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Acetophenone propionylhydrazone

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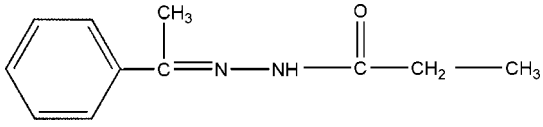
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.056; wR factor = 0.191; data-to-parameter ratio = 14.8.

In the crystal structure of the title compound, $C_{11}H_{14}N_2O$, there are two crystallographically independent molecules in the asymmetric unit, which are connected into dimers via N—H···O hydrogen bonding.



Experimental

Crystal data

$C_{11}H_{14}N_2O$
M_r = 190.24
Triclinic, $P\overline{1}$
a = 9.554 (7) Å
b = 10.007 (8) Å
c = 12.555 (9) Å
α = 76.603 (13)°
β = 68.836 (12)°
γ = 81.643 (13)°
V = 1086.4 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.22 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.983, T_{max} = 0.992
5630 measured reflections
3810 independent reflections
1798 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.191
S = 1.01
3810 reflections
258 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2^{i}	0.86	2.11	2.954 (3)	166
N4—H4···O1^{i}	0.86	2.10	2.937 (3)	166

Symmetry code: (i) $-x, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *SHELXTL/PC*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2042).

References

Bruker (1997). *SADABS*, *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1990). *SHELXTL/PC*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
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supplementary materials

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Acetophenone propionylhydrazone

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Comment

The structure determination of the title compound (I) was undertaken as a part of our project on the synthesis of new schiff base compounds. The crystal structure of the title compound consists of two crystallographically independent molecules of similar conformation. Both molecules are are connected into dimers *via* N—H···O hydrogen bonding between the amino and the carbonyl group. Bond lengths and angles of these hydrogen bonds shows, that this is a strong interaction.

Experimental

Acetophenone (0.1 mol)and propionylhydrazine (0.1 mol)were mixed in ethanol (30 ml) and were heated under reflux for 5 h. The mixture was transfered into water to afford a colourless solid if I, which were filtered off, washed with water and dried at room temperature. Single crystals of the title compound were obtained by recrystallization from EtOH at room temperature.

Refinement

C—H H atoms were positioned with idealized geometry and refined isotropic using a riding model with C—H distances of =0.93–0.97Å and U_{iso}=1.2–1.5U_{eq}(parent atom). The N—H H atoms were located in difference map, their bond lengths set to ideal values and afterwards they were refined using a riding model.

Figures

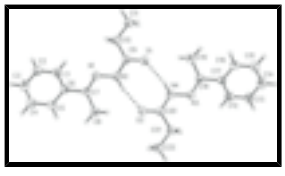


Fig. 1. The structure of the title compound showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Acetophenone propionylhydrazone

Crystal data

$C_{11}H_{14}N_2O$	$Z = 4$
$M_r = 190.24$	$F_{000} = 408$
Triclinic, $P\bar{1}$	$D_x = 1.163$ Mg m^{-3}
$a = 9.554$ (7) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 10.007$ (8) Å	Cell parameters from 1128 reflections
$c = 12.555$ (9) Å	$\theta = 2.3$–25.7º

$\alpha = 76.603\ (13)^{\circ}$	$\mu = 0.08\ mm^{-1}$
$\beta = 68.836\ (12)^{\circ}$	$T = 293\ (2)\ K$
$\gamma = 81.643\ (13)^{\circ}$	Block, colorless
$V = 1086.4\ (14)\ Å^3$	0.22 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3810 independent reflections
Radiation source: fine-focus sealed tube	1798 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.028$
$T = 293(2)$ K	$\theta_{max} = 25.0^{\circ}$
φ and ω scans	$\theta_{min} = 1.8^{\circ}$
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$h = -11 \rightarrow 10$
$T_{min} = 0.983$, $T_{max} = 0.992$	$k = -10 \rightarrow 11$
5630 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.057$	$w = 1/[\sigma^2(F_o^2) + (0.0791P)^2 + 0.1785P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.191$	$(\Delta/\sigma)_{max} = 0.002$
$S = 1.01$	$\Delta\rho_{max} = 0.18\ e\ Å^{-3}$
3810 reflections	$\Delta\rho_{min} = -0.13\ e\ Å^{-3}$
258 parameters	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.016 (3)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.1027 (3)	0.6056 (2)	0.53651 (18)	0.0901 (8)
O2	0.1040 (2)	0.1031 (2)	0.54184 (17)	0.0854 (7)
N1	0.1903 (2)	0.6784 (2)	0.2353 (2)	0.0581 (6)
N2	0.1246 (3)	0.6901 (2)	0.3508 (2)	0.0648 (7)
H2	0.0586	0.7565	0.3701	0.078*
N3	0.1916 (2)	0.1813 (2)	0.2399 (2)	0.0557 (6)
N4	0.1230 (3)	0.1879 (2)	0.3564 (2)	0.0634 (7)
H4	0.0524	0.2505	0.3769	0.076*
C1	0.3038 (3)	0.6283 (3)	0.0099 (3)	0.0641 (8)
H1	0.3030	0.5540	0.0703	0.077*
C2	0.3745 (4)	0.6114 (4)	−0.1036 (3)	0.0765 (10)
H2A	0.4200	0.5260	−0.1190	0.092*
C3	0.3779 (4)	0.7198 (4)	−0.1938 (3)	0.0876 (11)
H3	0.4252	0.7080	−0.2704	0.105*
C4	0.3116 (4)	0.8454 (4)	−0.1710 (3)	0.0891 (11)
H4A	0.3148	0.9192	−0.2323	0.107*
C5	0.2397 (3)	0.8634 (3)	−0.0571 (3)	0.0715 (9)
H5	0.1951	0.9494	−0.0428	0.086*
C6	0.2334 (3)	0.7548 (3)	0.0357 (2)	0.0530 (7)
C7	0.1579 (3)	0.7736 (3)	0.1579 (2)	0.0531 (7)
C8	0.0530 (4)	0.8986 (3)	0.1836 (3)	0.0752 (9)
H8A	−0.0313	0.8729	0.2528	0.113*
H8B	0.0181	0.9365	0.1193	0.113*
H8C	0.1053	0.9661	0.1950	0.113*
C9	0.1646 (3)	0.5966 (3)	0.4334 (3)	0.0653 (8)
C10	0.2856 (4)	0.4870 (3)	0.3955 (3)	0.0767 (10)
H10A	0.3757	0.5301	0.3409	0.092*
H10B	0.2535	0.4319	0.3555	0.092*
C11	0.3227 (4)	0.3942 (4)	0.4964 (3)	0.1062 (14)
H11A	0.3594	0.4475	0.5340	0.159*
H11B	0.3984	0.3242	0.4683	0.159*
H11C	0.2337	0.3518	0.5511	0.159*
C12	0.3670 (3)	0.1940 (3)	0.0065 (3)	0.0661 (9)
H12	0.4155	0.1613	0.0607	0.079*
C13	0.4412 (4)	0.1836 (4)	−0.1083 (3)	0.0777 (10)
H13	0.5387	0.1429	−0.1305	0.093*
C14	0.3726 (4)	0.2329 (4)	−0.1901 (3)	0.0799 (10)
H14	0.4234	0.2263	−0.2675	0.096*
C15	0.2291 (4)	0.2917 (3)	−0.1567 (3)	0.0796 (10)
H15	0.1822	0.3251	−0.2118	0.096*
C16	0.1530 (3)	0.3018 (3)	−0.0415 (3)	0.0676 (9)
H16	0.0553	0.3421	−0.0201	0.081*
C17	0.2206 (3)	0.2526 (3)	0.0425 (2)	0.0521 (7)
C18	0.1405 (3)	0.2647 (3)	0.1661 (2)	0.0525 (7)
C19	0.0089 (4)	0.3676 (3)	0.1965 (3)	0.0862 (11)

H19A	−0.0822	0.3205	0.2331	0.129*
H19B	0.0046	0.4302	0.1269	0.129*
H19C	0.0200	0.4181	0.2490	0.129*
C20	0.1663 (3)	0.0963 (3)	0.4384 (3)	0.0621 (8)
C21	0.2895 (3)	−0.0106 (3)	0.3990 (3)	0.0734 (9)
H21A	0.3785	0.0347	0.3451	0.088*
H21B	0.2589	−0.0650	0.3575	0.088*
C22	0.3283 (4)	−0.1046 (4)	0.4975 (3)	0.1058 (14)
H22A	0.3711	−0.0532	0.5327	0.159*
H22B	0.3999	−0.1768	0.4685	0.159*
H22C	0.2390	−0.1438	0.5545	0.159*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1141 (19)	0.0844 (16)	0.0533 (14)	0.0394 (13)	−0.0209 (13)	−0.0188 (12)
O2	0.1033 (17)	0.0857 (16)	0.0496 (14)	0.0328 (13)	−0.0186 (12)	−0.0157 (12)
N1	0.0622 (15)	0.0567 (15)	0.0493 (15)	0.0053 (12)	−0.0157 (12)	−0.0094 (12)
N2	0.0728 (17)	0.0587 (16)	0.0508 (15)	0.0214 (13)	−0.0159 (13)	−0.0118 (13)
N3	0.0602 (15)	0.0558 (15)	0.0482 (15)	0.0037 (12)	−0.0170 (12)	−0.0115 (12)
N4	0.0691 (16)	0.0602 (16)	0.0502 (15)	0.0189 (13)	−0.0159 (13)	−0.0120 (13)
C1	0.070 (2)	0.060 (2)	0.061 (2)	0.0004 (16)	−0.0227 (16)	−0.0115 (16)
C2	0.085 (2)	0.078 (2)	0.064 (2)	0.0070 (18)	−0.0194 (18)	−0.0261 (19)
C3	0.096 (3)	0.102 (3)	0.056 (2)	0.009 (2)	−0.0174 (18)	−0.022 (2)
C4	0.104 (3)	0.094 (3)	0.054 (2)	0.015 (2)	−0.0223 (19)	−0.006 (2)
C5	0.077 (2)	0.068 (2)	0.060 (2)	0.0120 (17)	−0.0219 (17)	−0.0083 (17)
C6	0.0500 (17)	0.0558 (18)	0.0537 (18)	0.0015 (14)	−0.0207 (14)	−0.0097 (15)
C7	0.0520 (17)	0.0542 (18)	0.0525 (18)	0.0002 (14)	−0.0180 (14)	−0.0114 (15)
C8	0.096 (2)	0.062 (2)	0.067 (2)	0.0168 (17)	−0.0329 (18)	−0.0168 (17)
C9	0.073 (2)	0.060 (2)	0.052 (2)	0.0120 (16)	−0.0153 (17)	−0.0118 (17)
C10	0.083 (2)	0.073 (2)	0.063 (2)	0.0287 (18)	−0.0220 (17)	−0.0167 (17)
C11	0.114 (3)	0.102 (3)	0.080 (3)	0.050 (2)	−0.033 (2)	−0.014 (2)
C12	0.0565 (19)	0.081 (2)	0.060 (2)	−0.0008 (16)	−0.0204 (15)	−0.0116 (17)
C13	0.060 (2)	0.101 (3)	0.065 (2)	−0.0006 (18)	−0.0099 (17)	−0.024 (2)
C14	0.087 (3)	0.092 (3)	0.055 (2)	−0.009 (2)	−0.0150 (19)	−0.0176 (19)
C15	0.098 (3)	0.084 (2)	0.060 (2)	0.003 (2)	−0.037 (2)	−0.0108 (18)
C16	0.070 (2)	0.068 (2)	0.063 (2)	0.0074 (16)	−0.0270 (17)	−0.0093 (17)
C17	0.0544 (18)	0.0485 (17)	0.0514 (18)	−0.0057 (14)	−0.0181 (15)	−0.0040 (14)
C18	0.0515 (17)	0.0495 (17)	0.0526 (18)	0.0038 (14)	−0.0185 (14)	−0.0055 (15)
C19	0.082 (2)	0.091 (3)	0.069 (2)	0.0302 (19)	−0.0219 (18)	−0.0112 (19)
C20	0.068 (2)	0.0589 (19)	0.051 (2)	0.0122 (16)	−0.0174 (16)	−0.0100 (16)
C21	0.076 (2)	0.078 (2)	0.058 (2)	0.0263 (18)	−0.0244 (16)	−0.0153 (17)
C22	0.110 (3)	0.110 (3)	0.075 (3)	0.053 (2)	−0.033 (2)	−0.011 (2)

Geometric parameters (Å, °)

O1—C9	1.233 (3)	C10—H10A	0.9700
O2—C20	1.231 (3)	C10—H10B	0.9700
N1—C7	1.285 (3)	C11—H11A	0.9600

N1—N2	1.383 (3)	C11—H11B	0.9600
N2—C9	1.352 (4)	C11—H11C	0.9600
N2—H2	0.8600	C12—C13	1.379 (4)
N3—C18	1.282 (3)	C12—C17	1.390 (4)
N3—N4	1.384 (3)	C12—H12	0.9300
N4—C20	1.353 (3)	C13—C14	1.373 (4)
N4—H4	0.8600	C13—H13	0.9300
C1—C2	1.377 (4)	C14—C15	1.366 (4)
C1—C6	1.395 (4)	C14—H14	0.9300
C1—H1	0.9300	C15—C16	1.385 (4)
C2—C3	1.369 (4)	C15—H15	0.9300
C2—H2A	0.9300	C16—C17	1.389 (4)
C3—C4	1.366 (5)	C16—H16	0.9300
C3—H3	0.9300	C17—C18	1.487 (4)
C4—C5	1.387 (4)	C18—C19	1.499 (4)
C4—H4A	0.9300	C19—H19A	0.9600
C5—C6	1.387 (4)	C19—H19B	0.9600
C5—H5	0.9300	C19—H19C	0.9600
C6—C7	1.485 (4)	C20—C21	1.495 (4)
C7—C8	1.504 (4)	C21—C22	1.498 (4)
C8—H8A	0.9600	C21—H21A	0.9700
C8—H8B	0.9600	C21—H21B	0.9700
C8—H8C	0.9600	C22—H22A	0.9600
C9—C10	1.497 (4)	C22—H22B	0.9600
C10—C11	1.508 (4)	C22—H22C	0.9600
C7—N1—N2	118.3 (2)	H11A—C11—H11B	109.5
C9—N2—N1	119.6 (2)	C10—C11—H11C	109.5
C9—N2—H2	120.2	H11A—C11—H11C	109.5
N1—N2—H2	120.2	H11B—C11—H11C	109.5
C18—N3—N4	118.1 (2)	C13—C12—C17	121.0 (3)
C20—N4—N3	120.4 (2)	C13—C12—H12	119.5
C20—N4—H4	119.8	C17—C12—H12	119.5
N3—N4—H4	119.8	C14—C13—C12	120.6 (3)
C2—C1—C6	121.2 (3)	C14—C13—H13	119.7
C2—C1—H1	119.4	C12—C13—H13	119.7
C6—C1—H1	119.4	C15—C14—C13	119.4 (3)
C3—C2—C1	120.3 (3)	C15—C14—H14	120.3
C3—C2—H2A	119.8	C13—C14—H14	120.3
C1—C2—H2A	119.8	C14—C15—C16	120.6 (3)
C4—C3—C2	119.7 (3)	C14—C15—H15	119.7
C4—C3—H3	120.1	C16—C15—H15	119.7
C2—C3—H3	120.1	C15—C16—C17	120.8 (3)
C3—C4—C5	120.4 (3)	C15—C16—H16	119.6
C3—C4—H4A	119.8	C17—C16—H16	119.6
C5—C4—H4A	119.8	C16—C17—C12	117.7 (3)
C4—C5—C6	120.9 (3)	C16—C17—C18	121.3 (3)
C4—C5—H5	119.6	C12—C17—C18	121.1 (3)
C6—C5—H5	119.6	N3—C18—C17	115.1 (3)
C5—C6—C1	117.4 (3)	N3—C18—C19	124.9 (3)

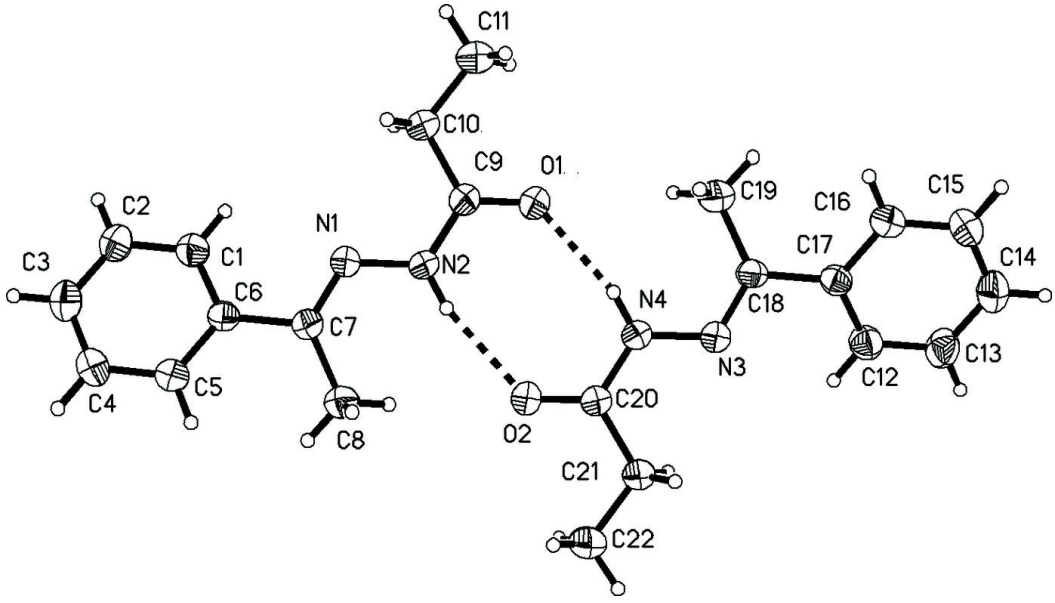
C5—C6—C7	121.2 (3)	C17—C18—C19	120.0 (3)
C1—C6—C7	121.4 (3)	C18—C19—H19A	109.5
N1—C7—C6	115.4 (3)	C18—C19—H19B	109.5
N1—C7—C8	124.7 (3)	H19A—C19—H19B	109.5
C6—C7—C8	119.9 (3)	C18—C19—H19C	109.5
C7—C8—H8A	109.5	H19A—C19—H19C	109.5
C7—C8—H8B	109.5	H19B—C19—H19C	109.5
H8A—C8—H8B	109.5	O2—C20—N4	119.7 (3)
C7—C8—H8C	109.5	O2—C20—C21	122.3 (3)
H8A—C8—H8C	109.5	N4—C20—C21	118.0 (3)
H8B—C8—H8C	109.5	C20—C21—C22	112.9 (3)
O1—C9—N2	119.3 (3)	C20—C21—H21A	109.0
O1—C9—C10	122.2 (3)	C22—C21—H21A	109.0
N2—C9—C10	118.4 (3)	C20—C21—H21B	109.0
C9—C10—C11	112.4 (3)	C22—C21—H21B	109.0
C9—C10—H10A	109.1	H21A—C21—H21B	107.8
C11—C10—H10A	109.1	C21—C22—H22A	109.5
C9—C10—H10B	109.1	C21—C22—H22B	109.5
C11—C10—H10B	109.1	H22A—C22—H22B	109.5
H10A—C10—H10B	107.8	C21—C22—H22C	109.5
C10—C11—H11A	109.5	H22A—C22—H22C	109.5
C10—C11—H11B	109.5	H22B—C22—H22C	109.5
C7—N1—N2—C9	−175.3 (3)	N2—C9—C10—C11	177.6 (3)
C18—N3—N4—C20	175.7 (3)	C17—C12—C13—C14	0.9 (5)
C6—C1—C2—C3	0.5 (5)	C12—C13—C14—C15	−0.5 (5)
C1—C2—C3—C4	0.4 (5)	C13—C14—C15—C16	0.0 (5)
C2—C3—C4—C5	−0.6 (6)	C14—C15—C16—C17	0.0 (5)
C3—C4—C5—C6	−0.1 (5)	C15—C16—C17—C12	0.4 (4)
C4—C5—C6—C1	0.9 (4)	C15—C16—C17—C18	179.2 (3)
C4—C5—C6—C7	179.4 (3)	C13—C12—C17—C16	−0.8 (4)
C2—C1—C6—C5	−1.2 (4)	C13—C12—C17—C18	−179.6 (3)
C2—C1—C6—C7	−179.6 (3)	N4—N3—C18—C17	179.5 (2)
N2—N1—C7—C6	179.6 (2)	N4—N3—C18—C19	−1.4 (4)
N2—N1—C7—C8	0.1 (4)	C16—C17—C18—N3	159.4 (3)
C5—C6—C7—N1	−163.5 (3)	C12—C17—C18—N3	−21.8 (4)
C1—C6—C7—N1	14.9 (4)	C16—C17—C18—C19	−19.8 (4)
C5—C6—C7—C8	16.0 (4)	C12—C17—C18—C19	159.0 (3)
C1—C6—C7—C8	−165.6 (3)	N3—N4—C20—O2	−179.8 (3)
N1—N2—C9—O1	−178.1 (3)	N3—N4—C20—C21	0.0 (4)
N1—N2—C9—C10	3.2 (4)	O2—C20—C21—C22	−0.8 (5)
O1—C9—C10—C11	−1.1 (5)	N4—C20—C21—C22	179.4 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2^{i}	0.86	2.11	2.954 (3)	166
N4—H4···O1^{i}	0.86	2.10	2.937 (3)	166

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1.

Fig. 1


C11
C10
C9
O1
C19
C16
C15
C2
N1
C17
C14
C3
C1
N2
C6
N4
C18
C7
N3
C13
C5
C12
C4
C20
C8
O2
C21
C22