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

**Hexahydro-1,3,5-trinitro-1,3,5-triazine**

**C<sub>3</sub>**

$r_g$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
C–N	1.464(6)	N–C–N	109.4(6)
N–N	1.413(5)	C–N–C	123.7(6)
N=O	1.213(2)	C–N–N	116.3(5)
C–H	1.089(27)	O–N–O	125.5(10)
		H–C–H	105.1(60)
		$\tau(\text{NN})$ <sup>b)</sup>	19.1(23)
		$\phi$ <sup>c)</sup>	33.9(29)
		$\delta$ <sup>d)</sup>	19.9(50) <sup>f)</sup>
		$\gamma$ <sup>e)</sup>	356.3(50) <sup>f)</sup>

The six-membered ring has a chair conformation with an axial positions of the NO<sub>2</sub> groups.

The N–NO<sub>2</sub> fragment was assumed to be planar with C<sub>2v</sub> local symmetry.

The nozzle temperature was 160 °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> will lie in a single plane.

<sup>c)</sup> Dihedral angle between the CNC plane and adjacent CN···NC plane; see figure.

<sup>d)</sup> Angle between the N–N bond and the CNC plane; see figure.

<sup>e)</sup> The sum of the bond angles at the amine N atom.

<sup>f)</sup> The uncertainty was not estimated in the original paper.

Shishkov, I.F., El'fimova, T.L., Vilkov, L.V.: Zh. Strukt. Khim. **33** (1992) No.1, 41; Russ. J. Struct. Chem. (Engl. Transl.) **33** (1992) 34.

Shishkov, I.F., Vilkov, L.V., Kolonits, M., Rozsondai, B.: Struct. Chem. **2** (1991) 57.

