

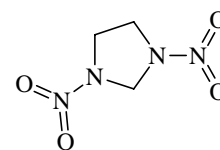
1263  
ED

**C<sub>3</sub>H<sub>6</sub>N<sub>4</sub>O<sub>4</sub>**

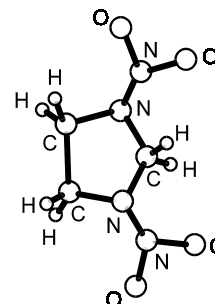
**1,3-Dinitroimidazolidine**

**C<sub>2</sub>**

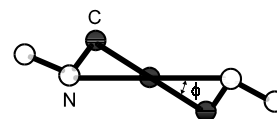
$r_g$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
C–N	1.483(8)	C–C–N	100.2(24)
C–C	1.528(61)	C–N–C	109.7(17)
N–N	1.393(8)	C–N–N	114.8(8)
N=O	1.226(2)	O=N=O	128.2(18)
C–H	1.112(22)	H–C–H	111.2(91)
		$\tau(\text{NN})$ <sup>b)</sup>	12.9(30)
		$\phi$ <sup>c)</sup>	37.3(18)
		$\delta$ <sup>d)</sup>	43.2(50) <sup>e)</sup>
		$\gamma$ <sup>f)</sup>	339.3(50) <sup>e)</sup>



The conformation of the five-membered ring is a half-chair of C<sub>2</sub> symmetry. The nitro groups are located in the equatorial positions. The NNO<sub>2</sub> geometry was assumed to be planar. The NNO<sub>2</sub> and CH<sub>2</sub> fragments were assumed to have C<sub>2v</sub> local symmetry. The nozzle temperature was 162 °C.



- <sup>a)</sup> Three times the estimated standard errors.  
<sup>b)</sup> Torsional angle about the N–N bond. The value 0° corresponds to a position of the NO<sub>2</sub> groups such that the line segments C–C and O–O for C<sub>2</sub>N–NO<sub>2</sub> lie in a single plane.  
<sup>c)</sup> Angle between the NCN plane and the plane containing C–C bond and C<sub>2</sub> symmetry axis; see figure.  
<sup>d)</sup> Angle between the CNC plane and the N–N bond  
<sup>e)</sup> The uncertainty was not estimated in the original paper.  
<sup>f)</sup> The sum of the bond angles at the amine N atom.



Shishkov, I.F., El'fimova, T.L., Vilkov, L.V., Ivshin, V.P.: Zh. Strukt. Khim. **33** No.1 (1992) 35; Russ. J. Struct. Chem. (Engl. Transl.) **33** (1992) 29.  
 Shishkov, I.F., Vilkov, L.V., Kolonits, M., Rozsondai, B.: Struct. Chem. **2** (1991) 57.