

228 IR	HNeO^+	Oxoniumylidene – neon (1/1) (weakly bound complex)	$\text{C}_{\infty v}$ (effective symmetry class) (large-amplitude motion) $\text{OH}^+ \cdot \text{Ne}$	

State	$R_{\text{cm}} [\text{\AA}]^{\text{a)}}$	$\text{H} \dots \text{Ne} [\text{\AA}]^{\text{a)}}$	$\theta [\text{deg}]^{\text{a) b)}$
$\nu=0$	2.6536(3)	1.6748(3)	19.6(3)
$\nu_1=1$	2.6320(1)	1.6307(1)	17.4(1)

The linear H-bound structures in the $^3\Sigma^-$ electronic ground state were determined from the IR predissociation spectrum of the ν_1 band (O–H stretch). The geometry of the OH^+ subunit was assumed to be unchanged upon complexation.

^{a)} Estimated standard errors.

^{b)} Angular oscillation of the OH^+ subunit.

Roth, D., Nizkorodov, S.A., Maier, J.P., Dopfer, O.: J. Chem. Phys. **109** (1998) 3841.