

Structure Data of Free Polyatomic Molecules

275 MW	H₅NS	Ammonia – hydrogen sulfide (1/1) (weakly bound complex)	C_s (effective symmetry class) (large-amplitude motion) NH ₃ · H ₂ S
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The *b*-type $\Delta K = \pm 2$, $\Delta m = 0$ transitions observed around 300 GHz are split into doublets with a 3:1 relative intensity ratio indicative of tunneling interchange of the two H₂S protons. The most likely interchange motion consists of a partial internal rotation of the H₂S unit about its *c* inertial axis, through a bifurcated, doubly hydrogen-bonded transition state. The proton interchange tunneling splittings of 859 – 864 MHz vary little between *K* and *m* states, indicating that the interchange motion is only weakly coupled to the internal motion. Two model potential functions, quartic and Fourier, for the H₂S proton interchange tunneling were used. The tunneling barrier was determined to be 510(3) cm⁻¹.

Hilpert, G., Fraser, G.T., Suenram, R.D., Karyakin, E.N.: J. Chem. Phys. **102** (1995) 4321.

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