Verification of Experimental Vibrational - Rotational Transitions of Hydrogen Sulfide and its Isotopologues between 0 and 16500 cm^{-1} based on an Effective Hamiltonian Approach and Variational Computations

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More than 50,000 published experimental rotation-vibration transitions of $H_2{}^{32}S$, $H_2{}^{34}S$, and $H_2{}^{33}S$ from 30 literature sources were combined to form and extensive compilation between 0 and 16500 cm^{-1}. The values were verified using both the effective Hamiltonian approach and variational nuclear motion computations. The methodology previously applied to large experimental H_2O datasets [1] was used to obtain accurate rovibrational energy levels for each isotopologue of H_2S. This approach is based on the Rydberg-Ritz system of linear equations implemented in the MARVEL computer code [2]. The experimental energy levels of the key (000) and (010) states were modeled close to experimental accuracy using rotational operators constructed on the basis of divergent series summation methods.

Detailed and extensive reference spectra of all considered isotopologues were generated in a wide spectral region considered based on the experimental energy levels and first-principles variational intensities. The numerical information obtained has been deposited in the Internet accessible information system W@DIS (http://wadis.saga.iao.ru).

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