UV excitations of halons

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Abstract

In the present study, we examined the UV excitations of a newly introduced molecular set, Halons-9, composed of nine gaseous halon molecules. The performance of the density functional-based multi-reference configuration interaction method (DFT/MRCI) and time-dependent density functional theory with CAM-B3LYP functional (TD-CAM-B3LYP) in the computation of singlet and triplet excited states of this set was evaluated against coupled-cluster with singles and doubles (CCSD). Excited states up to the corresponding ionization limits, including both localized and delocalized excitations, have been benchmarked. TD-CAM-B3LYP significantly underestimates excitation energies of the higher mixed valence-Rydberg and Rydberg states, with computed mean absolute deviations from the equation of motion (EOM)-CCSD results 1.06 and 0.76 eV, respectively. DFT/MRCI gives a significantly better description of higher excited states, albeit still poor, compared to the TD-CAM-B3LYP. The mean absolute deviations of mixed valence-Rydberg and Rydberg states from the reference EOM-CCSD values are 0.66 and 0.47 eV, respectively. The performance of DFT/MRCI for description of strongly correlated states with valence-Rydberg mixing is still not satisfactory enough. On the other hand, oscillator strengths of most of singlet states obtained with both methods are close to the EOM-CCSD values. The largest deviations, occurring in the case of several high-lying multiconfigurational states, are of an order of magnitude. Published by AIP Publishing.

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