Crystal structure of tris(diformylamino)methane, $C_7H_7N_3O_6$

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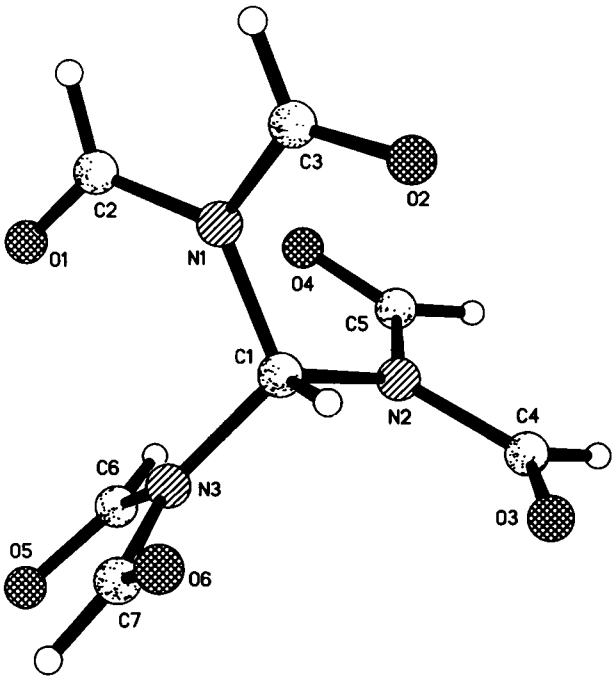

Abstract

$C_7H_7N_3O_6$, orthorhombic, *Pbca* (No. 61), $a = 12.159(2)$ Å, $b = 10.661(2)$ Å, $c = 14.813(2)$ Å, $V = 1920.2$ Å^3, $Z = 8$, $R_{gt}(F) = 0.043$, $wR_{obs}(F^2) = 0.107$, $T = 293$ K.

Source of material

The compound can be prepared by the reaction of triformylamine ('triformamide') with sodium diformamide in good yields [1]; mp. 425 K (decomposition).

Discussion

Tris(diformylamino)methane is a remarkable molecule; it contains seven carbons which are all part of a (masked) formyl group. As expected, the diformylamino moieties are nearly planar. In the plane-angles to each other we observe a slight difference, documented by the values 80.6°, 65.5° and 72.6°, respectively.

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.6 × 1.5 × 1.5 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.41 cm^{-1}
Diffractometer, scan mode:	Nicolet P3, Wyckoff
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2202, 2202
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1850
$N(param)_{refined}$:	146
Programs:	SHELXS-86 [2], SHELXL-93 [3]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1)	8c	0.3383(1)	0.2297(1)	0.35770(9)	0.032
H(2)	8c	0.3347(2)	−0.1262(2)	0.4245(1)	0.047
H(3)	8c	0.1782(1)	−0.0112(2)	0.4080(1)	0.049
H(4)	8c	0.3540(1)	0.2823(2)	0.1394(1)	0.045
H(5)	8c	0.4004(1)	0.0720(2)	0.1235(1)	0.046
H(6)	8c	0.5863(1)	0.0718(2)	0.3035(1)	0.046
H(7)	8c	0.5606(2)	0.2929(2)	0.4738(1)	0.045

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Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(1)	8*c*	0.3291(1)	0.0477(1)	0.37466(8)	0.0353(7)	0.0278(6)	0.0274(6)	–0.0029(5)	0.0045(5)	0.0018(5)
O(1)	8*c*	0.4768(1)	–0.0787(1)	0.40831(9)	0.0524(8)	0.0382(7)	0.0508(7)	0.0092(6)	–0.0026(6)	0.0083(5)
C(1)	8*c*	0.3848(1)	0.1589(1)	0.33969(9)	0.0305(7)	0.0261(7)	0.0233(6)	–0.0002(5)	0.0029(5)	0.0012(5)
N(2)	8*c*	0.3873(1)	0.1629(1)	0.24130(8)	0.0344(6)	0.0350(7)	0.0227(6)	–0.0017(5)	0.0001(5)	0.0032(5)
O(2)	8*c*	0.1638(1)	0.1485(1)	0.3633(1)	0.0356(7)	0.0463(8)	0.082(1)	0.0023(6)	0.0070(6)	–0.0036(7)
C(2)	8*c*	0.3800(2)	–0.0614(2)	0.4051(1)	0.053(1)	0.0290(8)	0.0348(8)	–0.0021(7)	0.0015(7)	0.0053(6)
N(3)	8*c*	0.4906(1)	0.1829(1)	0.38082(8)	0.0326(6)	0.0290(6)	0.0249(6)	–0.0012(5)	–0.0004(5)	–0.0004(5)
O(3)	8*c*	0.3264(1)	0.3653(1)	0.24492(9)	0.0610(8)	0.0348(6)	0.0513(7)	0.0012(6)	0.0001(6)	0.0099(6)
C(3)	8*c*	0.2159(1)	0.0571(2)	0.3841(1)	0.0370(8)	0.0382(9)	0.0463(9)	–0.0073(7)	0.0113(7)	–0.0032(7)
O(4)	8*c*	0.4355(1)	–0.0406(1)	0.21145(9)	0.0650(8)	0.0455(7)	0.0388(6)	0.0118(6)	–0.0001(6)	–0.0078(6)
C(4)	8*c*	0.3543(1)	0.2762(2)	0.2020(1)	0.0405(8)	0.0393(9)	0.0340(8)	–0.0064(7)	–0.0027(7)	0.0114(7)
O(5)	8*c*	0.6738(1)	0.1414(2)	0.3912(1)	0.0317(6)	0.079(1)	0.0555(8)	–0.0009(6)	–0.0037(6)	–0.0064(7)
C(5)	8*c*	0.4082(1)	0.0606(2)	0.1854(1)	0.0412(9)	0.0472(9)	0.0265(7)	–0.0005(7)	0.0013(6)	–0.0038(7)
O(6)	8*c*	0.4119(1)	0.3218(1)	0.47740(8)	0.0731(9)	0.0511(7)	0.0323(6)	0.0253(7)	–0.0090(6)	–0.0111(5)
C(6)	8*c*	0.5880(1)	0.1250(2)	0.3532(1)	0.0325(8)	0.0473(9)	0.0346(8)	–0.0002(7)	0.0040(6)	–0.0008(7)
C(7)	8*c*	0.4929(2)	0.2714(2)	0.4489(1)	0.0522(9)	0.0317(8)	0.0294(7)	0.0036(7)	–0.0098(7)	–0.0014(6)

References

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