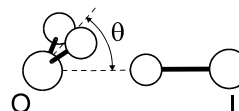


260	H₃IO	Hydrogen iodide – water (1/1)	C_s
MW		(weakly bound complex)	(effective symmetry class)
			(large-amplitude motion)
			HI · H ₂ O

r_0	Å	θ_0	deg
O...I	3.745(2)	θ_{av}^a	20.89(2)

Ab initio calculations support the conclusion that the ground vibrational state for the H₂O flapping mode is delocalized between two equilibrium structures at an energy above an inversion barrier.

^a) See figure for the definition. Average value.



McIntosh, A., Walther, T., Lucchese, R.R., Bevan, J.W., Suenram, R.D., Legon, A.C.: Chem. Phys. Lett. **314** (1999) 57.