

$C_6N_6O_3$ $hP30$ $(176) P6_3/m - h^5$ $C_6N_6O_3$ [1]

Structural features: Planar $C_6N_6O_3$ molecules (a C_6 hexagon with alternatively an N=N unit or an O atom bonded to each C) in a Mg-type (h.c.p.) arrangement.

Jones P.G. et al. (1997) [1]

 $C_6N_6O_3$ $a = 0.91599$, $c = 0.5445$ nm, $c/a = 0.594$, $V = 0.3956$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	$6h$	$m..$	0.00385	0.41446	$1/4$		single atom C
C2	$6h$	$m..$	0.15168	0.52808	$1/4$		coplanar triangle OC_2
N3	$6h$	$m..$	0.21895	0.20295	$1/4$		single atom N
N4	$6h$	$m..$	0.25478	0.33774	$1/4$		non-colinear NC
C5	$6h$	$m..$	0.29383	0.4986	$1/4$		coplanar triangle NC_2

Transformation from published data: $y, x, -z$; origin shift $0\ 0\ 1/2$ Experimental: single crystal, diffractometer, X-rays, $R = 0.029$, $T = 143$ K

Remarks: 2,4,6-tris(diazo)cyclohexane-1,3,5-trione.

References: [1] Jones P.G., Ahrens B., Höpfner T., Hopf H. (1997), Acta Crystallogr. C 53, 783-786.