

1262
ED

C₃H₆N₂O₄

2,2-Dinitropropane

C_{2v} (effective)

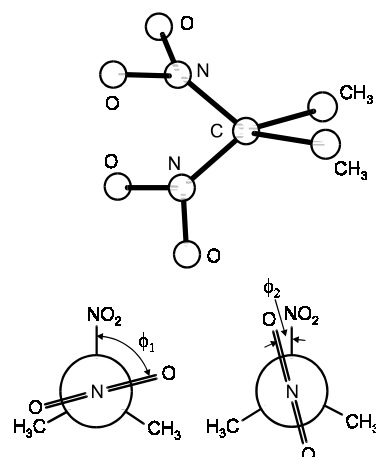
r_g	\AA^a	θ_g	deg^a
N=O	1.227(2)	O=N=O	124.5(6)
C–N,		N–C–N	111.6(12)
C–C (average)	1.517(15)	H–C–H	109.5 ^b
C–H	1.089(13)	C–C–C	113.1(23)

The experimental data were consistent with free internal rotation of the NO₂ groups retaining a nearly perpendicular conformation relative to each other ($\phi_1 + \phi_2 \approx 90^\circ$; see figure).

The nozzle temperatures were 45(5) °C and 60(5) °C.

^a) Uncertainties were unidentified, possibly estimated limits of error.

^b) Assumed.



Shishkov, I.F., Sadova, N.I., Vilkov, L.V., Pankrushev, Yu.A.: Zh. Strukt. Khim. **24** No.3 (1983) 173; Russ. J. Struct. Chem. (Engl. Transl.) **24** (1983) 485.