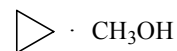


595
MW $C_4H_{10}O$ **Cyclopropane – methanol (1/1)**
(weakly bound complex) **C_1**
(effective symmetry class)
(large-amplitude motion)

r_0	Å
	fit 1, fit 2
$R^a)^b)$	3.28(1)

θ_0	deg	
	fit 1	fit 2
$\theta_{CYC}^a)$	90 °)	90 °)
$\phi_{CYC}^a)$	180 °)	180 °)
$\theta_{MET}^a)$	102.3(10)	102.6(9)
$\phi_{MET}^a)$	180 °)	180 °)
$\tau^a)$	42.5(8)	42.5(7)

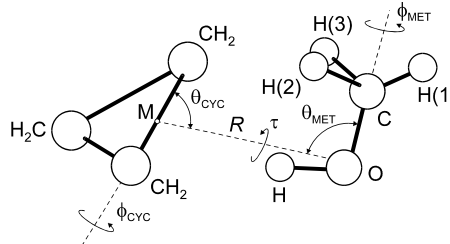


The observed microwave spectra exhibited complication and splittings from large-amplitude motions. Rotational transitions were assigned for two states and fit reasonably well with a normal semi-rigid Hamiltonian. Based on data from five isotopic species, a hydrogen-bonded structure was deduced in which the hydroxyl hydrogen is attracted to an edge of the cyclopropane ring.

^{a)} See figure for the definition. θ_{MET} is C–O...M; ϕ_{MET} denotes the out-of-plane tilt of the methanol, *i.e.*, the dihedral angle H(1)–C–O...M; τ means the torsional angle between the two monomers defined by the dihedral angle C–O...M–C_{CYC} with the origin $\tau = 0^\circ$ when the C atom of methanol lies in the cyclopropane carbon plane; θ_{CYC} is equal to O...M–C_{CYC}, and ϕ_{CYC} corresponds to the dihedral angle O...M–C_{CYC}–C_{CYC}, where M denotes the midpoint of the C–C bond of the cyclopropane to which the hydroxyl group of methanol is hydrogen-bonded.

^{b)} Distance from M to O of the methanol.

^{c)} Assumed.



Forest, S.E., Peebles, S.A., Sun, L.-H., Andrews, A.M., Kuczkowski, R.L.: J. Mol. Struct. **413-414** (1997) 255.