

Structure Data of Free Polyatomic Molecules

214 MW	HINe		Hydrogen iodide – neon (1/1)		C _s (large-amplitude motion) HI · Ne
			(weakly bound complex)		
	r_0	\AA	θ_0	deg	
	$R_{\text{cm}}(^{20}\text{Ne} \cdot \text{HI})$	4.1018(1)	$\langle P_2(\cos\theta) \rangle(^{20}\text{Ne} \cdot \text{HI})$	0.12527(1) ^{a)}	
	$R_{\text{cm}}(^{20}\text{Ne} \cdot \text{DI})$	3.9616(1)	$\langle P_2(\cos\theta) \rangle(^{20}\text{Ne} \cdot \text{DI})$	0.41110(1) ^{a) b)}	

In $^{20}\text{Ne} \cdot \text{HI}$, hydrogen iodide is a nearly free rotor.

^{a)} θ denotes the angle between R_{cm} and the molecular axis of hydrogen iodide.

^{b)} Corresponding to $\theta = 141.20(1)^\circ$, *i.e.*, to the isomeric structure: Ne · ID.

Lin, P., Jabs, W., Lucchese, R.R., Bevan, J.W., Brugh, D.J., Suenram, R.D.: Chem. Phys. Lett. **356** (2002) 101.