

1222
MW

C₃H₅NO₂

Nitrocyclopropane

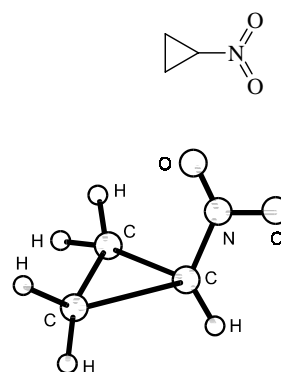
C_s

r_0	Å	θ_0	deg
C–C	1.511 ^{a)}	H–C–H	116.2 ^{a)}
C–H	1.080 ^{a)}	O=N=O	130.0 ^{a)}
C–N	1.488(20)	N–C–H	114.4(15)
N=O	1.213(20)	ϕ ^{b)}	122.6 ^{a)}

The NO₂ group was assumed to have twofold symmetry axis about the C–N bond. The conformation of the molecule was found to be such that the NO₂ plane was perpendicular to the ring plane.

^{a)} Assumed.

^{b)} Angle between the C–N bond and the plane of the ring.



Mochel, A.R., Britt, C.O., Boggs, J.E.: J. Chem. Phys. **58** (1973) 3221.