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Crystal structure of 3-nitroquinoline 1-oxide, $C_9H_6N_2O_3$

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Abstract

$C_9H_6N_2O_3$, monoclinic, $P2_1/n$ (no. 14), $a = 8.7156(3)$ Å, $b = 9.4003(3)$ Å, $c = 19.8188(7)$ Å, $V = 1610.12(10)$ Å³, $Z = 8$, $R_{gt}(F) = 0.0491$, $wR_{ref}(F^2) = 0.1347$, $T = 291(2)$ K.

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The asymmetric unit, containing two independent molecules, of the title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was prepared according to the reported method [4]. The compound was crystallized by slow

Table 1: Data collection and handling.

Crystal:	Yellow needle
Size:	$0.20 \times 0.17 \times 0.16$ mm
Wavelength:	Cu $K\alpha$ radiation (1.54184 Å)
μ :	1.03 mm^{-1}
Diffractometer, scan mode:	Xcalibur, ω
$\theta_{\max}$, completeness:	67.1° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	6132, 2882, 0.022
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2376
$N(\text{param})_{\text{refined}}$:	253
Programs:	CrysAlis ^{PRO} [1], Olex2 [2], SHELX [3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.4429(2)	0.1239(2)	0.58047(9)	0.0565(5)
O2	0.3112(2)	0.3027(2)	0.61027(9)	0.0646(5)
O3	−0.0138(2)	0.4577(2)	0.40873(9)	0.0611(5)
N1	0.3450(2)	0.2179(2)	0.56810(10)	0.0453(5)
N2	0.0891(2)	0.3590(2)	0.42195(10)	0.0422(4)
C1	0.2806(3)	0.0869(3)	0.32617(12)	0.0473(6)
H1	0.3524	0.0136	0.3338	0.057*
C2	0.2131(3)	0.1152(3)	0.26172(12)	0.0518(6)
H2	0.2406	0.0622	0.2255	0.062*
C3	0.1030(3)	0.2230(3)	0.24952(12)	0.0548(6)
H3	0.0574	0.2403	0.2052	0.066*
C4	0.0609(3)	0.3038(3)	0.30174(12)	0.0491(6)
H4	−0.0126	0.3754	0.2932	0.059*
C5	0.1305(3)	0.2765(2)	0.36809(11)	0.0394(5)
C6	0.2423(3)	0.1679(2)	0.38138(11)	0.0385(5)
C7	0.3135(3)	0.1466(2)	0.44879(11)	0.0400(5)
H7	0.3885	0.0767	0.4590	0.048*
C8	0.2689(3)	0.2314(2)	0.49809(11)	0.0390(5)
C9	0.1560(3)	0.3364(2)	0.48570(12)	0.0424(5)
H9	0.1275	0.3904	0.5214	0.051*
O1'	0.6543(2)	0.4153(2)	0.57929(9)	0.0617(5)
O2'	0.8159(3)	0.2475(2)	0.61189(9)	0.0747(6)
O3'	0.8993(2)	−0.0126(2)	0.41109(10)	0.0613(5)
N1'	0.7366(2)	0.3145(2)	0.56788(10)	0.0498(5)
N2'	0.8196(2)	0.0991(2)	0.42249(10)	0.0447(5)
C1'	0.5633(3)	0.3579(3)	0.32214(13)	0.0526(6)
H1'	0.5103	0.4419	0.3282	0.063*
C2'	0.5592(3)	0.3020(3)	0.25883(13)	0.0573(7)
H2'	0.5039	0.3481	0.2219	0.069*
C3'	0.6379(3)	0.1751(3)	0.24884(13)	0.0585(7)
H3'	0.6321	0.1364	0.2054	0.070*
C4'	0.7231(3)	0.1075(3)	0.30230(13)	0.0531(6)

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H4'	0.7763	0.0241	0.2953	0.064*
C5'	0.7292(3)	0.1654(2)	0.36770(12)	0.0424(5)
C6'	0.6472(3)	0.2901(2)	0.37913(12)	0.0416(5)
C7'	0.6491(3)	0.3421(2)	0.44592(12)	0.0439(5)
H7'	0.5939	0.4231	0.4549	0.053*
C8'	0.7350(3)	0.2689(2)	0.49686(11)	0.0405(5)
C9'	0.8225(3)	0.1493(2)	0.48569(11)	0.0424(5)
H9'	0.8824	0.1048	0.5219	0.051*

evaporation from a mixture solution of CH₂Cl₂ and hexane at room temperature.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

Nitro compounds are important and useful precursors for preparing dyes, plastics, explosives and pharmaceuticals [5–8]. The activating effect of the nitro group is exploited in many organic reactions, and its facile transformation into various functional groups has broadened the importance of nitro compounds in the synthesis of complicate and high valuable molecules [9, 10].

Furthermore, nitrones are important synthons in the organic synthesis [11]. The asymmetric unit of the title structure contains two crystallographically independent but chemically identical molecules (*cf.* the figure). All bond lengths are in normal ranges [12]. The quinoline ring in the structure is planar and the O1, O2 and O3 (O1', O2', O3') atoms are almost in the plane.

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