

A THEORETICAL RO-VIBRATIONAL LINE LIST OF H₂CS USING A NEW APPROACH TO CONSTRUCT THE EXACT KINETIC ENERGY OPERATOR

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A procedure to generate the exact kinetic energy operator in valence coordinates, based on Sørensen's method for constructing non-rigid Hamiltonians, is presented. This method is currently being applied to the thioformaldehyde (H₂CS) molecule, where the TROVE program is used to compute ro-vibrational energy levels and transition intensities. Moreover, the *ab initio* PES is refined with the MARVEL approach. The exact kinetic energy operator itself is produced using the symbolic computation program *Mathematica* and acts as TROVE input.