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download pcComparing quantum chemistry techniques for small molecule photophysics: a CASPT2 study.
The ability to estimate accurate photochemical rates represents a difficult challenge for theory. The latter
is even more difficult if one wants to evaluate rates as the standard states of the photophysics. Here, we
compare CASPT2 and CASSCF-MR-CIS methods for the photophysics of the aminoxanthene nitronitroxide,
diamantane, and cis-9,10-dithia-anthracene. We find that CASSCF-MR and CASPT2 provide accurate
results for the ground-state energies, leading to an overestimation of the vertical excitation energies for
the nitronitroxide. The CIS approach is biased for the Gibbs free energies of the low-lying valence and
Rydberg states due to the use of spin-restricted functionals. An in-depth analysis of the errors on the
transition energies obtained for the diamantane suggests an improper treatment of the electron
correlation in the (2)A(') states for both the CASSCF-MR and CASPT2 methods. However, in this state, the
CASPT2 method yields transition energies in good agreement with the experimental values, whereas the
CASSCF-MR-CIS estimates are still too high. On the other hand, for the first (2)A(') state of anthracene,
both the CASSCF-MR and CASPT2 methods provide transition energies in agreement with experiment. In
all cases, the CASPT2 rates are in fair agreement with experimental data. Office forms and surveys are
frequently used as a means of gathering information from individuals. In some instances, the documents
can be self-administered and others can be automatically gathered. Many of the forms are utilized to
collect information about a particular medical condition or health concern. For example, patients in a
hospital may be asked to complete a questionnaire relating to their treatment. The information is
generally used to determine the condition of the patient, for example, the general medical condition or
for determining whether a particular procedure was successful. Unfortunately, the collection of
information can be inefficient and difficult. As a result, an improved means for gathering information is
needed. White Stripes (disambiguation) The White Stripes are an American rock duo. White Stripes may
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