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Acetone 2-nitrophenylhydrazone

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean *σ*(C–C) = 0.002 Å
R factor = 0.054
wR factor = 0.153
Data-to-parameter ratio = 16.3

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

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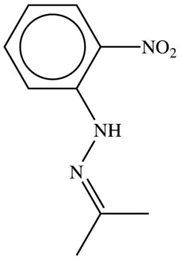
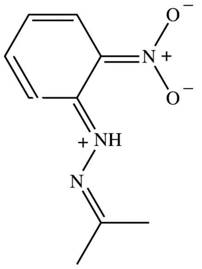
There are no direction-specific interactions between the almost-planar molecules of the title compound, $C_9H_{11}N_3O_2$.

Comment

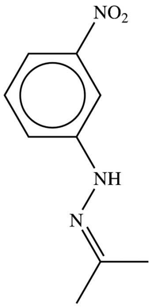
We report here the structure of acetone 2-nitrophenylhydrazone, (I) (Fig. 1), whose behaviour differs significantly from that of the isomeric compound acetone 3-nitrophenylhydrazone, (II) (Wardell *et al.*, 2006).



(I)



(Ia)



(II)

The non-H atoms in the molecule of (I) are virtually co-planar, as shown by the key torsion angles (Table 1). There is a short intermolecular N—H···O hydrogen bond (Table 2), which may assist in controlling the planar conformation. The bond distances (Table 1) show evidence for a significant contribution from the quinonoid form (I*a*). In particular, the bonds C3—C4 and C5—C6 are shorter than the remaining bonds in the ring, while C2—N21 is very short for its type and the N—O bonds are long (Allen *et al.*, 1987). In contrast, the bond distances in (II) show no unusual values (Wardell *et al.*, 2006).

Whereas the molecules of (II) are linked into complex sheets by a combination of N—H···O, C—H···O and C—H···N hydrogen bonds, there are no direction-specific intermolecular interactions in the structure of (I). In particular, hydrogen bonds of all types and aromatic *π*–*π* stacking interactions are absent.

Experimental

2-Nitrophenylhydrazine (3 mmol) was dissolved in acetone (30 ml) and the solution was heated under reflux for 1 h. The solution was then cooled and excess solvent was removed under reduced pressure. The resulting solid product, (I), was crystallized from ethanol (m.p. 339–341 K).

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Crystal data

$C_9H_{11}N_3O_2$
$M_r = 193.21$
Monoclinic, $P2_1/c$
$a = 3.8451\ (2)$ Å
$b = 11.4926\ (8)$ Å
$c = 21.3214\ (13)$ Å
$\beta = 92.208\ (4)°$
$V = 941.50\ (10)$ Å^3
$Z = 4$
$D_x = 1.363$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 120\ (2)$ K
Needle, orange
0.40 × 0.04 × 0.04 mm

Data collection

Bruker Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.971$, $T_{max} = 0.996$
10829 measured reflections
2104 independent reflections
1738 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 27.8°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.153$
$S = 1.06$
2104 reflections
129 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0854P)^2 + 0.2667P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.417 (2)	C1—N1	1.3637 (17)
C2—C3	1.4027 (19)	N1—N2	1.3799 (17)
C3—C4	1.370 (2)	N2—C7	1.2877 (18)
C4—C5	1.398 (2)	C2—N21	1.4387 (18)
C5—C6	1.3772 (19)	N21—O21	1.2513 (16)
C6—C1	1.4100 (19)	N21—O22	1.2267 (17)
C1—C2—N21—O21	−0.3 (2)	C1—N1—N2—C7	175.80 (12)
C1—C2—N21—O22	178.88 (13)	N1—N2—C7—C8	179.80 (12)
C2—C1—N1—N2	−175.52 (12)	N1—N2—C7—C9	0.2 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O21	0.88	1.97	2.6010 (17)	128

All H atoms were located in a difference map and then treated as riding, with C—H distances of 0.95 or 0.98 Å and N—H distances of 0.88 Å, and with $U_{iso}(H) = kU_{eq}(C,N)$ where $k = 1.5$ for methyl groups and 1.2 for all other H.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *FLIPPER* (Oszlányi & Sütő, 2004, 2005; Spek, 2003); program(s) used to refine structure: *OSCAIL* (McArdle, 2003) and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

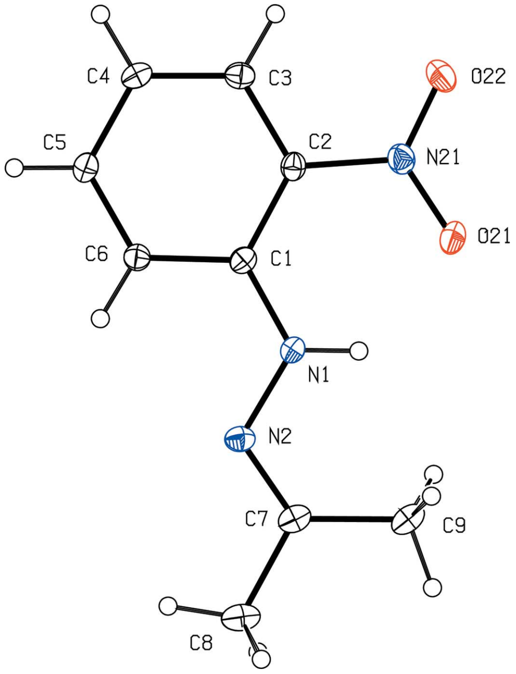

Figure 1
The molecular structure of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

The X-ray data were collected at the EPSRC X-Ray Crystallographic Service, University of Southampton, UK; the authors thank the staff of the Service for all their help and advice. JLW thanks CNPq and FAPERJ for financial support.

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