

## The challenging equilibrium structure of HSSH: Another success of the rotational spectroscopy / quantum chemistry synergism

### Autorzy

Hexu Ye

Marco Mendolicchio

Holger Kruse

Cristina Puzzarini

Małgorzata Biczysko

Vincenzo Barone

### Rok wydania

2020

### Czasopismo

Journal of Molecular  
Structure

### Numer woluminu

1211

### Strony

127933/1-127933/10

### DOI

10.1016/j.molstruc.2020.127933

### Kolekcja

Naukowa

### Język

Angielski

### Typ publikacji

Artykuł

### Streszczenie

The simplest molecule with a disulfide bond, hydrogen disulfide (HSSH), represents an ideal test model for the determination of accurate gas-phase equilibrium structures for molecules containing third-row elements. First, pure theoretical composite schemes based on the coupled-cluster (CC) theory, which take into account the extrapolation to the complete basis set limit, core-valence correlation contributions, higher excitations in the CC expansion, and relativistic effects, allow for calculating accurate reference geometrical parameters. Second, using experimental vibrational ground-state rotational constants for a set of isotopologues, in conjunction with vibrational corrections based on second-order vibrational perturbation theory formulation and the recently developed Molecular Structure Refinement (MSR) software, we have determined the semi-experimental (SE) equilibrium structure of HSSH. The comparison of SE parameters with the computational best estimates shows an agreement within 0.001 Å for distances and 0.1° for angles, thus further validating the SE approach as cost-effective, provided that the required experimental data are available. Together with the intrinsic interest of HSSH, also in connection with astrochemistry, highly accurate structural properties of a prototypical disulfide bond can serve as references for future studies of larger molecules of biological interest containing this challenging moiety.

### Słowa kluczowe

Semi-experimental, Composite scheme, Equilibrium structure, Coupled cluster, CBS, Disulfide

### Adres publiczny

<http://dx.doi.org/10.1016/j.molstruc.2020.127933>

### Strona internetowa wydawcy

<http://www.elsevier.com>

Plik został wygenerowany dnia 2026-10-11 08:05:38

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/tGAQUkP>.