

1430
MW

C₃H₁₀O

Propane – water (1/1)
(weakly bound complex)

C_{2v}
(effective symmetry class)
H₃C–CH₂–CH₃ · H₂O

r_0	Å
R_{cm}	3.76(2)
cm(H ₂ O)...methylene C	4.35(2)

All four heavy atoms are coplanar, with the cm(H₂O) lying on or near the C₂ axis of propane, inside the C–C–C angle. The Stark effect indicates that one of the protons of H₂O lies on the C₂ axis of the propane monomer, which is also the axis connecting the subunit centers of mass and is most consistent with an equilibrium structure in which all three atoms of H₂O lie in the CCC plane of propane, with torsional tunneling about the hydrogen bond occurring on the same time scale as the overall rotation.

Steyert, D.W., Elrod, M.J., Saykally, R.J., Lovas, F.J., Suenram, R.D.: J. Chem. Phys. **99** (1993) 7424.

See also: (Far-IR) Steyert, D.W., Elrod, M.J., Saykally, R.J.: J. Chem. Phys. **99** (1993) 7431.