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1-(2,4-Dinitrophenyl)-2-(propan-2-ylidene)hydrazine

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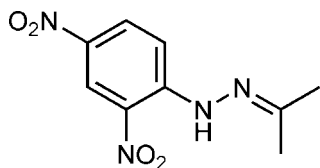
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.058; wR factor = 0.141; data-to-parameter ratio = 12.2.

The asymmetric unit of the title compound, $\text{C}_9\text{H}_{10}\text{N}_4\text{O}_4$, consists of two crystallographically independent molecules, which are held together by $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds. Each molecule is essentially planar.

Related literature

For related literature, see: Saraçoğlu *et al.* (2004).

Experimental

Crystal data

 $\text{C}_9\text{H}_{10}\text{N}_4\text{O}_4$ $M_r = 238.21$ Monoclinic, $P2_1/n$ $a = 5.3299$ (11) Å $b = 11.189$ (2) Å $c = 37.172$ (7) Å $\beta = 93.31$ (3)° $V = 2213.1$ (7) Å³ $Z = 8$ Mo $K\alpha$ radiation $\mu = 0.12$ mm⁻¹ $T = 293$ (2) K

0.12 × 0.10 × 0.08 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan
(*CrystalClear*; Rigaku, 2004)
 $T_{\min} = 0.986$, $T_{\max} = 0.991$ 12591 measured reflections
3859 independent reflections
2695 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.045$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.058$ $wR(F^2) = 0.141$ $S = 1.12$

3859 reflections

317 parameters

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\max} = 0.13$ e Å⁻³ $\Delta\rho_{\min} = -0.14$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C2}-\text{H2}\cdots\text{O1}^i$	0.93	2.42	3.300 (3)	157
$\text{C8}-\text{H8B}\cdots\text{O2}^{ii}$	0.96	2.58	3.506 (3)	163
$\text{C18}-\text{H18C}\cdots\text{O3}^{iii}$	0.96	2.56	3.389 (4)	144
$\text{C10}-\text{H10}\cdots\text{O5}^{iv}$	0.93	2.46	3.295 (4)	150

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

Data collection: *CrystalClear* (Rigaku, 2004); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2160).

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supplementary materials

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1-(2,4-Dinitrophenyl)-2-(propan-2-ylidene)hydrazine

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Comment

Schiff base and its complexes are widely used in the fields of biology, catalysis and material. In this paper, the structure of the title compound, (I), is reported. The asymmetric unit of (I) consists of two independent molecules (Fig. 1). The bond lengths and angles agree with those in the compound 3-[(2,4-dinitrophenyl)hydrazono]butan-2-one oxime (Saracoglu *et al.*, 2004). The all non-H atoms of each independent molecule are essentially coplanar, within 0.052 (2) and 0.055 (3) Å. The dihedral angle between two independent molecules is 76.4 (2)°. The crystal structure is stabilized by C—H···O hydrogen bonds (Fig. 2 and Table 1).

Experimental

1-(2,4-Dinitrophenyl)hydrazine (10 mmol) in propanone (20 ml) was refluxed for 2 h. After cooling, the solution was kept at room temperature for 10 d. Natural evaporation gave yellow single crystals of (I) suitable for X-ray analysis.

Refinement

N-bound H atoms were located in a difference map and their positional parameters were refined, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$. Other H atoms were positioned geometrically (C—H = 0.93 Å or 0.96 Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$.

Figures

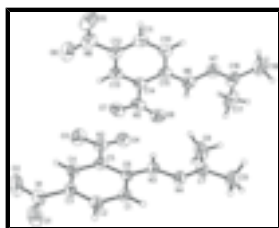


Fig. 1. The asymmetric unit of (I), drawn with 30% probability ellipsoids.

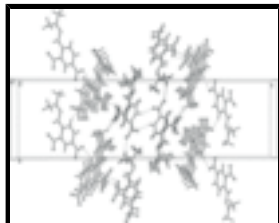


Fig. 2. A packing view of (I) along the *a* axis. Hydrogen bonds are indicated by dashed lines.

1-(2,4-Dinitrophenyl)-2-(propan-2-ylidene)hydrazine

Crystal data

$C_9H_{10}N_4O_4$	$F_{000} = 992$
$M_r = 238.21$	$D_x = 1.430 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
Hall symbol: -P 2yn	$\lambda = 0.71073 \text{ \AA}$
$a = 5.3299 (11) \text{ \AA}$	Cell parameters from 2238 reflections
$b = 11.189 (2) \text{ \AA}$	$\theta = 2.3\text{--}22.5^\circ$
$c = 37.172 (7) \text{ \AA}$	$\mu = 0.12 \text{ mm}^{-1}$
$\beta = 93.31 (3)^\circ$	$T = 293 (2) \text{ K}$
$V = 2213.1 (7) \text{ \AA}^3$	Block, yellow
$Z = 8$	$0.12 \times 0.10 \times 0.08 \text{ mm}$

Data collection

Rigaku Saturn diffractometer	$R_{\text{int}} = 0.045$
Radiation source: rotating anode	$\theta_{\text{max}} = 25.0^\circ$
Monochromator: confocal	$\theta_{\text{min}} = 1.9^\circ$
$T = 293(2) \text{ K}$	$h = -6 \rightarrow 2$
ω scans	$k = -12 \rightarrow 13$
Absorption correction: multi-scan (CrystalClear; Rigaku, 2004)	$l = -44 \rightarrow 44$
$T_{\text{min}} = 0.986$, $T_{\text{max}} = 0.991$	Standard reflections: .;
12591 measured reflections	every . reflections
3859 independent reflections	intensity decay: .
2695 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.058$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.141$	$w = 1/[\sigma^2(F_o^2) + (0.0628P)^2 + 0.0593P]$
$S = 1.12$	where $P = (F_o^2 + 2F_c^2)/3$
3859 reflections	$(\Delta/\sigma)_{\text{max}} = 0.002$
317 parameters	$\Delta\rho_{\text{max}} = 0.13 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.14 \text{ e \AA}^{-3}$
	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	−0.4124 (4)	1.13689 (16)	0.02987 (6)	0.0944 (7)
O2	−0.1589 (4)	1.22257 (15)	0.06903 (7)	0.1047 (8)
O3	0.5342 (4)	1.01915 (16)	0.12217 (6)	0.0882 (6)
O4	0.6236 (3)	0.83732 (16)	0.10960 (5)	0.0700 (5)
O5	0.2146 (4)	0.8646 (2)	0.25369 (7)	0.1055 (8)
O6	0.4578 (5)	0.9955 (2)	0.23075 (7)	0.1078 (8)
O7	1.1155 (3)	0.87148 (18)	0.15955 (5)	0.0847 (6)
O8	1.1459 (4)	0.6908 (2)	0.14115 (6)	0.0903 (6)
N1	−0.2260 (4)	1.13669 (17)	0.05044 (7)	0.0701 (6)
N2	0.4892 (4)	0.9265 (2)	0.10567 (5)	0.0607 (5)
N3	0.3397 (4)	0.71717 (16)	0.06354 (6)	0.0576 (5)
H3	0.454 (5)	0.714 (2)	0.0802 (7)	0.069*
N4	0.2541 (4)	0.61533 (16)	0.04575 (6)	0.0608 (5)
N5	1.0493 (4)	0.7669 (2)	0.15980 (6)	0.0687 (6)
N6	0.9126 (4)	0.5189 (2)	0.17335 (6)	0.0684 (6)
H6	1.040 (5)	0.542 (2)	0.1593 (8)	0.082*
N7	0.8486 (4)	0.4022 (2)	0.18100 (6)	0.0741 (6)
N8	0.3933 (5)	0.8921 (3)	0.23606 (7)	0.0825 (7)
C1	−0.0081 (4)	0.82699 (19)	0.03643 (6)	0.0546 (6)
H1	−0.0556	0.7608	0.0225	0.066*
C2	−0.1472 (4)	0.92925 (19)	0.03302 (6)	0.0560 (6)
H2	−0.2880	0.9325	0.0171	0.067*
C3	−0.0761 (4)	1.02841 (18)	0.05361 (6)	0.0528 (6)
C4	0.1303 (4)	1.02565 (18)	0.07705 (6)	0.0544 (6)
H4	0.1754	1.0929	0.0906	0.065*
C5	0.2725 (4)	0.92244 (19)	0.08053 (6)	0.0500 (5)
C6	0.2055 (4)	0.81925 (17)	0.06047 (6)	0.0471 (5)
C7	0.3855 (5)	0.5209 (2)	0.05221 (7)	0.0650 (7)
C8	0.6148 (6)	0.5150 (2)	0.07713 (10)	0.0907 (10)
H8A	0.7477	0.5599	0.0672	0.136*
H8B	0.6660	0.4332	0.0802	0.136*
H8C	0.5782	0.5481	0.1001	0.136*
C9	0.2987 (6)	0.4098 (2)	0.03317 (9)	0.0887 (9)

supplementary materials

H9A	0.1543	0.4274	0.0174	0.133*
H9B	0.2550	0.3509	0.0505	0.133*
H9C	0.4311	0.3794	0.0193	0.133*
C10	0.5939 (4)	0.5876 (2)	0.21139 (6)	0.0623 (6)
H10	0.5500	0.5089	0.2161	0.075*
C11	0.4674 (5)	0.6777 (2)	0.22648 (7)	0.0654 (7)
H11	0.3361	0.6608	0.2411	0.078*
C12	0.5341 (5)	0.7961 (2)	0.22007 (7)	0.0632 (7)
C13	0.7241 (5)	0.8237 (2)	0.19851 (7)	0.0623 (6)
H13	0.7669	0.9029	0.1945	0.075*
C14	0.8516 (4)	0.7320 (2)	0.18281 (6)	0.0570 (6)
C15	0.7918 (4)	0.6108 (2)	0.18860 (6)	0.0574 (6)
C16	0.9862 (6)	0.3210 (3)	0.16758 (8)	0.0804 (8)
C17	1.2042 (6)	0.3440 (3)	0.14543 (11)	0.1074 (11)
H17A	1.1481	0.3845	0.1237	0.161*
H17B	1.2807	0.2694	0.1395	0.161*
H17C	1.3247	0.3929	0.1588	0.161*
C18	0.9177 (7)	0.1943 (3)	0.17554 (10)	0.1160 (13)
H18A	0.7805	0.1933	0.1912	0.174*
H18B	1.0600	0.1544	0.1871	0.174*
H18C	0.8688	0.1539	0.1535	0.174*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0796 (13)	0.0767 (12)	0.1238 (19)	0.0243 (11)	-0.0213 (13)	0.0016 (11)
O2	0.1113 (17)	0.0509 (10)	0.149 (2)	0.0149 (11)	-0.0200 (15)	-0.0195 (12)
O3	0.0856 (14)	0.0816 (12)	0.0942 (15)	-0.0194 (11)	-0.0227 (11)	-0.0216 (11)
O4	0.0554 (10)	0.0801 (11)	0.0729 (12)	0.0017 (10)	-0.0110 (9)	0.0050 (9)
O5	0.0700 (13)	0.1395 (19)	0.1079 (18)	0.0167 (13)	0.0133 (13)	-0.0320 (14)
O6	0.1090 (18)	0.0868 (14)	0.126 (2)	0.0116 (14)	-0.0036 (15)	-0.0260 (13)
O7	0.0706 (12)	0.0946 (14)	0.0878 (15)	-0.0246 (11)	-0.0041 (10)	0.0233 (10)
O8	0.0825 (14)	0.1085 (15)	0.0831 (14)	-0.0009 (12)	0.0310 (12)	0.0047 (12)
N1	0.0724 (15)	0.0512 (12)	0.0870 (17)	0.0066 (12)	0.0063 (13)	0.0055 (11)
N2	0.0562 (12)	0.0684 (13)	0.0569 (13)	-0.0116 (11)	-0.0025 (10)	0.0010 (10)
N3	0.0564 (12)	0.0536 (11)	0.0619 (13)	0.0030 (10)	-0.0049 (10)	-0.0037 (9)
N4	0.0633 (12)	0.0512 (11)	0.0676 (13)	0.0065 (10)	-0.0003 (10)	-0.0070 (9)
N5	0.0534 (13)	0.0928 (17)	0.0587 (14)	-0.0061 (13)	-0.0066 (11)	0.0164 (12)
N6	0.0619 (13)	0.0757 (15)	0.0683 (15)	-0.0008 (12)	0.0087 (12)	-0.0036 (11)
N7	0.0750 (15)	0.0729 (14)	0.0737 (15)	-0.0054 (13)	-0.0025 (12)	-0.0067 (11)
N8	0.0667 (16)	0.0973 (19)	0.0817 (18)	0.0129 (15)	-0.0112 (14)	-0.0193 (14)
C1	0.0563 (14)	0.0525 (13)	0.0545 (15)	-0.0010 (11)	-0.0007 (12)	-0.0064 (10)
C2	0.0542 (13)	0.0579 (13)	0.0549 (15)	0.0044 (12)	-0.0044 (11)	0.0028 (11)
C3	0.0548 (14)	0.0451 (12)	0.0588 (15)	0.0009 (11)	0.0069 (12)	0.0020 (10)
C4	0.0578 (14)	0.0474 (12)	0.0583 (15)	-0.0089 (11)	0.0057 (12)	-0.0054 (10)
C5	0.0484 (12)	0.0550 (12)	0.0462 (13)	-0.0073 (11)	-0.0007 (10)	0.0033 (10)
C6	0.0485 (12)	0.0447 (11)	0.0482 (13)	0.0011 (10)	0.0043 (11)	0.0026 (9)
C7	0.0633 (15)	0.0540 (13)	0.0782 (19)	0.0081 (13)	0.0086 (14)	0.0018 (12)

C8	0.0768 (19)	0.0681 (16)	0.125 (3)	0.0201 (15)	-0.0160 (19)	0.0074 (16)
C9	0.100 (2)	0.0564 (15)	0.109 (2)	0.0165 (15)	-0.0041 (19)	-0.0122 (14)
C10	0.0558 (14)	0.0724 (15)	0.0586 (16)	-0.0039 (13)	0.0015 (13)	0.0065 (12)
C11	0.0506 (14)	0.0881 (18)	0.0574 (16)	-0.0004 (14)	0.0026 (12)	0.0031 (13)
C12	0.0521 (14)	0.0794 (17)	0.0565 (16)	0.0102 (14)	-0.0117 (13)	-0.0060 (12)
C13	0.0558 (14)	0.0701 (15)	0.0592 (16)	-0.0011 (13)	-0.0121 (13)	0.0039 (12)
C14	0.0451 (12)	0.0772 (16)	0.0480 (14)	-0.0041 (13)	-0.0031 (11)	0.0083 (11)
C15	0.0482 (13)	0.0760 (16)	0.0471 (14)	-0.0033 (13)	-0.0053 (11)	0.0019 (11)
C16	0.081 (2)	0.0822 (19)	0.075 (2)	-0.0002 (17)	-0.0193 (16)	-0.0245 (15)
C17	0.082 (2)	0.115 (2)	0.127 (3)	-0.0005 (19)	0.014 (2)	-0.047 (2)
C18	0.147 (3)	0.080 (2)	0.118 (3)	-0.008 (2)	-0.017 (3)	-0.0247 (18)

Geometric parameters (Å, °)

O1—N1	1.218 (3)	C4—H4	0.9300
O2—N1	1.225 (3)	C5—C6	1.409 (3)
O3—N2	1.221 (2)	C7—C9	1.491 (4)
O4—N2	1.232 (2)	C7—C8	1.492 (4)
O5—N8	1.226 (3)	C8—H8A	0.9600
O6—N8	1.226 (3)	C8—H8B	0.9600
O7—N5	1.222 (3)	C8—H8C	0.9600
O8—N5	1.230 (3)	C9—H9A	0.9600
N1—C3	1.452 (3)	C9—H9B	0.9600
N2—C5	1.444 (3)	C9—H9C	0.9600
N3—C6	1.349 (3)	C10—C11	1.353 (3)
N3—N4	1.382 (3)	C10—C15	1.414 (3)
N3—H3	0.84 (2)	C10—H10	0.9300
N4—C7	1.282 (3)	C11—C12	1.396 (3)
N5—C14	1.449 (3)	C11—H11	0.9300
N6—C15	1.355 (3)	C12—C13	1.362 (4)
N6—N7	1.383 (3)	C13—C14	1.378 (3)
N6—H6	0.92 (3)	C13—H13	0.9300
N7—C16	1.286 (3)	C14—C15	1.412 (3)
N8—C12	1.457 (3)	C16—C17	1.484 (5)
C1—C2	1.365 (3)	C16—C18	1.498 (4)
C1—C6	1.409 (3)	C17—H17A	0.9600
C1—H1	0.9300	C17—H17B	0.9600
C2—C3	1.388 (3)	C17—H17C	0.9600
C2—H2	0.9300	C18—H18A	0.9600
C3—C4	1.364 (3)	C18—H18B	0.9600
C4—C5	1.383 (3)	C18—H18C	0.9600
?...?	?		
O1—N1—O2	123.6 (2)	H8A—C8—H8B	109.5
O1—N1—C3	118.5 (2)	C7—C8—H8C	109.5
O2—N1—C3	117.9 (2)	H8A—C8—H8C	109.5
O3—N2—O4	122.1 (2)	H8B—C8—H8C	109.5
O3—N2—C5	118.6 (2)	C7—C9—H9A	109.5
O4—N2—C5	119.27 (19)	C7—C9—H9B	109.5
C6—N3—N4	119.9 (2)	H9A—C9—H9B	109.5

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C6—N3—H3	116.9 (16)	C7—C9—H9C	109.5
N4—N3—H3	121.5 (16)	H9A—C9—H9C	109.5
C7—N4—N3	115.3 (2)	H9B—C9—H9C	109.5
O7—N5—O8	121.9 (2)	C11—C10—C15	121.2 (2)
O7—N5—C14	118.9 (2)	C11—C10—H10	119.4
O8—N5—C14	119.2 (2)	C15—C10—H10	119.4
C15—N6—N7	120.1 (2)	C10—C11—C12	119.9 (2)
C15—N6—H6	114.1 (16)	C10—C11—H11	120.1
N7—N6—H6	125.7 (16)	C12—C11—H11	120.1
C16—N7—N6	115.7 (2)	C13—C12—C11	121.4 (2)
O6—N8—O5	123.8 (3)	C13—C12—N8	119.4 (3)
O6—N8—C12	118.3 (3)	C11—C12—N8	119.2 (3)
O5—N8—C12	117.9 (3)	C12—C13—C14	118.8 (2)
C2—C1—C6	121.7 (2)	C12—C13—H13	120.6
C2—C1—H1	119.2	C14—C13—H13	120.6
C6—C1—H1	119.2	C13—C14—C15	121.9 (2)
C1—C2—C3	119.3 (2)	C13—C14—N5	116.3 (2)
C1—C2—H2	120.3	C15—C14—N5	121.8 (2)
C3—C2—H2	120.3	N6—C15—C14	123.2 (2)
C4—C3—C2	121.2 (2)	N6—C15—C10	120.0 (2)
C4—C3—N1	119.4 (2)	C14—C15—C10	116.8 (2)
C2—C3—N1	119.4 (2)	N7—C16—C17	125.1 (3)
C3—C4—C5	119.7 (2)	N7—C16—C18	116.2 (3)
C3—C4—H4	120.1	C17—C16—C18	118.7 (3)
C5—C4—H4	120.1	C16—C17—H17A	109.5
C4—C5—C6	120.9 (2)	C16—C17—H17B	109.5
C4—C5—N2	116.6 (2)	H17A—C17—H17B	109.5
C6—C5—N2	122.5 (2)	C16—C17—H17C	109.5
N3—C6—C1	120.7 (2)	H17A—C17—H17C	109.5
N3—C6—C5	122.1 (2)	H17B—C17—H17C	109.5
C1—C6—C5	117.13 (19)	C16—C18—H18A	109.5
N4—C7—C9	116.6 (2)	C16—C18—H18B	109.5
N4—C7—C8	124.9 (2)	H18A—C18—H18B	109.5
C9—C7—C8	118.6 (2)	C16—C18—H18C	109.5
C7—C8—H8A	109.5	H18A—C18—H18C	109.5
C7—C8—H8B	109.5	H18B—C18—H18C	109.5
C6—N3—N4—C7	-175.5 (2)	N3—N4—C7—C8	0.6 (4)
C15—N6—N7—C16	-174.7 (2)	C15—C10—C11—C12	-1.0 (3)
C6—C1—C2—C3	0.3 (3)	C10—C11—C12—C13	0.6 (4)
C1—C2—C3—C4	0.2 (4)	C10—C11—C12—N8	179.0 (2)
C1—C2—C3—N1	-179.0 (2)	O6—N8—C12—C13	-3.0 (3)
O1—N1—C3—C4	-178.7 (2)	O5—N8—C12—C13	176.0 (2)
O2—N1—C3—C4	0.5 (3)	O6—N8—C12—C11	178.5 (2)
O1—N1—C3—C2	0.6 (3)	O5—N8—C12—C11	-2.4 (3)
O2—N1—C3—C2	179.8 (2)	C11—C12—C13—C14	0.1 (4)
C2—C3—C4—C5	0.0 (3)	N8—C12—C13—C14	-178.4 (2)
N1—C3—C4—C5	179.3 (2)	C12—C13—C14—C15	-0.3 (3)
C3—C4—C5—C6	-0.7 (3)	C12—C13—C14—N5	179.2 (2)
C3—C4—C5—N2	179.6 (2)	O7—N5—C14—C13	10.2 (3)

O3—N2—C5—C4	0.0 (3)	O8—N5—C14—C13	-170.0 (2)
O4—N2—C5—C4	-179.4 (2)	O7—N5—C14—C15	-170.3 (2)
O3—N2—C5—C6	-179.7 (2)	O8—N5—C14—C15	9.5 (3)
O4—N2—C5—C6	0.9 (3)	N7—N6—C15—C14	178.2 (2)
N4—N3—C6—C1	-6.5 (3)	N7—N6—C15—C10	-2.2 (3)
N4—N3—C6—C5	174.2 (2)	C13—C14—C15—N6	179.5 (2)
C2—C1—C6—N3	179.7 (2)	N5—C14—C15—N6	0.0 (3)
C2—C1—C6—C5	-1.0 (3)	C13—C14—C15—C10	0.0 (3)
C4—C5—C6—N3	-179.5 (2)	N5—C14—C15—C10	-179.5 (2)
N2—C5—C6—N3	0.2 (3)	C11—C10—C15—N6	-178.9 (2)
C4—C5—C6—C1	1.2 (3)	C11—C10—C15—C14	0.7 (3)
N2—C5—C6—C1	-179.12 (19)	N6—N7—C16—C17	0.7 (4)
N3—N4—C7—C9	-179.5 (2)	N6—N7—C16—C18	-179.7 (2)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C2—H2 \cdots O1 ⁱ	0.93	2.42	3.300 (3)	157
C8—H8B \cdots O2 ⁱⁱ	0.96	2.58	3.506 (3)	163
C18—H18C \cdots O3 ⁱⁱⁱ	0.96	2.56	3.389 (4)	144
C10—H10 \cdots O5 ^{iv}	0.93	2.46	3.295 (4)	150

Symmetry codes: (i) $-x-1, -y+2, -z$; (ii) $x+1, y-1, z$; (iii) $x, y-1, z$; (iv) $-x+1/2, y-1/2, -z+1/2$.

Fig. 1

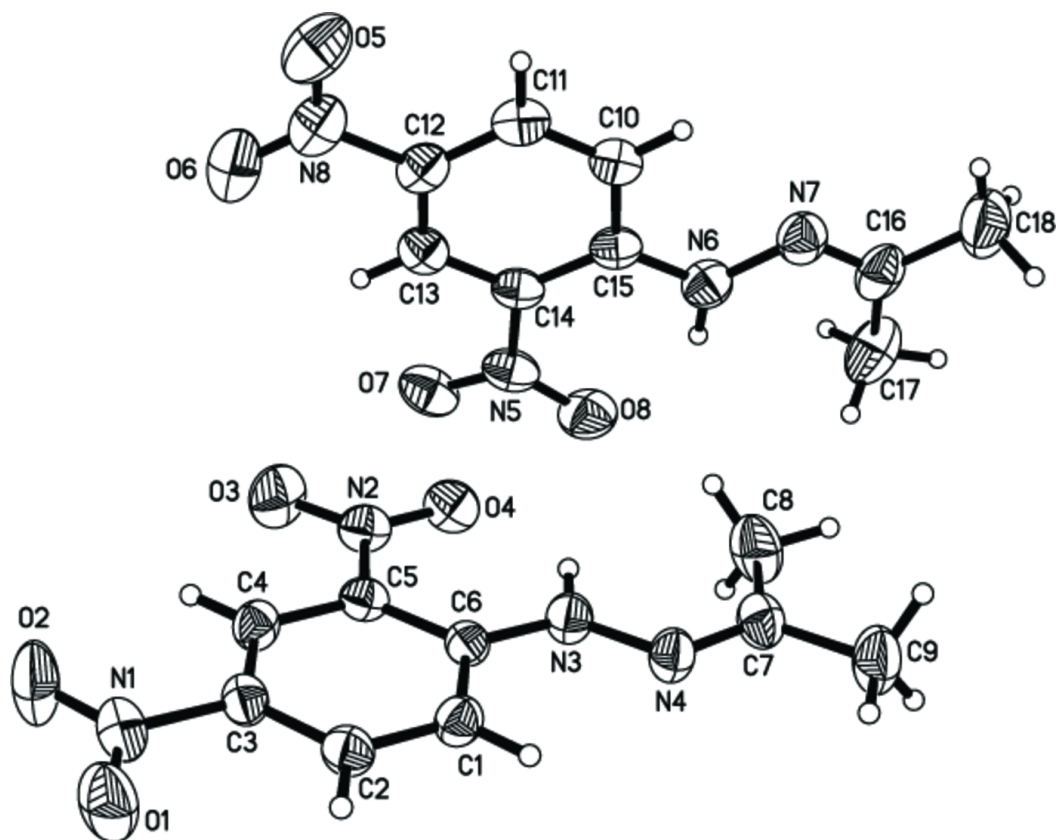


Fig. 2

