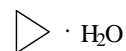


1346  
MW

**C<sub>3</sub>H<sub>8</sub>O**

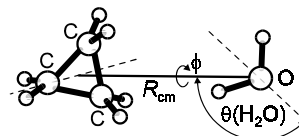
**Cyclopropane – water (1/1)**  
(weakly bound complex)

**C<sub>s</sub>**  
(effective symmetry class)



	$\theta_0$ (H <sub>2</sub> O) [deg] <sup>a)</sup>	$r_0(R_{\text{cm}})$ [Å] <sup>a)</sup>	$R$ (H-bond) [Å] <sup>b)</sup>	$\theta_0$ (H-bond) [deg] <sup>b)</sup>
$\phi = 0^\circ$	124.8(40)	3.712(1)	2.342	3
$\phi = 90^\circ$	123.0(63)	3.713(2)	2.343	4

The water is hydrogen-bonded to the center of an edge of the cyclopropane; the hydrogen bond is nearly linear (bond center–H–O angle = 180(5)°) with the O and hydrogen-bonded H in the CCC plane. The hydrogen bond length (H-to-edge distance) is 2.34 Å. The position of the free H is uncertain. Nuclear spin statistics indicate that the splittings in the spectrum arise from a high-barrier internal motion of the water subunit which exchanges the two hydrogen atoms; a nearly free rotation of the water about the hydrogen bond is postulated to explain anomalous dipole moment and nuclear quadrupole coupling results.



<sup>a)</sup> The  $r_0$  structures.

<sup>b)</sup> Calculated parameter (not explicitly fit).  $R$ (H-bond) is the distance from the hydrogen-bonded H to the C–C bond center.  $\theta$ (H-bond) is the deviation from 180° of the angle subtended by the C–C bond center, the hydrogen-bonded H, and the O.

Andrews, A.M., Hillig, K.W., Kuczkowski, R.L.: J. Am. Chem. Soc. **114** (1992) 6765.