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1-[3-(1*H*-Indol-2-yl)-2-furyl]ethanone

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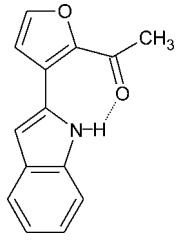
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.100; data-to-parameter ratio = 8.7.

En route to furostifoline, we synthesized the title compound, $C_{14}H_{11}NO_2$, as a yellow crystalline material, with two independent molecules in the asymmetric unit, related by a *pseudo*-centre of inversion; they have an approximately planar conformation, and similar bond lengths and angles. An intramolecular N—H···O hydrogen bond was observed for each molecule, as well as several intermolecular C—H···O interactions, linking the two molecules together into dimers. The dimers themselves are linked to neighbouring dimers by C—H···O and C—H···π interactions.

Related literature

For details of the preparation and use of the title compound, see Pelly *et al.* (2005).

For related literature, see: Bernstein *et al.* (1995); Etter *et al.* (1990); Furukawa & Ito (1990); Knölker & Reddy (2002); Omura *et al.* (1977); de Koning *et al.* (2000).



Experimental

Crystal data

$C_{14}H_{11}NO_2$
M_r = 225.24
Monoclinic, $P2_1$
a = 7.2780 (2) Å
b = 14.3556 (3) Å
c = 10.7002 (2) Å
β = 99.433 (1)°
V = 1102.84 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 173 (2) K
0.35 × 0.23 × 0.14 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: none
21468 measured reflections
2768 independent reflections
2212 reflections with $I > 2\sigma(I)$
R_{int} = 0.075

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.100
S = 1.06
2768 reflections
317 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Selected torsion angles (°).

N1*A*—C1*A*—C9*A*—C12*A*	5.8 (4)	C1*A*—C9*A*—C12*A*—C13*A*	0.9 (5)
C13*B*—C12*B*—C9*B*—C1*B*	−0.8 (5)	O2*A*—C13*A*—C12*A*—C9*A*	−1.1 (4)
N1*B*—C1*B*—C9*B*—C12*B*	−8.7 (4)	C9*B*—C12*B*—C13*B*—O2*B*	5.0 (4)

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

Cg is the centroid of atoms C3*B*–C8*B*.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···O2*A*	0.93 (3)	1.91 (3)	2.739 (3)	148 (2)
N1*B*—H1*B*···O2*B*	0.97 (3)	1.90 (3)	2.730 (3)	143 (3)
C4*A*—H4*A*···*Cg*^{i}	0.95	2.94	3.695 (2)	137
C7*A*—H7*A*···O2*B*	0.95	2.55	3.472 (3)	163
C7*B*—H7*B*···O2*A*	0.95	2.62	3.546 (3)	163
C11*A*—H11*A*···O2*A*^{ii}	0.95	2.53	3.231 (3)	131 (1)
C11*B*—H11*B*···O2*B*^{iii}	0.95	2.55	3.234 (3)	129 (1)

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

Data collection: *APEX2* (Bruker, 2005*a*); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005*b*); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2046).

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supplementary materials

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1-[3-(1*H*-Indol-2-yl)-2-furyl]ethanone

M. A. Fernandes, C. B. de Koning, C. B. Perry and S. C. Pelly

Comment

The carbazole structure is found in many naturally occurring compounds which possess interesting and potentially useful biological properties (Knölker & Reddy, 2002). For example, staurosporine, an indolo[3,2-*a*]carbazole isolated from *Streptomyces staurosporeus*, is a potent protein kinase C (PKC) inhibitor and therefore interest in compounds of this type exists due to their potential use as anti-cancer agents (Omura *et al.*, 1977). Our research group has been interested in the synthesis of carbazoles and in continuing this work (de Koning *et al.*, 2000), we sought to synthesize the naturally occurring furo[3,2-*a*]carbazole, furostifoline, first isolated by Furukawa and co-workers from *Murraya euchrestifolia* in 1990 (Furukawa & Ito, 1990).

En route to furostifoline, we synthesized the title compound in two steps starting from previously synthesized 1-(*tert*-butoxycarbonyl)-1*H*-indol-2-yl-2-boronic acid and 2-acetyl-3-bromofuran. (de Koning *et al.*, 2000).

The title compound crystallizes with two molecules (designated A and B) in the asymmetric unit related by a pseudo centre of inversion (Fig. 1). Both molecules have an approximate planar conformation and similar bond lengths and angles. Selected bond lengths and angles are given in Table 1. Molecules in the structure pack in a herring bone type arrangement. There is within each molecule an intramolecular N—H···O H bond (Table 2) which can be described by the graph set S(7) (Etter *et al.*, 1990; Bernstein *et al.*, 1995). Acting between molecule A and B are weak C—H···O contacts (Table 2) linking these two molecules together into a dimer. Each of these dimers interact through C—H···O and C—H···π interactions with neighbouring dimers to form a stack of dimer molecules related by translation along the *a* axis (Fig. 2). The kink in the herring bone is generated by dimers related by the 2-fold screw axis along b. These interact with molecules in the original stack through C—H···π interactions (Table 2).

Experimental

The title compound, 2-(2-Acetylfuran-3-yl)-1*H*-indole, was prepared in 85% yield by $AlCl_3$ facilitated deprotection of *tert*-butyl 2-(2-acetylfuran-3-yl)-1*H*-indole-1-carboxylate as described previously (de Koning *et al.*, 2000). Crystals suitable for X-ray crystallography were obtained as yellow needles by recrystallization from n-hexane–ethyl acetate (*ca* 4:1).

Refinement

The structure is chiral but does not contain any atoms capable of significant anomalous dispersion under the experimental conditions used. As a consequence, a total of 2556 Friedel pairs were merged (92% of all possible pairs were collected) before the final refinement was performed. The indole N—H atoms were placed from the difference map and refined freely. All remaining H atoms were positioned geometrically, and allowed to ride on their parent atoms, with C—H bond lengths of 0.99 Å (CH_2), 0.98 Å (CH_3), or 0.95 Å (aromatic CH). Isotropic displacement parameters for these atoms were set equal to 1.2 (CH_2 and aromatic CH), or 1.5 (CH_3) times U_{eq} of the parent atom.

Figures

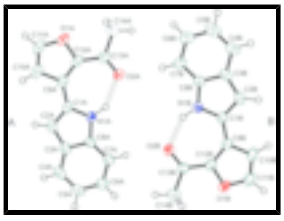

Fig. 1. The molecular structure of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The intramolecular N—H···O hydrogen bonds are indicated as dashed lines.

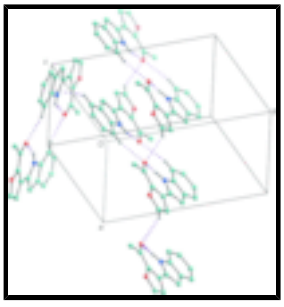

Fig. 2. Packing diagram showing the intramolecular N—H···O hydrogen bonding, as well as the intermolecular C—H···O interactions in the crystal structure of the title compound. All hydrogen atoms not involved in these interactions have been omitted for clarity.

1-[3-(1*H*-Indol-2-yl)-2-furyl]ethanone

Crystal data

$C_{14}H_{11}NO_2$	F_{000} = 472
M_r = 225.24	D_x = 1.357 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 6968 reflections
a = 7.2780 (2) Å	θ = 2.4–27.1º
b = 14.3556 (3) Å	μ = 0.09 mm^{-1}
c = 10.7002 (2) Å	T = 173 (2) K
β = 99.4330 (10)º	Block, yellow
V = 1102.84 (4) Å^3	0.35 × 0.23 × 0.14 mm
Z = 4	

Data collection

CCD area-detector diffractometer	2212 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.075
Monochromator: graphite	θ_{max} = 28.0º
T = 173(2) K	θ_{min} = 1.9º
φ and ω scans	h = −9→9
Absorption correction: none	k = −18→18
21468 measured reflections	l = −14→14
2768 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.036$	$w = 1/[\sigma^2(F_o^2) + (0.0635P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.100$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.06$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
2768 reflections	$\Delta\rho_{min} = -0.18$ e Å^{-3}
317 parameters	Extinction correction: none
1 restraint	
Primary atom site location: structure-invariant direct methods	
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 $F^2 > 2$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}
C1A	0.1578 (3)	0.21152 (16)	0.4829 (2)	0.0323 (5)
C2A	0.1439 (3)	0.18270 (16)	0.6032 (2)	0.0364 (6)
H2A	0.0375	0.1554	0.6293	0.044*
C3A	0.3167 (4)	0.20099 (16)	0.6816 (2)	0.0349 (5)
C4A	0.3883 (4)	0.18930 (17)	0.8110 (2)	0.0417 (6)
H4A	0.3139	0.1618	0.8662	0.050*
C5A	0.5660 (4)	0.2179 (2)	0.8565 (2)	0.0453 (6)
H5A	0.6148	0.2096	0.9437	0.054*
C6A	0.6766 (4)	0.2590 (2)	0.7770 (3)	0.0458 (7)
H6A	0.7991	0.2786	0.8115	0.055*
C7A	0.6131 (4)	0.27201 (18)	0.6500 (2)	0.0382 (6)
H7A	0.6893	0.3000	0.5963	0.046*
C8A	0.4337 (3)	0.24268 (15)	0.6035 (2)	0.0318 (5)
C9A	0.0165 (3)	0.21028 (16)	0.3723 (2)	0.0336 (5)
C10A	−0.1737 (3)	0.18362 (17)	0.3743 (3)	0.0434 (6)

H10A	−0.2244	0.1636	0.4461	0.052*
C11A	−0.2652 (3)	0.1923 (2)	0.2564 (3)	0.0493 (7)
H11A	−0.3940	0.1793	0.2319	0.059*
C12B	1.1820 (3)	0.46577 (16)	0.4771 (2)	0.0320 (5)
C13A	0.1643 (3)	0.26771 (16)	0.1773 (2)	0.0344 (5)
C14A	0.1071 (4)	0.28415 (19)	0.0385 (2)	0.0421 (6)
H14A	0.2151	0.3048	0.0020	0.063*
H14B	0.0102	0.3322	0.0251	0.063*
H14C	0.0584	0.2262	−0.0026	0.063*
N1A	0.3340 (3)	0.24717 (13)	0.48294 (19)	0.0319 (4)
O1A	−0.1524 (2)	0.22201 (13)	0.17585 (18)	0.0422 (4)
O2A	0.3235 (2)	0.28245 (13)	0.23032 (16)	0.0401 (4)
H1A	0.376 (4)	0.2655 (19)	0.410 (3)	0.037 (7)*
C1B	1.0474 (3)	0.49080 (15)	0.2418 (2)	0.0308 (5)
C2B	1.0589 (3)	0.52566 (16)	0.1234 (2)	0.0360 (5)
H2B	1.1643	0.5549	0.0985	0.043*
C3B	0.8846 (4)	0.50997 (15)	0.0456 (2)	0.0333 (5)
C4B	0.8092 (4)	0.52995 (18)	−0.0817 (2)	0.0435 (6)
H4B	0.8826	0.5603	−0.1351	0.052*
C5B	0.6294 (4)	0.50511 (19)	−0.1272 (2)	0.0482 (7)
H5B	0.5783	0.5183	−0.2129	0.058*
C6B	0.5188 (4)	0.4603 (2)	−0.0492 (3)	0.0483 (7)
H6B	0.3941	0.4440	−0.0832	0.058*
C7B	0.5868 (4)	0.43953 (18)	0.0748 (2)	0.0397 (6)
H7B	0.5120	0.4087	0.1269	0.048*
C8B	0.7690 (3)	0.46518 (15)	0.1213 (2)	0.0310 (5)
C9B	1.1889 (3)	0.48966 (16)	0.3528 (2)	0.0317 (5)
C10B	1.3770 (3)	0.51843 (19)	0.3530 (3)	0.0421 (6)
H10B	1.4276	0.5403	0.2820	0.051*
C11B	1.4689 (3)	0.5088 (2)	0.4713 (3)	0.0450 (7)
H11B	1.5972	0.5225	0.4969	0.054*
C12A	0.0223 (3)	0.23417 (16)	0.2476 (2)	0.0345 (5)
C13B	1.0363 (3)	0.43421 (15)	0.5458 (2)	0.0324 (5)
C14B	1.0873 (4)	0.42508 (19)	0.6865 (2)	0.0433 (6)
H14D	0.9756	0.4104	0.7228	0.065*
H14E	1.1408	0.4839	0.7221	0.065*
H14F	1.1789	0.3750	0.7067	0.065*
N1B	0.8714 (3)	0.45416 (13)	0.24001 (18)	0.0305 (4)
O1B	1.3545 (2)	0.47702 (12)	0.54965 (16)	0.0396 (4)
O2B	0.8787 (2)	0.41725 (13)	0.49107 (16)	0.0399 (4)
H1B	0.833 (4)	0.423 (2)	0.312 (3)	0.054 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1A	0.0270 (11)	0.0269 (10)	0.0440 (13)	−0.0004 (9)	0.0088 (10)	−0.0018 (9)
C2A	0.0355 (13)	0.0311 (12)	0.0462 (15)	−0.0014 (10)	0.0177 (11)	0.0015 (10)
C3A	0.0395 (13)	0.0292 (12)	0.0386 (13)	0.0034 (10)	0.0144 (11)	0.0002 (9)

C4A	0.0594 (18)	0.0339 (12)	0.0359 (14)	0.0057 (11)	0.0195 (13)	0.0049 (10)
C5A	0.0642 (18)	0.0436 (14)	0.0274 (12)	0.0019 (13)	0.0055 (12)	0.0017 (11)
C6A	0.0479 (16)	0.0471 (16)	0.0391 (14)	−0.0075 (13)	−0.0028 (12)	0.0022 (12)
C7A	0.0391 (13)	0.0410 (13)	0.0342 (13)	−0.0045 (11)	0.0048 (10)	0.0059 (10)
C8A	0.0342 (12)	0.0290 (11)	0.0320 (12)	0.0008 (9)	0.0048 (10)	0.0044 (9)
C9A	0.0277 (12)	0.0272 (11)	0.0466 (14)	0.0025 (9)	0.0077 (10)	−0.0033 (10)
C10A	0.0278 (13)	0.0407 (14)	0.0624 (18)	−0.0029 (11)	0.0090 (12)	−0.0043 (13)
C11A	0.0231 (13)	0.0499 (16)	0.073 (2)	−0.0001 (11)	0.0029 (13)	−0.0080 (14)
C12B	0.0258 (11)	0.0315 (12)	0.0375 (12)	0.0021 (9)	0.0013 (9)	−0.0024 (10)
C13A	0.0322 (13)	0.0313 (12)	0.0389 (13)	0.0058 (10)	0.0035 (10)	−0.0032 (10)
C14A	0.0422 (14)	0.0444 (14)	0.0374 (13)	0.0049 (11)	−0.0002 (11)	−0.0048 (11)
N1A	0.0276 (10)	0.0354 (10)	0.0328 (10)	−0.0041 (8)	0.0057 (8)	0.0034 (8)
O1A	0.0261 (8)	0.0460 (10)	0.0515 (11)	0.0015 (8)	−0.0030 (8)	−0.0069 (8)
O2A	0.0300 (9)	0.0545 (11)	0.0352 (9)	−0.0006 (8)	0.0038 (7)	0.0019 (8)
C1B	0.0292 (11)	0.0291 (11)	0.0353 (12)	0.0001 (9)	0.0085 (9)	−0.0049 (9)
C2B	0.0393 (13)	0.0323 (12)	0.0400 (13)	−0.0024 (10)	0.0167 (11)	−0.0017 (10)
C3B	0.0448 (14)	0.0267 (11)	0.0303 (12)	0.0037 (10)	0.0114 (10)	−0.0013 (9)
C4B	0.0666 (18)	0.0346 (13)	0.0307 (13)	0.0046 (12)	0.0122 (12)	0.0011 (11)
C5B	0.0673 (19)	0.0444 (15)	0.0307 (13)	0.0071 (13)	0.0012 (13)	0.0004 (11)
C6B	0.0520 (16)	0.0480 (15)	0.0399 (14)	0.0019 (13)	−0.0074 (12)	−0.0068 (12)
C7B	0.0395 (14)	0.0399 (14)	0.0374 (14)	−0.0027 (11)	−0.0006 (11)	−0.0028 (11)
C8B	0.0371 (13)	0.0273 (11)	0.0283 (11)	0.0038 (9)	0.0044 (9)	−0.0024 (9)
C9B	0.0279 (11)	0.0297 (11)	0.0390 (12)	0.0015 (9)	0.0097 (10)	−0.0045 (10)
C10B	0.0286 (12)	0.0471 (14)	0.0535 (16)	−0.0025 (11)	0.0149 (12)	−0.0076 (12)
C11B	0.0253 (13)	0.0530 (16)	0.0566 (17)	−0.0014 (11)	0.0066 (12)	−0.0114 (13)
C12A	0.0236 (11)	0.0323 (12)	0.0454 (14)	0.0026 (9)	−0.0006 (10)	−0.0074 (10)
C13B	0.0328 (12)	0.0328 (12)	0.0304 (12)	0.0044 (10)	0.0018 (10)	0.0002 (9)
C14B	0.0488 (15)	0.0455 (14)	0.0346 (13)	0.0014 (12)	0.0036 (11)	0.0004 (11)
N1B	0.0308 (10)	0.0321 (9)	0.0287 (9)	−0.0031 (8)	0.0050 (8)	−0.0001 (8)
O1B	0.0273 (8)	0.0460 (10)	0.0437 (10)	0.0031 (7)	0.0004 (7)	−0.0059 (8)
O2B	0.0299 (9)	0.0521 (10)	0.0376 (9)	−0.0022 (8)	0.0048 (7)	0.0070 (8)

Geometric parameters (Å, °)

C1A—C2A	1.371 (3)	C14A—H14C	0.9800
C1A—N1A	1.381 (3)	N1A—H1A	0.93 (3)
C1A—C9A	1.435 (3)	O1A—C12A	1.384 (3)
C2A—C3A	1.417 (3)	C1B—C2B	1.378 (3)
C2A—H2A	0.9500	C1B—N1B	1.382 (3)
C3A—C4A	1.407 (4)	C1B—C9B	1.439 (3)
C3A—C8A	1.420 (3)	C2B—C3B	1.416 (4)
C4A—C5A	1.368 (4)	C2B—H2B	0.9500
C4A—H4A	0.9500	C3B—C4B	1.413 (3)
C5A—C6A	1.395 (4)	C3B—C8B	1.414 (3)
C5A—H5A	0.9500	C4B—C5B	1.367 (4)
C6A—C7A	1.374 (4)	C4B—H4B	0.9500
C6A—H6A	0.9500	C5B—C6B	1.407 (4)
C7A—C8A	1.385 (3)	C5B—H5B	0.9500
C7A—H7A	0.9500	C6B—C7B	1.370 (4)

C8A—N1A	1.374 (3)	C6B—H6B	0.9500
C9A—C12A	1.385 (3)	C7B—C8B	1.388 (3)
C9A—C10A	1.440 (3)	C7B—H7B	0.9500
C10A—C11A	1.332 (4)	C8B—N1B	1.373 (3)
C10A—H10A	0.9500	C9B—C10B	1.430 (3)
C11A—O1A	1.353 (3)	C10B—C11B	1.339 (4)
C11A—H11A	0.9500	C10B—H10B	0.9500
C12B—O1B	1.373 (3)	C11B—O1B	1.354 (3)
C12B—C9B	1.382 (3)	C11B—H11B	0.9500
C12B—C13B	1.457 (3)	C13B—O2B	1.224 (3)
C13A—O2A	1.222 (3)	C13B—C14B	1.497 (3)
C13A—C12A	1.456 (4)	C14B—H14D	0.9800
C13A—C14A	1.494 (4)	C14B—H14E	0.9800
C14A—H14A	0.9800	C14B—H14F	0.9800
C14A—H14B	0.9800	N1B—H1B	0.97 (3)
C2A—C1A—N1A	108.8 (2)	C2B—C1B—N1B	108.7 (2)
C2A—C1A—C9A	128.1 (2)	C2B—C1B—C9B	128.3 (2)
N1A—C1A—C9A	123.0 (2)	N1B—C1B—C9B	122.94 (19)
C1A—C2A—C3A	107.7 (2)	C1B—C2B—C3B	107.4 (2)
C1A—C2A—H2A	126.1	C1B—C2B—H2B	126.3
C3A—C2A—H2A	126.1	C3B—C2B—H2B	126.3
C4A—C3A—C2A	135.2 (2)	C4B—C3B—C8B	118.1 (2)
C4A—C3A—C8A	118.0 (2)	C4B—C3B—C2B	134.7 (2)
C2A—C3A—C8A	106.8 (2)	C8B—C3B—C2B	107.2 (2)
C5A—C4A—C3A	119.3 (2)	C5B—C4B—C3B	119.3 (2)
C5A—C4A—H4A	120.3	C5B—C4B—H4B	120.4
C3A—C4A—H4A	120.3	C3B—C4B—H4B	120.4
C4A—C5A—C6A	121.1 (2)	C4B—C5B—C6B	121.0 (3)
C4A—C5A—H5A	119.4	C4B—C5B—H5B	119.5
C6A—C5A—H5A	119.4	C6B—C5B—H5B	119.5
C7A—C6A—C5A	121.8 (3)	C7B—C6B—C5B	121.5 (3)
C7A—C6A—H6A	119.1	C7B—C6B—H6B	119.2
C5A—C6A—H6A	119.1	C5B—C6B—H6B	119.2
C6A—C7A—C8A	117.3 (2)	C6B—C7B—C8B	117.5 (3)
C6A—C7A—H7A	121.4	C6B—C7B—H7B	121.3
C8A—C7A—H7A	121.4	C8B—C7B—H7B	121.3
N1A—C8A—C7A	130.2 (2)	N1B—C8B—C7B	130.0 (2)
N1A—C8A—C3A	107.3 (2)	N1B—C8B—C3B	107.4 (2)
C7A—C8A—C3A	122.5 (2)	C7B—C8B—C3B	122.6 (2)
C12A—C9A—C1A	131.3 (2)	C12B—C9B—C10B	104.9 (2)
C12A—C9A—C10A	105.2 (2)	C12B—C9B—C1B	131.5 (2)
C1A—C9A—C10A	123.5 (2)	C10B—C9B—C1B	123.6 (2)
C11A—C10A—C9A	107.0 (3)	C11B—C10B—C9B	107.5 (2)
C11A—C10A—H10A	126.5	C11B—C10B—H10B	126.3
C9A—C10A—H10A	126.5	C9B—C10B—H10B	126.3
C10A—C11A—O1A	111.8 (2)	C10B—C11B—O1B	111.0 (2)
C10A—C11A—H11A	124.1	C10B—C11B—H11B	124.5
O1A—C11A—H11A	124.1	O1B—C11B—H11B	124.5
O1B—C12B—C9B	109.9 (2)	O1A—C12A—C9A	109.4 (2)

O1B—C12B—C13B	115.1 (2)	O1A—C12A—C13A	114.9 (2)
C9B—C12B—C13B	134.9 (2)	C9A—C12A—C13A	135.7 (2)
O2A—C13A—C12A	121.1 (2)	O2B—C13B—C12B	121.5 (2)
O2A—C13A—C14A	121.5 (2)	O2B—C13B—C14B	121.5 (2)
C12A—C13A—C14A	117.4 (2)	C12B—C13B—C14B	117.0 (2)
C13A—C14A—H14A	109.5	C13B—C14B—H14D	109.5
C13A—C14A—H14B	109.5	C13B—C14B—H14E	109.5
H14A—C14A—H14B	109.5	H14D—C14B—H14E	109.5
C13A—C14A—H14C	109.5	C13B—C14B—H14F	109.5
H14A—C14A—H14C	109.5	H14D—C14B—H14F	109.5
H14B—C14A—H14C	109.5	H14E—C14B—H14F	109.5
C8A—N1A—C1A	109.3 (2)	C8B—N1B—C1B	109.31 (19)
C8A—N1A—H1A	127.6 (17)	C8B—N1B—H1B	127.0 (18)
C1A—N1A—H1A	122.9 (17)	C1B—N1B—H1B	123.6 (18)
C11A—O1A—C12A	106.5 (2)	C11B—O1B—C12B	106.7 (2)
N1A—C1A—C2A—C3A	0.2 (3)	C6B—C7B—C8B—C3B	−0.8 (4)
C9A—C1A—C2A—C3A	−177.6 (2)	C4B—C3B—C8B—N1B	−179.4 (2)
C1A—C2A—C3A—C4A	178.7 (3)	C2B—C3B—C8B—N1B	−0.3 (2)
C1A—C2A—C3A—C8A	0.5 (3)	C4B—C3B—C8B—C7B	0.8 (3)
C2A—C3A—C4A—C5A	−178.2 (3)	C2B—C3B—C8B—C7B	179.9 (2)
C8A—C3A—C4A—C5A	−0.2 (3)	O1B—C12B—C9B—C10B	−1.1 (3)
C3A—C4A—C5A—C6A	0.5 (4)	C13B—C12B—C9B—C10B	177.5 (3)
C4A—C5A—C6A—C7A	−0.5 (4)	O1B—C12B—C9B—C1B	−179.4 (2)
C5A—C6A—C7A—C8A	0.1 (4)	C13B—C12B—C9B—C1B	−0.8 (5)
C6A—C7A—C8A—N1A	179.5 (2)	C2B—C1B—C9B—C12B	171.7 (3)
C6A—C7A—C8A—C3A	0.2 (4)	N1B—C1B—C9B—C12B	−8.7 (4)
C4A—C3A—C8A—N1A	−179.6 (2)	C2B—C1B—C9B—C10B	−6.3 (4)
C2A—C3A—C8A—N1A	−1.0 (2)	N1B—C1B—C9B—C10B	173.3 (2)
C4A—C3A—C8A—C7A	−0.2 (3)	C12B—C9B—C10B—C11B	1.2 (3)
C2A—C3A—C8A—C7A	178.4 (2)	C1B—C9B—C10B—C11B	179.6 (2)
C2A—C1A—C9A—C12A	−176.8 (3)	C9B—C10B—C11B—O1B	−0.8 (3)
N1A—C1A—C9A—C12A	5.8 (4)	C11A—O1A—C12A—C9A	1.0 (3)
C2A—C1A—C9A—C10A	5.1 (4)	C11A—O1A—C12A—C13A	−179.1 (2)
N1A—C1A—C9A—C10A	−172.4 (2)	C1A—C9A—C12A—O1A	−179.2 (2)
C12A—C9A—C10A—C11A	0.3 (3)	C10A—C9A—C12A—O1A	−0.8 (3)
C1A—C9A—C10A—C11A	178.9 (2)	C1A—C9A—C12A—C13A	0.9 (5)
C9A—C10A—C11A—O1A	0.3 (3)	C10A—C9A—C12A—C13A	179.3 (3)
C7A—C8A—N1A—C1A	−178.2 (2)	O2A—C13A—C12A—O1A	179.0 (2)
C3A—C8A—N1A—C1A	1.1 (2)	C14A—C13A—C12A—O1A	−0.5 (3)
C2A—C1A—N1A—C8A	−0.8 (3)	O2A—C13A—C12A—C9A	−1.1 (4)
C9A—C1A—N1A—C8A	177.1 (2)	C14A—C13A—C12A—C9A	179.4 (3)
C10A—C11A—O1A—C12A	−0.8 (3)	O1B—C12B—C13B—O2B	−176.5 (2)
N1B—C1B—C2B—C3B	−0.1 (3)	C9B—C12B—C13B—O2B	5.0 (4)
C9B—C1B—C2B—C3B	179.5 (2)	O1B—C12B—C13B—C14B	4.6 (3)
C1B—C2B—C3B—C4B	179.2 (3)	C9B—C12B—C13B—C14B	−174.0 (3)
C1B—C2B—C3B—C8B	0.2 (2)	C7B—C8B—N1B—C1B	−180.0 (2)
C8B—C3B—C4B—C5B	−0.4 (3)	C3B—C8B—N1B—C1B	0.2 (2)
C2B—C3B—C4B—C5B	−179.2 (3)	C2B—C1B—N1B—C8B	−0.1 (3)
C3B—C4B—C5B—C6B	0.1 (4)	C9B—C1B—N1B—C8B	−179.69 (19)

C4B—C5B—C6B—C7B	−0.2 (4)	C10B—C11B—O1B—C12B	0.1 (3)
C5B—C6B—C7B—C8B	0.6 (4)	C9B—C12B—O1B—C11B	0.6 (3)
C6B—C7B—C8B—N1B	179.4 (2)	C13B—C12B—O1B—C11B	−178.3 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1A—H1A···O2A	0.93 (3)	1.91 (3)	2.739 (3)	148 (2)
N1B—H1B···O2B	0.97 (3)	1.90 (3)	2.730 (3)	143 (3)
C4A—H4A···Cg^{i}	0.95	2.94	3.695 (2)	137
C7A—H7A···O2B	0.95	2.55	3.472 (3)	163
C7B—H7B···O2A	0.95	2.62	3.546 (3)	163
C11A—H11A···O2A^{ii}	0.95	2.53	3.231 (3)	131 (1)
C11B—H11B···O2B^{iii}	0.95	2.55	3.234 (3)	129 (1)

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1; (ii) *x*−1, *y*, *z*; (iii) *x*+1, *y*, *z*.

Fig. 1

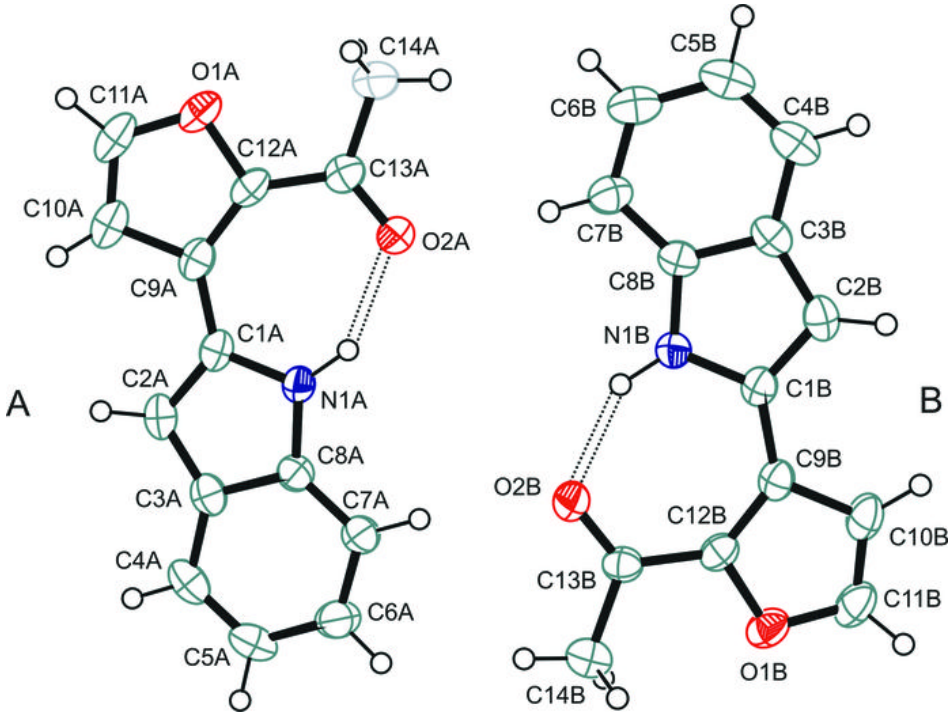
A
C14A
O1A
C11A
C12A
C13A
C10A
O2A
C9A
C1A
C2A
N1A
C8A
C3A
C7A
C4A
C6A
C5A
B
C5B
C6B
C4B
C7B
C3B
C8B
C2B
N1B
C1B
C9B
O2B
C12B
C10B
C13B
C11B
O1B
C14B

Fig. 2