

267
MW H_3O^+

Oxonium

 C_{3v}
 H_3O^+

Isotopic species

(inversion states) $r_0(\text{H-O})$ [Å] $\theta_0(\text{H-O-H})$ [deg] $\text{H}_3\text{O}^+(0^+)^a)$ 0.978229(62) 114.9680(181) $\text{H}_3\text{O}^+(0^-)^a)$ 0.981178(60) 113.2585(175) $\text{D}_3\text{O}^+(0^+)^a)$ 0.9762(23) 113.25(99) $\text{D}_3\text{O}^+(0^-)^a)$ 0.9774(22) 112.58(98)

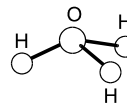
Isotopic species

(inversion states) $r_z(\text{H-O})$ [Å] $\theta_z(\text{H-O-H})$ [deg] $\text{H}_3\text{O}^+(0^+)^a)$ 0.985419(134) 114.307(32) $\text{H}_3\text{O}^+(0^-)^a)$ 0.988525(135) 112.587(32) $\text{D}_3\text{O}^+(0^+)^a)$ 0.9818(23) 112.68(100) $\text{D}_3\text{O}^+(0^-)^a)$ 0.9830(23) 112.02(100) $r_e^b)$ Å

H-O 0.9702(89)

 $\theta_e^b)$ deg

H-O-H 109.4(38)

The inversion splitting in D_3O^+ is determined to be $15.35550338(107) \text{ cm}^{-1}$.^{a)} 0^+ and 0^- denote the symmetric and antisymmetric inversion states, respectively.^{b)} Estimated from the r_z structures of H_3O^+ and D_3O^+ .Araki, M., Ozeki, H., Saito, S.: Mol. Phys. **97** (1999) 177.

IR

 r_e Å

O-H 0.9744(9)

 θ_e deg

H-O-H 113.58(7)

Tang, J., Oka, T.: J. Mol. Spectrosc. **196** (1999) 120.Replaces [II/25A\(2, 741\)](#)