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6-Nitroquinolin-2(1*H*)-one

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.004 Å
R factor = 0.055
wR factor = 0.149
Data-to-parameter ratio = 10.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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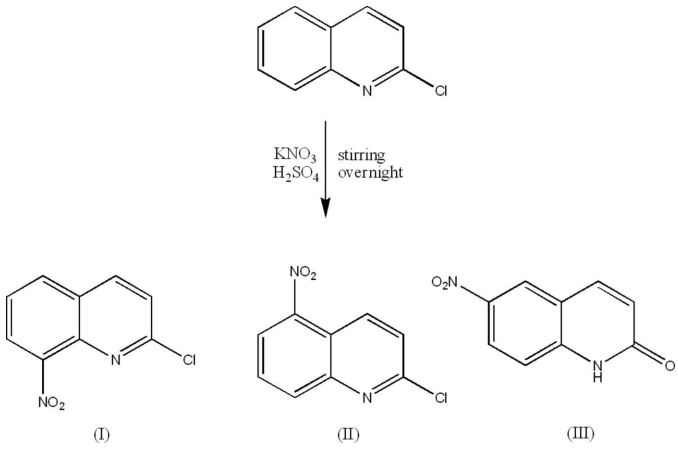
The title compound, $C_9H_6N_2O_3$, is nearly planar, with maximum deviations from the mean plane of −0.024 (3) Å for the C atom *para* to the ring N atom and 0.048 (2) Å for one of the nitro O atoms. Three C—H···O and one N—H···O intermolecular hydrogen bonds stabilize the crystal structure.

Comment

As part of our ongoing studies on quinoline derivatives as fluorophores, we attempted to prepare, by treatment of 2-chloroquinoline with potassium nitrate and sulfuric acid, the corresponding nitroquinoline derivatives (I) and (II) (Kimber *et al.*, 2003). However, analytical data from the reaction mixture indicated, besides (I) and (II) as the main products, the presence of another compound whose structure could not be resolved unequivocally by spectroscopic methods. This minor product is the title compound, (III); in order to identify the structure of (III), and hence to help in clarifying the reaction mechanism, its crystal structure was determined by X-ray diffraction.



Four intermolecular hydrogen bonds, *viz*. one N—H···O and three C—H···O, form a three-dimensional network (Fig. 2). Details of the hydrogen-bonding geometry are given in Table 1. The title compound is nearly planar, with maximum deviations from the mean plane of −0.024 (3) Å for C3 and 0.048 (2) Å for O2.

Experimental

The title compound, (III), was obtained as a minor product from a mixture of 2-chloroquinoline, potassium nitrate and sulfuric acid, according to the literature procedure of Kimber *et al.* (2003). Crystals suitable for X-ray data collection were obtained by recrystallization from dichloromethane–hexane (1:1).

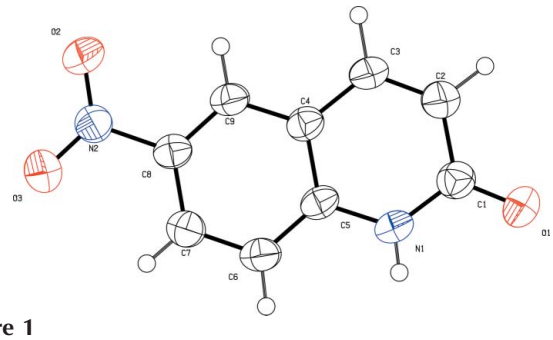


Figure 1
The molecular structure of (III), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level.

Crystal data

$C_9H_6N_2O_3$
M_r = 190.16
Monoclinic, $P2_1/c$
a = 11.470 (2) Å
b = 4.8880 (6) Å
c = 15.065 (2) Å
β = 99.53 (1)°
V = 833.0 (2) Å^3
Z = 4
D_x = 1.516 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 6.6–26.7°
μ = 1.00 mm^{-1}
T = 299 (2) K
Prism, orange
0.18 × 0.10 × 0.05 mm

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
1941 measured reflections
1504 independent reflections
892 reflections with $I > 2\sigma(I)$
R_{int} = 0.069
θ_{max} = 68.0°
$h = -13 \rightarrow 13$
$k = 0 \rightarrow 5$
$l = -18 \rightarrow 18$
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.149
S = 1.01
1504 reflections
146 parameters
Only H-atom coordinates refined
$w = 1/[\sigma^2(F_o^2) + (0.0734P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0053 (11)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2^{i}	1.04 (3)	2.48 (3)	3.377 (4)	145 (2)
C3—H3···O3^{ii}	1.04 (3)	2.50 (3)	3.230 (4)	127 (2)
C9—H9···O2^{i}	0.95 (3)	2.53 (3)	3.371 (4)	147 (2)
N1—H1*N*···O1^{iii}	0.83 (3)	1.97 (3)	2.794 (3)	175 (3)

Symmetry codes: (i) $-x+2, -y, -z+1$; (ii) $x, -y-\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x+1, -y-2, -z+1$.

The H atoms were located in a difference map and refined with U_{iso}(H) = 1.2U_{eq}(parent atom).

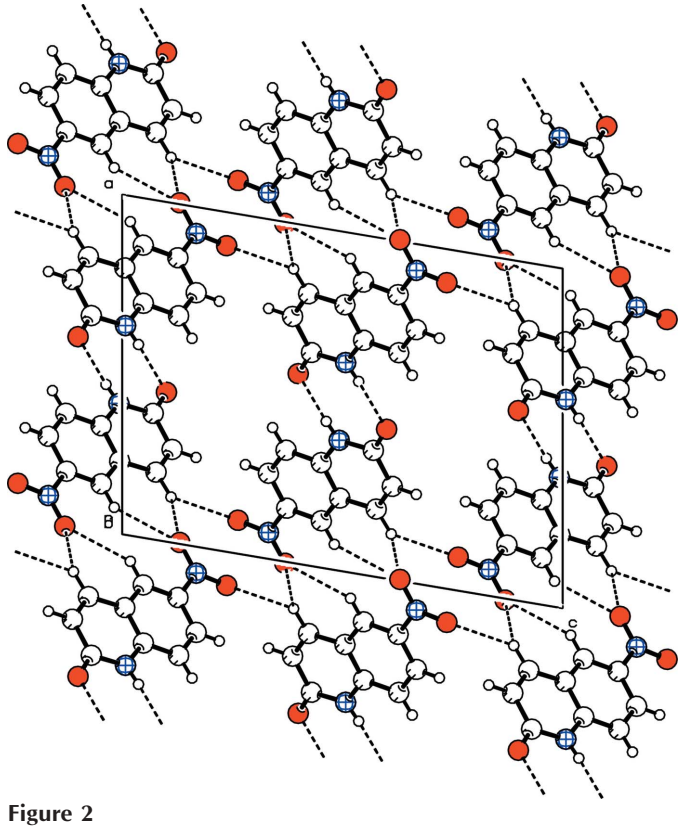


Figure 2
The molecular packing of (III), with hydrogen bonds shown as dashed lines.

Data collection: *CAD-4/PC Software* (Nonius, 1996); cell refinement: *CAD-4/PC Software*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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References

Kimber, M. C., Geue, J. P., Lincoln, S. F., Ward, A. D. & Tiekink, E. R. T. (2003). *Aust. J. Chem.* **56**, 39–44.
Nonius (1996). *CAD-4/PC Software*. Version 2.0. Nonius GmbH, Solingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (1987). *REDU4*. Version 6.2c. Stoe & Cie GmbH, Darmstadt, Germany.