed an ab initio study of the singlet−triplet gap in trimethylenmethane (TMM) and of the ring-opening of methylenecyclopropane by the multireference BWCC method. Since the singlet states of TMM and intermediates between TMM and methylenecyclopropane have a strong multiconfigurational character, it is necessary to use a multireference method. The cc-pVDZ and cc-pVTZ basis sets were used. We compared our results with experiments, where available, and with previous calculations performed by MCSCF and spin-flip coupled-cluster-type methods.