

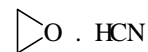
1220
MW

C₃H₅NO

Hydrogen cyanide – oxirane (1/1)
(weakly bound complex)

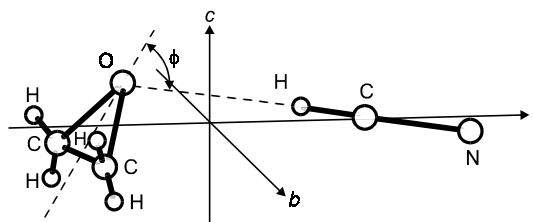
C_s
(effective symmetry class)

Isotopic species	State ^{a)}	$r_0(\text{O}\cdots\text{C})$ [Å]	ϕ_0 [deg]	θ_{av} [deg] ^{b)}
(CH ₂) ₂ O · HC ¹⁴ N	A	3.035(4)	52.2(3)	17.1(5)
	B	3.130(4)	61.1(3)	16.6(5)
(CH ₂) ₂ O · HC ¹⁵ N	A	3.035(4)	52.2(3)	
	B	3.129(4)	61.2(3)	
(CH ₂) ₂ O · DC ¹⁴ N	A	3.063(3)	55.7(3)	15.5(7)
	B	3.129(4)	61.7(3)	14.5(7)



^{a)} The states A and B correspond to the ground state and the $\nu = 1$ state of the low-frequency hydrogen bond bending mode.

^{b)} Angle between the a -axis and the molecular axis of HCN.



Goodwin, E.J., Legon, A.C., Millen, D.J.: J. Chem. Phys. **85** (1986) 676.