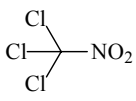


Structure Data of Free Polyatomic Molecules

27 MW	CCl₃NO₂		Trichloronitromethane		G₁₂ 
	r_0	Å	θ_0	deg	
	C–N	1.52(3)	Cl–C–Cl	109.8 ^{a)}	
	C–Cl	1.76 ^{a)}	O=N=O	125.8 ^{a)}	
	Cl...Cl	2.881(6)			
	N=O	1.220 ^{a)}			
	O...O	2.172(5) ^{b)}			

The barrier height to internal rotation was determined to be $V_6 = 306.43 \text{ J mol}^{-1}$.

^{a)} Assumed.

^{b)} Uncertainty was not estimated in the original paper.

Cox, A.P., Ellis, M.C.: J. Mol. Struct. **445** (1998) 287.

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