Describing the Disulfide Bond: From the Density Functional Theory and Back through the “Lego Brick” Approach

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Rok wydania

2024

Czasopismo

Journal of Physical Chemistry A

Numer woluminu

128

Strony

9383-9397

DOI

10.1021/acs.jpca.4c05198

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Selected molecular species containing the disulfide bond, RSSR, have been considered, these ranging from hydrogen disulfide, H_2S_2 (R = H), to diphenyl disulfide with R = C_6H_5. The aim of this work is two-fold: (i) to investigate different computational approaches in order to derive accurate equilibrium structures at an affordable cost, (ii) to employ the results from the first goal in order to benchmark cheaper methodologies rooted in the density functional theory. Among the strategies used for the accurate geometrical determinations, the semiexperimental approach has been exploited in combination with a reduced-dimensionality VPT2 model, without however obtaining satisfactory results. Instead, the so-called “Lego brick” approach turned out to be very effective despite the flexibility of the systems investigated. Concerning the second target of this work, the focus was mainly on the S–S bond and the structural parameters related to it. Among those tested, PBE0(-D3BJ), M06-2X(-D3) and DSD-PBEP86-D3BJ have been found to be the best-performing functionals.

Słowa kluczowe

Basis Sets, Disulfides, Energy Levels, Equilibrium, Molecules

Adres publiczny

http://dx.doi.org/10.1021/acs.jpca.4c05198

Strona internetowa wydawcy

https://www.acs.org/content/acs/en.html