

C_6N_{16} $hP44$ $(176) P6_3/m - h^7c$ C_6N_{16} [1]

Structural features: Planar C_6N_{16} molecules (three edge-linked (C_3N_3) hexagons with a $N=N=N$ unit bonded to each of the three not shared C atoms).

Miller D.R. et al. (2004) [1]

 C_6N_{16} $a = 1.02163$, $c = 0.59707$ nm, $c/a = 0.584$, $V = 0.5397$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	$6h$	$m..$	0.05678	0.44102	$\frac{1}{4}$		coplanar triangle N_3
N2	$6h$	$m..$	0.07028	0.57747	$\frac{1}{4}$		non-colinear C_2
N3	$6h$	$m..$	0.16545	0.40449	$\frac{1}{4}$		non-colinear C_2
N4	$6h$	$m..$	0.20327	0.12659	$\frac{1}{4}$		single atom N
N5	$6h$	$m..$	0.29795	0.10265	$\frac{1}{4}$		non-colinear N_2
C6	$6h$	$m..$	0.30686	0.51837	$\frac{1}{4}$		coplanar triangle N_3
N7	$6h$	$m..$	0.4166	0.09361	$\frac{1}{4}$		non-colinear NC
N8	$2c$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle C_3

Transformation from published data: $y, x, -z$; origin shift $0\ 0\ \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.035$, $T = 190$ K

Remarks: 2,5,8-triazido-s-heptazine.

References: [1] Miller D.R., Swenson D.C., Gillan E.G. (2004), J. Am. Chem. Soc. 126, 5372-5373.