

## Structure Data of Free Polyatomic Molecules

211 IR	$\text{HHeO}^+$	<b>Oxoniumylidene – helium (1/1)</b> (weakly bound complex)	$\text{C}_{\infty v}$ (effective symmetry class) (large-amplitude motion) $\text{OH}^+ \cdot \text{He}$
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State	$R_{\text{cm}} [\text{\AA}]^{\text{a)}}$	$r(\text{H} \dots \text{He}) [\text{\AA}]^{\text{a)}}$	$\theta [\text{deg}]^{\text{a) b)}$
$\nu=0$	2.6018(2)	1.6230(2)	24.7(2)
$\nu_1=1$	2.5761(1)	1.5748(1)	21.3(2)
$\nu_1=\nu_b=1$	2.5911(7)	1.5898(7)	39.5(3)

The linear H-bound structures in the  $^3\Sigma^-$  electronic ground state were determined from the IR predissociation spectra of the  $\nu_1$  (O–H stretch) and its combination band with the intermolecular vibration ( $\nu_1+\nu_b$ ). The geometry of the  $\text{OH}^+$  subunit was assumed to be unchanged upon complexation.

<sup>a)</sup> Estimated standard errors.

<sup>b)</sup> Angular oscillation of the  $\text{OH}^+$  subunit.

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