

GLOBAL ROVIBRATIONAL ANALYSIS FOR THE 20 LOWEST VIBRATIONAL BANDS OF HYDROGEN SULFIDE (H₂³²S)

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The rovibrational energy structure of H₂S has been analysed simultaneously for the 20 lowest energy vibrational bands up to J=20. We have used a global analysis rovibrational algebraic approach of which the effective Hamiltonian interaction terms are constructed as products of powers of the angular momentum components and an algebraic realization of the vibrational interactions. The algebraic vibrational terms are obtained as a set of anharmonic Morse ladder operators based on the dynamical algebra U(2), one for every internal coordinate ^a.

The parameters of the effective rovibrational Hamiltonian have been determined by a nonlinear least-squares fitting to the available experimental rovibrational energies ^b. More than 2500 experimental rovibrational energies, up to J=20 for the 20 lowest vibrational bands, have been fitted with a *rms* of the order of 10⁻³ cm⁻¹. In total, around 8000 rovibrational energy term values have been calculated.

^aM. Carvajal, R. Lemus, *J. Phys. Chem. A* 119 (2015) 12823.

^bK.L. Chubb *et al.*, *J. Quant. Spectrosc. Rad. Transf.* 218 (2018) 178–186.