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4a,5-Dihydro-2*H*-chromeno[4,3-*c*]-pyridazin-3(4*H*)-one

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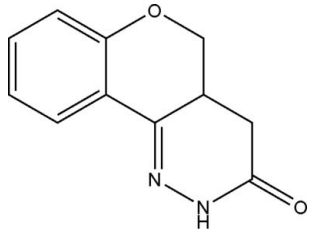
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.010 Å; R factor = 0.057; wR factor = 0.179; data-to-parameter ratio = 7.0.

In the crystal structure of the title compound, $C_{11}H_{10}N_2O_2$, there are two independent molecules, *A* and *B*, with different conformations. In molecule *A*, the pyran ring adopts a half-chair conformation, and in molecule *B*, it adopts an envelope conformation. The structure is stabilized by N—H···O hydrogen-bonding interactions, resulting in chains of molecules. Further stability is provided by offset π–π stacking interactions between the benzene rings in adjacent chains, with centroid–centroid distances of 3.860 (5) Å for the benzene rings in molecules *A* [symmetry codes: $-x$, $-\frac{1}{2}+y$, $z-x$; $-x$, $\frac{1}{2}+y$, z] and 3.860 (5) Å for molecules *B* [symmetry codes: $1-x$, $-\frac{1}{2}+y$, z; $1-x$, $\frac{1}{2}+y$, z].

Related literature

For background literature, see: Potts & Dery (1986), Ren *et al.* (2003) and Wang & Tunge (2006).

For related literature, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{11}H_{10}N_2O_2$
M_r = 202.21
Orthorhombic, $Pca2_1$
a = 7.6838 (10) Å
b = 7.4659 (9) Å
c = 33.322 (4) Å
V = 1911.6 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 292 (2) K
0.40 × 0.30 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.961, T_{max} = 0.990
9576 measured reflections
1906 independent reflections
1211 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.179
S = 1.00
1906 reflections
271 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*A*···O4	0.86	2.11	2.902 (7)	154
N4—H4*A*···O2^{i}	0.86	2.07	2.891 (7)	159
C21—H21*B*···O4^{ii}	0.97	2.44	3.312 (8)	149

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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: *SHELXTL* (Bruker, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2364).

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supplementary materials

Acta Cryst. (2007). E**63**, o2512 [**doi:10.1107/S1600536807017837**]

4a,5-Dihydro-2*H*-chromeno[4,3-*c*]pyridazin-3(4*H*)-one

Z.-Z. Zhou and H.-B. Zhou

Comment

Flavonoids, occurring widely throughout the plant kingdom, are one of the most representative families of plant secondary metabolites and display a remarkable

spectrum of biological activities. They are used as a synthetic lead for drug discovery (Ren *et al.*, 2003). The title compound, (I) (Fig. 1), is an important intermediate for the synthesis of flavonoid derivatives.

Compound (I) contains two independent molecules (A and B) in the asymmetric unit, with bond lengths and angles within normal ranges (Allen *et al.*, 1987). The six-membered pyran ring adopts a half-chair conformation in molecule A (atoms C1/C6–C9/O3) and an envelope conformation in molecule B (atoms C12/C17–C20/O1). The fused heterocyclic ring (atoms C7/C8/C10/C11/N4/N3 in A; atoms C18/C19/C21/C22/N1/N2 in B) adopts a sofa conformation in both molecules.

The structure is stabilised by weak N—H···O hydrogen-bonding interactions (Table 1). The hydrogen bonds link pairs of independent molecules into dimers, while the N—H···O interactions link pairs of dimers into chains in the bc plane. A short C—H···O contact is also present. Further stability is provided

by offset π–π stacking interactions between adjacent C1–C6 and C12–C17 benzene rings. The centroid–centroid distance is 3.860 (5) Å.

Experimental

The title compound was synthesized according to the literature procedure of Cignarella *et al.* (1992). Crystals of (I) suitable for X-ray crystallographic analysis were recrystallised from dichloromethane at 277 K.

Refinement

The H atoms were placed in idealized positions, with C—H = 0.93–0.97 Å and N—H = 0.86 Å, and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Figures

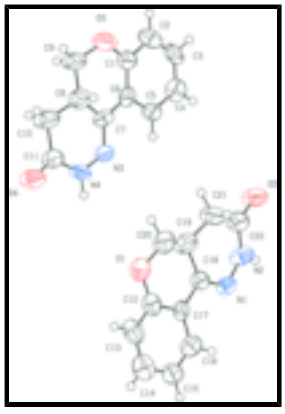

Fig. 1. A perspective view of the asymmetric unit of the title compound, with displacement ellipsoids drawn at the 50% probability level (arbitrary spheres for the H atoms).

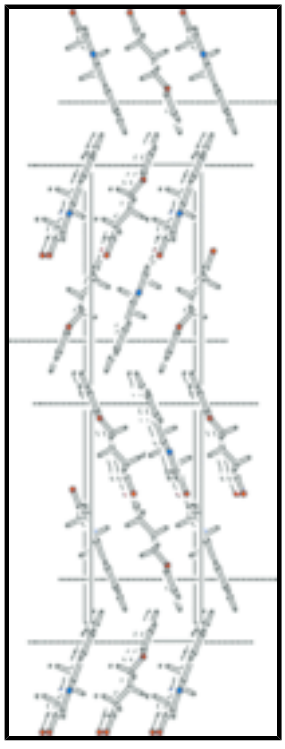

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as thin dashed lines [None visible] and π–π stacking contacts as thick dashed lines.

4a,5-Dihydro-2*H*-chromeno[4,3-c]pyridazin-3(4*H*)-one

Crystal data

$C_{11}H_{10}N_2O_2$	F_{000} = 848
M_r = 202.21	D_x = 1.405 Mg m^{-3}
Orthorhombic, *Pca*2$_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2c -2ac	Cell parameters from 1006 reflections
a = 7.6838 (10) Å	θ = 2.4–19.8º
b = 7.4659 (9) Å	μ = 0.10 mm^{-1}
c = 33.322 (4) Å	*T* = 292 (2) K

V = 1911.6 (4) Å^3	Block, colourless
Z = 8	0.40 × 0.30 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer	1906 independent reflections
Radiation source: fine-focus sealed tube	1211 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.057
T = 292(2) K	θ_{max} = 26.0º
ω scans	θ_{min} = 1.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −9→9
T_{min} = 0.961, T_{max} = 0.990	k = −8→9
9576 measured reflections	l = −41→36

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.057	H-atom parameters constrained
$wR(F^2)$ = 0.179	$w = 1/[\sigma^2(F_o^2) + (0.1059P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max} < 0.001$
1906 reflections	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
271 parameters	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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	0.0527 (7)	0.8659 (5)	0.46763 (15)	0.0732 (14)
O2	0.3726 (8)	0.6504 (6)	0.30959 (14)	0.0791 (15)

N1	0.2055 (7)	0.4405 (7)	0.39697 (15)	0.0498 (13)
N2	0.2621 (11)	0.4758 (7)	0.3587 (2)	0.0586 (18)
H2A	0.2644	0.3867	0.3423	0.070*
C12	0.0380 (9)	0.6931 (10)	0.4825 (2)	0.0565 (17)
C13	−0.0268 (11)	0.6771 (12)	0.5207 (2)	0.069 (2)
H13	−0.0574	0.7775	0.5357	0.083*
C14	−0.0450 (13)	0.5037 (13)	0.5364 (3)	0.077 (3)
H14	−0.0935	0.4879	0.5617	0.093*
C15	0.0090 (12)	0.3538 (12)	0.5143 (2)	0.067 (2)
H15	−0.0014	0.2394	0.5250	0.081*
C16	0.0767 (10)	0.3773 (10)	0.4771 (2)	0.0600 (19)
H16	0.1156	0.2770	0.4632	0.072*
C17	0.0910 (8)	0.5450 (10)	0.45849 (18)	0.0461 (16)
C18	0.1612 (8)	0.5739 (9)	0.41872 (17)	0.0483 (15)
C19	0.1671 (11)	0.7619 (8)	0.4037 (2)	0.070 (2)
H19	0.0555	0.7799	0.3901	0.083*
C20	0.1670 (11)	0.8928 (8)	0.4369 (2)	0.074 (2)
H20A	0.2834	0.8961	0.4482	0.089*
H20B	0.1440	1.0101	0.4256	0.089*
C21	0.2986 (12)	0.7876 (8)	0.3726 (2)	0.080 (2)
H21A	0.4107	0.8052	0.3854	0.096*
H21B	0.2713	0.8960	0.3579	0.096*
C22	0.3133 (10)	0.6356 (8)	0.34363 (18)	0.0614 (18)
O3	0.6970 (7)	0.3665 (6)	0.15967 (16)	0.0803 (15)
O4	0.3727 (8)	0.1510 (6)	0.31826 (13)	0.0788 (15)
N3	0.5429 (7)	−0.0626 (7)	0.23097 (16)	0.0487 (13)
N4	0.4795 (11)	−0.0232 (7)	0.26994 (17)	0.0588 (19)
H4A	0.4693	−0.1125	0.2860	0.071*
C1	0.7049 (9)	0.1930 (9)	0.1460 (2)	0.0535 (17)
C2	0.7724 (11)	0.1683 (11)	0.1079 (2)	0.064 (2)
H2	0.8062	0.2672	0.0928	0.076*
C3	0.7898 (13)	0.0023 (9)	0.0922 (2)	0.059 (2)
H3	0.8326	−0.0114	0.0663	0.071*
C4	0.7455 (11)	−0.1456 (10)	0.1141 (2)	0.060 (2)
H4	0.7629	−0.2600	0.1038	0.072*
C5	0.6731 (8)	−0.1215 (9)	0.15232 (19)	0.0497 (16)
H5	0.6402	−0.2212	0.1672	0.060*
C6	0.6500 (8)	0.0464 (10)	0.16813 (18)	0.0447 (14)
C7	0.5879 (8)	0.0760 (7)	0.20934 (18)	0.0455 (14)
C8	0.5825 (11)	0.2660 (9)	0.2245 (2)	0.0686 (19)
H8	0.6940	0.2851	0.2381	0.082*
C9	0.5791 (12)	0.3946 (7)	0.1915 (2)	0.075 (2)
H9A	0.4624	0.3958	0.1804	0.090*
H9B	0.6011	0.5126	0.2026	0.090*
C10	0.4477 (12)	0.2895 (8)	0.2557 (2)	0.078 (2)
H10A	0.3362	0.3079	0.2427	0.094*
H10B	0.4742	0.3968	0.2710	0.094*
C11	0.4322 (9)	0.1362 (8)	0.28399 (18)	0.0553 (17)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.097 (4)	0.052 (3)	0.070 (3)	0.009 (2)	0.022 (3)	−0.017 (2)
O2	0.130 (4)	0.053 (2)	0.054 (3)	0.000 (3)	0.020 (3)	0.005 (2)
N1	0.072 (4)	0.044 (3)	0.034 (3)	0.002 (3)	−0.003 (2)	−0.002 (2)
N2	0.088 (5)	0.037 (3)	0.051 (4)	−0.006 (3)	−0.015 (3)	0.000 (2)
C12	0.058 (4)	0.059 (4)	0.052 (4)	−0.002 (3)	0.003 (3)	−0.016 (3)
C13	0.065 (5)	0.076 (5)	0.066 (5)	−0.011 (4)	0.013 (4)	−0.022 (4)
C14	0.052 (6)	0.115 (9)	0.066 (6)	−0.003 (4)	−0.011 (4)	−0.013 (4)
C15	0.063 (5)	0.082 (6)	0.057 (5)	0.006 (4)	0.002 (4)	0.008 (4)
C16	0.065 (5)	0.058 (4)	0.056 (5)	0.005 (4)	−0.011 (4)	0.004 (4)
C17	0.047 (4)	0.050 (3)	0.041 (4)	0.018 (3)	0.000 (3)	−0.006 (3)
C18	0.051 (4)	0.056 (4)	0.037 (3)	0.002 (3)	0.002 (3)	−0.004 (3)
C19	0.105 (6)	0.041 (4)	0.062 (4)	0.005 (3)	0.010 (4)	−0.002 (3)
C20	0.107 (6)	0.056 (4)	0.060 (4)	0.014 (4)	0.015 (4)	−0.009 (3)
C21	0.133 (7)	0.047 (4)	0.059 (4)	−0.008 (4)	0.035 (5)	0.000 (3)
C22	0.093 (6)	0.053 (4)	0.038 (3)	0.004 (4)	0.003 (4)	−0.005 (3)
O3	0.109 (4)	0.056 (3)	0.075 (3)	−0.009 (3)	0.031 (3)	0.011 (2)
O4	0.143 (5)	0.050 (2)	0.043 (2)	0.006 (3)	0.025 (3)	−0.001 (2)
N3	0.065 (4)	0.040 (3)	0.041 (3)	0.001 (3)	0.002 (2)	0.003 (2)
N4	0.094 (5)	0.045 (3)	0.037 (3)	−0.005 (3)	0.032 (3)	0.006 (2)
C1	0.053 (4)	0.049 (4)	0.059 (4)	−0.003 (3)	0.004 (3)	0.008 (3)
C2	0.065 (5)	0.081 (5)	0.045 (4)	−0.011 (4)	0.007 (3)	0.010 (4)
C3	0.067 (6)	0.078 (6)	0.032 (4)	0.004 (3)	0.018 (4)	0.001 (3)
C4	0.072 (5)	0.064 (4)	0.044 (4)	0.007 (4)	−0.006 (3)	−0.017 (4)
C5	0.052 (4)	0.054 (4)	0.043 (3)	−0.002 (3)	0.002 (3)	0.005 (3)
C6	0.032 (3)	0.058 (4)	0.044 (3)	0.015 (3)	−0.013 (3)	0.002 (3)
C7	0.054 (4)	0.035 (3)	0.048 (3)	−0.001 (2)	−0.012 (3)	0.006 (3)
C8	0.096 (5)	0.049 (4)	0.061 (4)	0.002 (3)	0.011 (4)	0.001 (3)
C9	0.116 (6)	0.038 (3)	0.073 (5)	−0.003 (3)	0.023 (5)	0.005 (3)
C10	0.125 (7)	0.041 (4)	0.068 (4)	−0.001 (4)	0.009 (4)	0.005 (3)
C11	0.078 (5)	0.042 (3)	0.046 (4)	0.001 (3)	0.002 (3)	−0.003 (3)

Geometric parameters (Å, °)

O1—C20	1.363 (8)	O3—C1	1.374 (8)
O1—C12	1.386 (8)	O3—C9	1.411 (8)
O2—C22	1.228 (7)	O4—C11	1.235 (7)
N1—C18	1.278 (8)	N3—C7	1.308 (8)
N1—N2	1.373 (9)	N3—N4	1.418 (8)
N2—C22	1.353 (8)	N4—C11	1.330 (7)
N2—H2A	0.8611	N4—H4A	0.8591
C12—C13	1.373 (10)	C1—C2	1.385 (10)
C12—C17	1.425 (9)	C1—C6	1.386 (10)
C13—C14	1.403 (13)	C2—C3	1.350 (11)
C13—H13	0.9300	C2—H2	0.9300
C14—C15	1.402 (12)	C3—C4	1.365 (10)

C14—H14	0.9300	C3—H3	0.9300
C15—C16	1.355 (11)	C4—C5	1.403 (10)
C15—H15	0.9300	C4—H4	0.9300
C16—C17	1.401 (9)	C5—C6	1.371 (9)
C16—H16	0.9300	C5—H5	0.9300
C17—C18	1.447 (9)	C6—C7	1.470 (9)
C18—C19	1.490 (9)	C7—C8	1.506 (9)
C19—C21	1.460 (9)	C8—C9	1.458 (9)
C19—C20	1.475 (9)	C8—C10	1.480 (10)
C19—H19	0.9800	C8—H8	0.9800
C20—H20A	0.9700	C9—H9A	0.9700
C20—H20B	0.9700	C9—H9B	0.9700
C21—C22	1.495 (8)	C10—C11	1.487 (8)
C21—H21A	0.9700	C10—H10A	0.9700
C21—H21B	0.9700	C10—H10B	0.9700
C20—O1—C12	117.3 (5)	C1—O3—C9	114.7 (5)
C18—N1—N2	117.5 (6)	C7—N3—N4	115.5 (5)
C22—N2—N1	127.3 (6)	C11—N4—N3	127.1 (5)
C22—N2—H2A	116.1	C11—N4—H4A	116.7
N1—N2—H2A	116.6	N3—N4—H4A	116.2
C13—C12—O1	116.2 (6)	O3—C1—C2	116.5 (6)
C13—C12—C17	123.9 (8)	O3—C1—C6	123.7 (6)
O1—C12—C17	119.9 (6)	C2—C1—C6	119.8 (7)
C12—C13—C14	117.5 (8)	C3—C2—C1	120.9 (7)
C12—C13—H13	121.3	C3—C2—H2	119.6
C14—C13—H13	121.3	C1—C2—H2	119.6
C15—C14—C13	120.8 (9)	C2—C3—C4	120.8 (7)
C15—C14—H14	119.6	C2—C3—H3	119.6
C13—C14—H14	119.6	C4—C3—H3	119.6
C16—C15—C14	119.4 (9)	C3—C4—C5	118.6 (7)
C16—C15—H15	120.3	C3—C4—H4	120.7
C14—C15—H15	120.3	C5—C4—H4	120.7
C15—C16—C17	123.4 (7)	C6—C5—C4	121.2 (6)
C15—C16—H16	118.3	C6—C5—H5	119.4
C17—C16—H16	118.3	C4—C5—H5	119.4
C16—C17—C12	115.0 (6)	C5—C6—C1	118.6 (6)
C16—C17—C18	124.6 (7)	C5—C6—C7	122.6 (7)
C12—C17—C18	120.3 (7)	C1—C6—C7	118.5 (6)
N1—C18—C17	120.1 (7)	N3—C7—C6	118.8 (6)
N1—C18—C19	122.4 (6)	N3—C7—C8	123.6 (6)
C17—C18—C19	117.3 (6)	C6—C7—C8	117.6 (5)
C21—C19—C20	116.4 (6)	C9—C8—C10	116.1 (6)
C21—C19—C18	112.5 (5)	C9—C8—C7	111.6 (5)
C20—C19—C18	111.9 (6)	C10—C8—C7	111.5 (6)
C21—C19—H19	104.9	C9—C8—H8	105.6
C20—C19—H19	104.9	C10—C8—H8	105.6
C18—C19—H19	104.9	C7—C8—H8	105.6
O1—C20—C19	117.7 (6)	O3—C9—C8	117.2 (6)
O1—C20—H20A	107.9	O3—C9—H9A	108.0

C19—C20—H20A	107.9	C8—C9—H9A	108.0
O1—C20—H20B	107.9	O3—C9—H9B	108.0
C19—C20—H20B	107.9	C8—C9—H9B	108.0
H20A—C20—H20B	107.2	H9A—C9—H9B	107.2
C19—C21—C22	114.3 (6)	C8—C10—C11	114.3 (6)
C19—C21—H21A	108.7	C8—C10—H10A	108.7
C22—C21—H21A	108.7	C11—C10—H10A	108.7
C19—C21—H21B	108.7	C8—C10—H10B	108.7
C22—C21—H21B	108.7	C11—C10—H10B	108.7
H21A—C21—H21B	107.6	H10A—C10—H10B	107.6
O2—C22—N2	122.0 (6)	O4—C11—N4	120.4 (5)
O2—C22—C21	123.9 (6)	O4—C11—C10	123.1 (6)
N2—C22—C21	114.0 (6)	N4—C11—C10	116.4 (6)
C18—N1—N2—C22	15.7 (12)	C7—N3—N4—C11	13.0 (12)
C20—O1—C12—C13	158.2 (7)	C9—O3—C1—C2	160.0 (7)
C20—O1—C12—C17	−21.0 (10)	C9—O3—C1—C6	−20.1 (10)
O1—C12—C13—C14	179.3 (7)	O3—C1—C2—C3	178.2 (8)
C17—C12—C13—C14	−1.6 (12)	C6—C1—C2—C3	−1.7 (12)
C12—C13—C14—C15	3.0 (13)	C1—C2—C3—C4	−1.7 (15)
C13—C14—C15—C16	−1.2 (14)	C2—C3—C4—C5	3.2 (14)
C14—C15—C16—C17	−2.2 (12)	C3—C4—C5—C6	−1.3 (11)
C15—C16—C17—C12	3.4 (11)	C4—C5—C6—C1	−2.0 (10)
C15—C16—C17—C18	−179.4 (7)	C4—C5—C6—C7	−174.9 (6)
C13—C12—C17—C16	−1.5 (11)	O3—C1—C6—C5	−176.4 (6)
O1—C12—C17—C16	177.6 (6)	C2—C1—C6—C5	3.5 (10)
C13—C12—C17—C18	−178.8 (7)	O3—C1—C6—C7	−3.2 (10)
O1—C12—C17—C18	0.3 (10)	C2—C1—C6—C7	176.7 (6)
N2—N1—C18—C17	176.5 (6)	N4—N3—C7—C6	−178.2 (6)
N2—N1—C18—C19	0.8 (10)	N4—N3—C7—C8	2.8 (10)
C16—C17—C18—N1	4.3 (10)	C5—C6—C7—N3	−4.2 (9)
C12—C17—C18—N1	−178.6 (6)	C1—C6—C7—N3	−177.1 (6)
C16—C17—C18—C19	−179.8 (7)	C5—C6—C7—C8	174.8 (6)
C12—C17—C18—C19	−2.8 (10)	C1—C6—C7—C8	1.9 (9)
N1—C18—C19—C21	−27.9 (10)	N3—C7—C8—C9	−159.9 (7)
C17—C18—C19—C21	156.3 (7)	C6—C7—C8—C9	21.1 (9)
N1—C18—C19—C20	−161.1 (7)	N3—C7—C8—C10	−28.3 (10)
C17—C18—C19—C20	23.1 (9)	C6—C7—C8—C10	152.8 (6)
C12—O1—C20—C19	44.5 (9)	C1—O3—C9—C8	45.9 (9)
C21—C19—C20—O1	−176.1 (6)	C10—C8—C9—O3	−175.0 (7)
C18—C19—C20—O1	−44.8 (10)	C7—C8—C9—O3	−45.7 (10)
C20—C19—C21—C22	170.1 (6)	C9—C8—C10—C11	168.0 (7)
C18—C19—C21—C22	39.1 (10)	C7—C8—C10—C11	38.7 (9)
N1—N2—C22—O2	175.1 (7)	N3—N4—C11—O4	177.3 (7)
N1—N2—C22—C21	−2.1 (12)	N3—N4—C11—C10	−0.1 (12)
C19—C21—C22—O2	156.8 (7)	C8—C10—C11—O4	155.8 (7)
C19—C21—C22—N2	−26.0 (10)	C8—C10—C11—N4	−26.9 (10)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O4	0.86	2.11	2.902 (7)	154
N4—H4A···O2^{i}	0.86	2.07	2.891 (7)	159
C21—H21B···O4^{ii}	0.97	2.44	3.312 (8)	149

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

Fig. 1

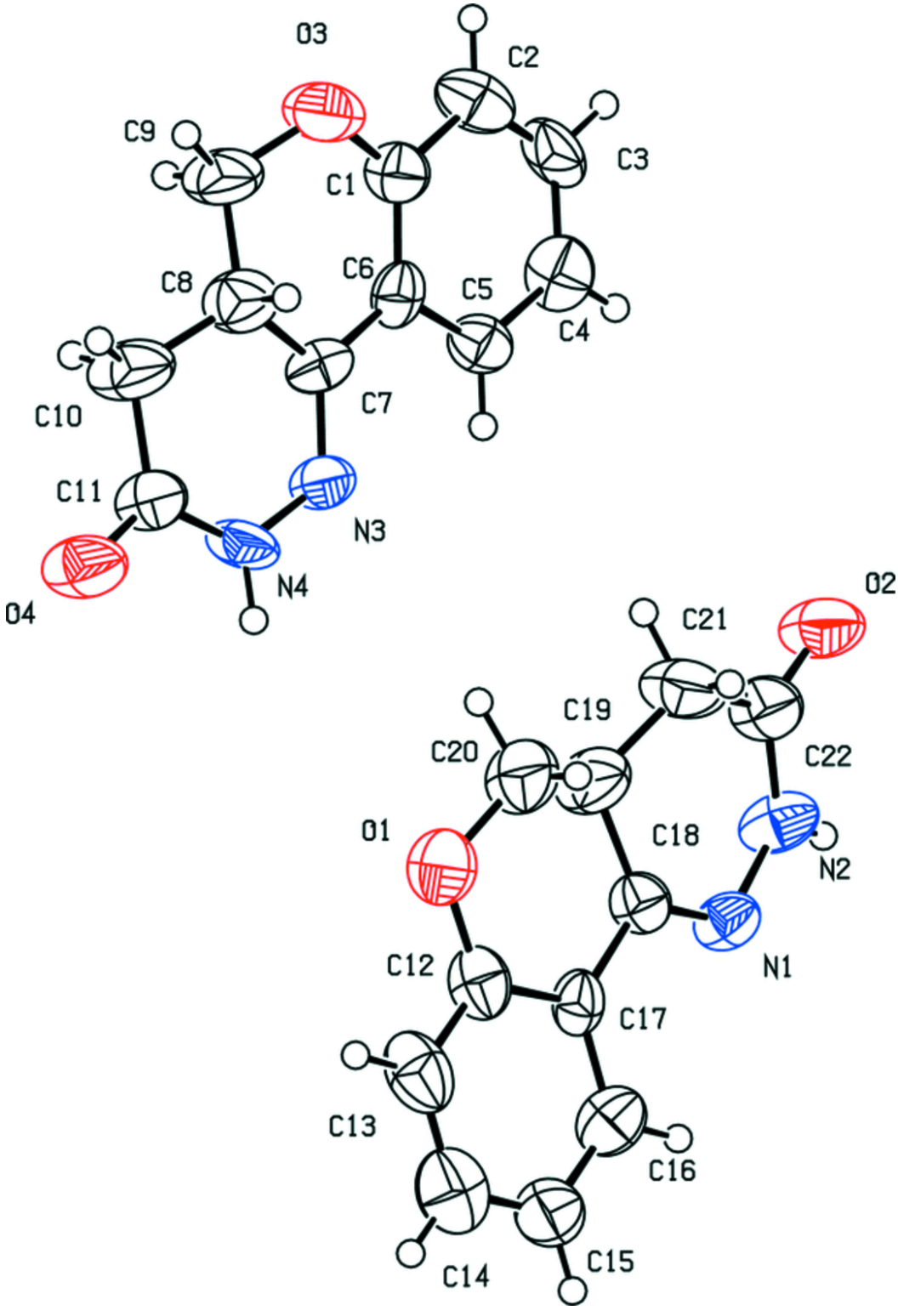
O3
C2
C9
C3
C1
C8
C6
C5
C4
C10
C7
C11
N3
N4
O4
O2
C21
C19
C20
C22
O1
C18
N2
C12
N1
C17
C13
C16
C14
C15

Fig. 2