Crystal structure of 1,3,5-tri-2-propyl-2,4-dioxohexahydro-1,3,5-triazine, $C_{12}H_{23}N_3O_2$

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Received August 14, 2002; accepted and available on-line October 2, 2002; CCDC-No. 1267/916

Abstract

$C_{12}H_{23}N_3O_2$, orthorhombic, $P2_12_12_1$ (No. 19), $a = 6.033(2)$ Å, $b = 17.658(8)$ Å, $c = 13.224(5)$ Å, $V = 1408.8$ Å³, $Z = 4$, $R_{gt}(F) = 0.046$, $wR_{obs}(F^2) = 0.048$, $T = 294$ K.

Source of material

The title compound can be obtained by reacting 2,4-dioxohexahydro-1,3,5-triazine with 2-chloropropane and powdered potassium hydroxide in anhydrous dimethylsulfoxide [1].

Discussion

The 1,3,5-tri-2-propyl-2,4-dioxohexahydro-1,3,5-triazine molecule is characterized by a puckered ring which adopts a boatlike conformation (upper figure). The atoms C1, C2, N1 and N2 are in a virtually planar arrangement (mean deviation 0.008 Å) from

which C3 and N3 are offset by 0.578 Å and 0.305 Å, respectively. These values are distinctly larger than the corresponding displacements observed for 1,3,5-trimethyl-2,4-dioxohexahydro-1,3,5-triazine [2]. In the crystal structure, the molecules are stacked in piles along [100] which in turn are arranged in a distorted hexagonal rod packing (lower figure).

Table 1. Data collection and handling.

Crystal:	colourless prism, size 0.25 × 0.30 × 0.45 mm
Wavelength:	Mo $K\alpha$ radiation (0.7107 Å)
μ :	0.78 cm ⁻¹
Diffractionmeter, scan mode:	CAD4, $\omega/2\theta$
$2\theta_{max}$:	53.92°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1795, 1795
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1280
$N(param)_{refined}$:	178
Programs:	SIR92 [3], CRYSTALS [4]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
H(1)	4a	0.4684(5)	0.0164(1)	0.5742(2)	0.067(1)
H(2)	4a	0.2247(5)	0.0385(1)	0.5969(2)	0.067
H(6)	4a	0.2011(6)	-0.1153(2)	0.7094(3)	0.109(2)
H(7)	4a	0.3632(6)	-0.1130(2)	0.6184(3)	0.109
H(8)	4a	0.4068(6)	-0.1681(2)	0.7076(3)	0.109
H(9)	4a	0.4663(6)	-0.0692(2)	0.8094(3)	0.085(1)
H(10)	4a	0.2850(6)	0.1725(2)	0.4464(2)	0.093(2)
H(11)	4a	0.5003(6)	0.1755(2)	0.3824(2)	0.093(2)
H(12)	4a	0.4087(6)	0.0982(2)	0.4192(2)	0.093
H(13)	4a	0.7648(5)	0.0715(2)	0.5101(3)	0.117(2)
H(14)	4a	0.8540(5)	0.1488(2)	0.4720(3)	0.117
H(15)	4a	0.8524(5)	0.1308(2)	0.5868(3)	0.117
H(16)	4a	0.5690(5)	0.2088(2)	0.5475(2)	0.073(1)
H(17)	4a	-0.2130(7)	0.1377(3)	0.7891(4)	0.201(3)
H(18)	4a	-0.1129(7)	0.0977(3)	0.8831(4)	0.201
H(19)	4a	-0.2129(7)	0.1783(3)	0.8931(4)	0.201
H(20)	4a	0.3237(7)	0.2382(2)	0.8870(2)	0.103(2)
H(21)	4a	0.1170(7)	0.2371(2)	0.9567(2)	0.103
H(22)	4a	0.2734(7)	0.1674(2)	0.9526(2)	0.103
H(23)	4a	0.0413(6)	0.2127(2)	0.7929(3)	0.112(2)
H(3)	4a	0.7750(6)	-0.1139(2)	0.7281(3)	0.138(2)
H(4)	4a	0.7405(6)	-0.0554(2)	0.6419(3)	0.138
H(5)	4a	0.8017(6)	-0.0281(2)	0.7499(3)	0.138

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
O(1)	4a	0.2655(5)	0.0341(1)	0.8786(1)	0.125(2)	0.094(2)	0.056(1)	−0.015(2)	0.017(2)	0.002(1)
O(2)	4a	0.3247(4)	0.2360(1)	0.6821(2)	0.096(2)	0.055(1)	0.084(1)	0.008(1)	0.001(1)	−0.011(1)
N(1)	4a	0.3926(5)	0.0158(1)	0.7197(2)	0.082(2)	0.054(1)	0.053(1)	0.006(1)	0.004(1)	0.001(1)
N(2)	4a	0.4306(4)	0.1224(1)	0.6175(2)	0.069(2)	0.047(1)	0.057(1)	0.001(1)	0.008(1)	−0.003(1)
N(3)	4a	0.2161(4)	0.1271(1)	0.7611(2)	0.057(1)	0.059(1)	0.061(1)	−0.000(1)	0.009(1)	−0.017(1)
C(3)	4a	0.3742(5)	0.0436(1)	0.6177(2)	0.067(2)	0.050(2)	0.050(1)	0.005(1)	0.004(1)	−0.005(1)
C(2)	4a	0.3253(5)	0.1670(2)	0.6849(2)	0.056(2)	0.056(2)	0.061(2)	0.004(1)	−0.005(2)	−0.010(1)
C(1)	4a	0.2909(5)	0.0565(2)	0.7930(2)	0.069(2)	0.066(2)	0.055(1)	−0.013(2)	0.001(2)	−0.007(1)
C(4)	4a	0.0772(6)	0.1715(2)	0.8317(3)	0.067(2)	0.108(3)	0.104(3)	−0.003(2)	0.022(2)	−0.056(2)
C(5)	4a	0.2096(7)	0.2078(2)	0.9140(2)	0.100(3)	0.087(2)	0.070(2)	−0.007(2)	0.016(2)	−0.028(2)
C(6)	4a	−0.1327(7)	0.1450(3)	0.8502(4)	0.074(3)	0.249(6)	0.180(5)	−0.004(4)	0.025(3)	−0.130(5)
C(7)	4a	0.4822(6)	−0.0595(2)	0.7395(3)	0.083(2)	0.060(2)	0.069(2)	0.009(2)	−0.004(2)	0.012(2)
C(8)	4a	0.3504(6)	−0.1199(2)	0.6882(3)	0.106(3)	0.057(2)	0.109(3)	0.008(2)	0.008(3)	−0.001(2)
C(9)	4a	0.7215(6)	−0.0648(2)	0.7121(3)	0.076(2)	0.106(3)	0.164(4)	0.020(2)	−0.009(3)	0.026(3)
C(10)	4a	0.5521(5)	0.1564(2)	0.5327(2)	0.060(2)	0.056(2)	0.065(2)	−0.009(1)	0.004(2)	0.004(1)
C(11)	4a	0.7805(5)	0.1242(2)	0.5239(3)	0.063(2)	0.134(3)	0.097(3)	0.001(2)	0.011(2)	0.026(3)
C(12)	4a	0.4243(6)	0.1509(2)	0.4363(2)	0.081(2)	0.082(2)	0.069(2)	−0.010(2)	−0.006(2)	0.016(2)

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