

Accurate structure, thermodynamics, and spectroscopy of medium-sized radicals by hybrid coupled cluster/density functional theory approaches: The case of phenyl radical

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Streszczenie

The coupled-cluster singles doubles model with perturbative treatment of triples (CCSD(T)) coupled with extrapolation to the complete basis-set limit and additive approaches represent the “golden standard” for the structural and spectroscopic characterization of building blocks of biomolecules and nanosystems. However, when open-shell systems are considered, additional problems related to both specific computational difficulties and the need of obtaining spin-dependent properties appear. In this contribution, we present a comprehensive study of the molecular structure and spectroscopic (IR, Raman, EPR) properties of the phenyl radical with the aim of validating an accurate computational protocol able to deal with conjugated open-shell species. We succeeded in obtaining reliable and accurate results, thus confirming and, partly, extending the available experimental data. The main issue to be pointed out is the need of going beyond the CCSD(T) level by including a full treatment of triple excitations in order to fulfil the accuracy requirements. On the other hand, the reliability of density functional theory in properly treating open-shell systems has been further confirmed.

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