

MICROWAVE SPECTROSCOPY AND LARGE AMPLITUDE MOTION OF CHLOROSULFONIC ACID (ClSO₂OH)

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The high-resolution rotational spectrum of chlorosulfonic acid (ClSO₂OH) was studied using both broadband chirped pulse and cavity-based Fourier transform microwave spectrometers over the frequency range of 5–18 GHz for the first time. The observation of *a*-, *b*-, and *c*-type transitions for both ³⁵Cl and ³⁷Cl isotopomers suggests that the molecule exhibits large amplitude motion of the hydroxyl hydrogen flipping between two equivalent structures. The rotational constants, the centrifugal distortion constants, and the nuclear quadrupole coupling constants for the chlorine nucleus have been determined. The quantum chemical calculations were carried out using MP2 and B3LYP density functional theory (DFT) with aug-cc-pVTZ basis set. The rotational constants from the optimized geometric structures were in good agreement with the experimental values. The energy barrier of the large amplitude motion was calculated to be 12 kJ/mol. The effect of the large amplitude motion will be compared to the recent rotational spectroscopic study on triflic acid.^a

^aAnna K.Huff, Nathan Love, C. J. Smith Kenneth R. Leopold; Parent, 34S, and deuterated triflic acid: Microwave spectra and tunneling splittings due to hydroxyl torsion, *J. Mol. Spectrosc.*, 2022, 385, 111623.