The intramolecular conversion of monothioformic acid: An ab initio study

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A complete description of the rotational isomerism of monothioformic acid is presented. Ab initio results concerning the barrier heights and the energy difference between the stable isomers are in good agreement with the experimental data. A reduced potential function deduced from our calculations has been used to characterize the kinetics and thermodynamics of the rotational isomerization. The reported ab initio values of equilibrium constants are in good agreement with the experimental ones. From the analysis of the available experimental data, we have found that the free energy and enthalpy behavior are quite similar and that no noticeable entropy contributions are involved in the internal rotation, in agreement with previous studies on unimolecular isomerization processes.