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3-(9*H*-Carbazol-9-yl)propanoic acid

Manpreet Kaur,[a] Shaaban K. Mohamed,[b,c] Mehmet Akkurt,[d] Jerry P. Jasinski,[a] Talaat I. El-Emary[e] and Mustafa R. Albayati[f]*

[a]Department of Chemistry, Keene State College, 229 Main Street, Keene, NH 03435-2001, USA, [b]Chemistry and Environmental Division, Manchester Metropolitan University, Manchester M1 5GD, England, [c]Chemistry Department, Faculty of Science, Minia University, 61519 El-Minia, Egypt, [d]Department of Physics, Faculty of Sciences, Erciyes University, 38039 Kayseri, Turkey, [e]Department of Chemistry, Faculty of Science, Assiut University, 71515 Assiut, Egypt, and [f]Kirkuk University, College of Science, Department of Chemistry, Kirkuk, Iraq. *Correspondence e-mail: shaabankamel@yahoo.com

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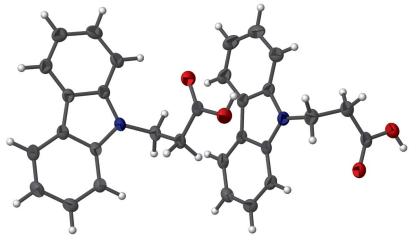
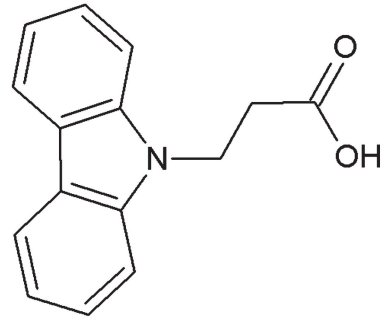
The title compound, $C_{15}H_{13}NO_2$, crystallizes with two molecules (*A* and *B*) in the asymmetric unit. The carbazole ring systems of both molecules are close to planar (r.m.s deviations = 0.035 and 0.053 Å). In the crystal, *A*+*A* and *B*+*B* inversion dimers linked by pairs of O—H···O hydrogen bonds generate $R_2^2(8)$ loops and weak C—H···π interactions link the dimers into a three-dimensional network.

3D view



Chemical scheme



Structure description

Compounds based on carbazole ring systems have been reported to exhibit diverse biological activities such as cytotoxic, antitumor, antiviral, antimicrobial, antiparasitics, antiserotonin and anti-inflammatory activities (*e.g.*: Kumara Swamy *et al.*, 2009; Broadbent *et al.*, 1998; Xia *et al.*, 2008). As part of our studies in this area, we herein report the synthesis and crystal structure of the title compound.

As shown in Fig. 1, there are two molecules (*A* and *B*) in the asymmetric unit: the carbazole ring systems of both molecules are close to planar (r.m.s deviation = 0.035 and 0.053 Å). The bond-length distributions within the molecules *A* and *B* of the title compound are almost identical. These values are in good agreement with those observed in related structures (Akkurt *et al.*, 2015; Fun *et al.*, 2010; Archana *et al.*, 2010).

In the crystal, pairwise O—H···O hydrogen bonds link pairs of molecules into *A*+*A* and *B*+*B* inversion dimers with $R_2^2(8)$ ring motifs (Fig. 2, Table 1). The three-dimensional architecture is consolidated by C—H···π interactions (Table 1).

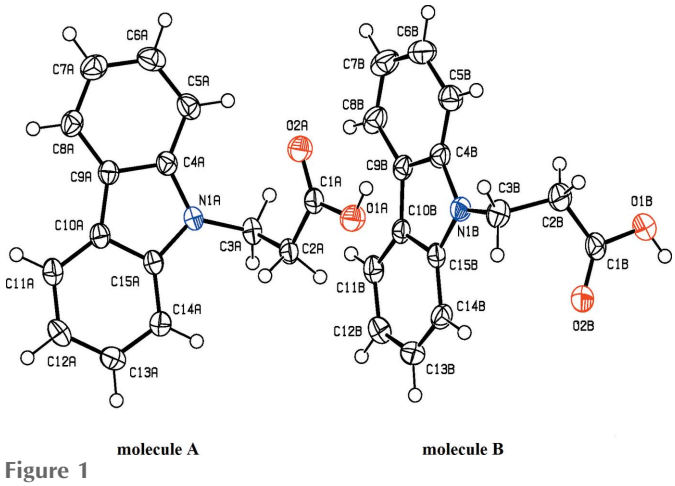


Figure 1
The title compound with 50% probability displacement ellipsoids.

Synthesis and crystallization

The title compound was obtained as an unexpected product of the reaction of 9,9a-dihydro-4a*H*-carbazole (0.01 mol, 1.69 g) with an excess of ethyl 3-chloropropanoate (0.1 mol, 13.7 g) in the presence of potassium carbonate under reflux for 3 h. The intended product was the corresponding ethyl ester, {ethyl 3-[4a*H*-carbazol-9(9a*H*)-yl]propanoate}. We assume that the ester has been hydrolysed under the basic reaction conditions employed into the corresponding carboxylic acid (title compound). The title compound was isolated by plate-layer chromatography (PLC) then the extracted product was dissolved in dimethylsulfoxide and left to evaporate slowly at room temperature to give colourless plates. The purity of the product was confirmed by TLC using ethyl acetate:cyclohexane (10: 1) as the mobile phase.

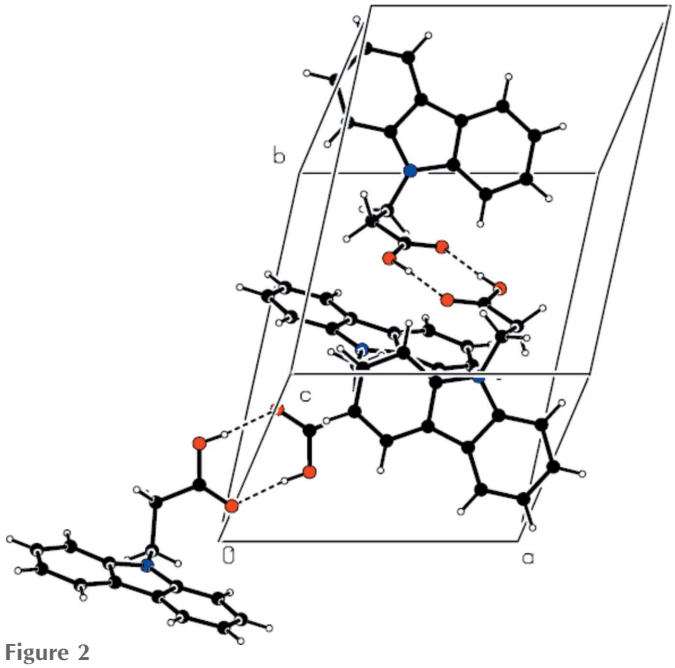


Figure 2
A view of the dimers in the unit cell with the hydrogen bonds shown by dotted lines.

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

*Cg*2 and *Cg*9 are the centroids of the C4*A*–C9*A* ring of molecule *A*, and the C10*B*–C15*B* ring of molecule *B*, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*A*—H1*A*···O2*A*^{i}	0.84	1.79	2.6310 (17)	177
O1*B*—H1*B*···O2*B*^{ii}	0.84	1.85	2.6867 (18)	174
C2*A*—H2*AB*···*Cg*9	0.99	2.64	3.5319 (19)	150
C2*B*—H2*BB*···*Cg*2^{i}	0.99	2.94	3.805 (2)	147

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{13}NO_2$
M_r	239.26
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	173
a, *b*, *c* (Å)	9.4550 (5), 11.9077 (6), 12.2120 (7)
α, β, γ (°)	62.429 (5), 79.276 (4), 77.627 (4)
V (Å^3)	1184.47 (12)
Z	4
Radiation type	Cu *K*α
μ (mm^{-1})	0.72
Crystal size (mm)	0.38 × 0.24 × 0.02
Data collection	
Diffractometer	Rigaku Oxford Diffraction Eos Gemini
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.804, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8217, 4490, 3605
R_{int}	0.041
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.615
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.045, 0.125, 1.03
No. of reflections	4490
No. of parameters	327
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.25

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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References

Agilent (2014). *CrysAlis PRO*. Agilent Technologies Ltd, Yarnton, England.
Akkurt, M., Jasinski, J. P., Mohamed, S. K., El-Emary, T. I. & Albayati, M. R. (2015). *Acta Cryst.* E**71**, o937–o938.
Archana, R., Prabakaran, K., Rajendra Prasad, K. J., Thiruvalluvar, A. & Butcher, R. J. (2010). *Acta Cryst.* E**66**, o3146.

Broadbent, A., Thomas, H. & Broadbent, S. (1998). *Curr. Med. Chem.* **5**, 469–491.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Fun, H.-K., Goh, J. H., Asiri, A. M., Khan, S. A. & Khan, K. A. (2010). *Acta Cryst.* E**66**, o1200–o1201.
Kumara Swamy, K. C., Bhuvan Kumar, N. N., Balaraman, E. & Pavan Kumar, K. V. P. (2009). *Chem. Rev.* **109**, 2551–2651.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Xia, Y., Fan, C.-D., Zhao, B.-X., Zhao, J., Shin, D.-S. & Miao, J.-Y. (2008). *Eur. J. Med. Chem.* **43**, 2347–2353.

full crystallographic data

IUCrData (2016). **1**, x161787 [https://doi.org/10.1107/S2414314616017879]

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3-(9*H*-Carbazol-9-yl)propanoic acid

Crystal data

$C_{15}H_{13}NO_2$
M_r = 239.26
Triclinic, $P\overline{1}$
a = 9.4550 (5) Å
b = 11.9077 (6) Å
c = 12.2120 (7) Å
α = 62.429 (5)°
β = 79.276 (4)°
γ = 77.627 (4)°
V = 1184.47 (12) Å^3
Z = 4
$F(000)$ = 504
D_x = 1.342 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 3450 reflections
θ = 4.1–71.2°
μ = 0.72 mm^{-1}
T = 173 K
Plate, colourless
0.38 × 0.24 × 0.02 mm

Data collection

Rigaku Oxford Diffraction Eos Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.804, T_{max} = 1.000
8217 measured reflections
4490 independent reflections
3605 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 71.4°, θ_{min} = 4.1°
h = −8→11
k = −14→13
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.125
S = 1.03
4490 reflections
327 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.070P)^2 + 0.1104P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1A	0.30384 (13)	0.53906 (11)	0.50496 (11)	0.0368 (3)
H1A	0.3728	0.4870	0.5440	0.055*
O2A	0.48660 (13)	0.63144 (11)	0.36956 (11)	0.0363 (3)
N1A	0.34738 (14)	0.92232 (12)	0.18471 (12)	0.0276 (3)
C1A	0.35653 (17)	0.62751 (14)	0.40047 (14)	0.0280 (3)
C2A	0.24026 (17)	0.72309 (14)	0.32348 (15)	0.0295 (3)
H2AA	0.1885	0.7761	0.3657	0.035*
H2AB	0.1688	0.6766	0.3179	0.035*
C3A	0.29874 (18)	0.81094 (14)	0.19250 (15)	0.0296 (3)
H3AA	0.3812	0.7615	0.1629	0.035*
H3AB	0.2214	0.8401	0.1365	0.035*
C4A	0.48895 (17)	0.94769 (14)	0.16488 (14)	0.0269 (3)
C5A	0.62051 (19)	0.87355 (16)	0.15129 (15)	0.0334 (4)
H5A	0.6234	0.7909	0.1567	0.040*
C6A	0.74688 (19)	0.92506 (17)	0.12951 (16)	0.0380 (4)
H6A	0.8380	0.8769	0.1190	0.046*
C7A	0.74389 (19)	1.04588 (17)	0.12266 (16)	0.0379 (4)
H7A	0.8327	1.0780	0.1080	0.045*
C8A	0.61415 (18)	1.11927 (15)	0.13675 (15)	0.0320 (4)
H8A	0.6129	1.2011	0.1328	0.038*
C9A	0.48409 (17)	1.07082 (14)	0.15706 (14)	0.0266 (3)
C10A	0.33290 (17)	1.12215 (14)	0.17007 (13)	0.0268 (3)
C11A	0.25935 (18)	1.23829 (15)	0.16644 (15)	0.0318 (4)
H11A	0.3119	1.3032	0.1552	0.038*
C12A	0.10905 (19)	1.25785 (16)	0.17948 (16)	0.0356 (4)
H12A	0.0580	1.3368	0.1769	0.043*
C13A	0.03124 (18)	1.16260 (16)	0.19641 (16)	0.0347 (4)
H13A	−0.0721	1.1780	0.2056	0.042*
C14A	0.10125 (18)	1.04660 (15)	0.20008 (15)	0.0307 (3)
H14A	0.0479	0.9822	0.2115	0.037*
C15A	0.25248 (17)	1.02766 (14)	0.18644 (14)	0.0264 (3)
O1B	0.19516 (14)	−0.03589 (12)	0.49393 (13)	0.0418 (3)
H1B	0.1181	−0.0596	0.4929	0.063*
O2B	0.03890 (13)	0.12573 (11)	0.51304 (12)	0.0386 (3)
N1B	0.29252 (14)	0.34102 (12)	0.39404 (12)	0.0280 (3)
C1B	0.16291 (19)	0.06936 (14)	0.50979 (14)	0.0316 (4)
C2B	0.2935 (2)	0.10816 (16)	0.52860 (17)	0.0379 (4)
H2BA	0.3736	0.1027	0.4654	0.046*
H2BB	0.3249	0.0457	0.6111	0.046*

C3B	0.27139 (19)	0.24259 (16)	0.52076 (15)	0.0337 (4)
H3BA	0.1716	0.2613	0.5569	0.040*
H3BB	0.3407	0.2452	0.5709	0.040*
C4B	0.42766 (17)	0.36444 (15)	0.32828 (15)	0.0289 (3)
C5B	0.56543 (18)	0.30203 (17)	0.36535 (17)	0.0352 (4)
H5B	0.5771	0.2303	0.4439	0.042*
C6B	0.68471 (19)	0.34902 (19)	0.28274 (19)	0.0408 (4)
H6B	0.7799	0.3092	0.3059	0.049*
C7B	0.6682 (2)	0.4534 (2)	0.16639 (18)	0.0423 (4)
H7B	0.7521	0.4831	0.1119	0.051*
C8B	0.53203 (19)	0.51376 (17)	0.12957 (17)	0.0356 (4)
H8B	0.5216	0.5843	0.0501	0.043*
C9B	0.40870 (17)	0.46945 (15)	0.21127 (14)	0.0276 (3)
C10B	0.25444 (17)	0.51095 (14)	0.20579 (14)	0.0261 (3)
C11B	0.16898 (19)	0.60655 (15)	0.11495 (15)	0.0318 (4)
H11B	0.2129	0.6587	0.0355	0.038*
C12B	0.01968 (19)	0.62424 (16)	0.14224 (16)	0.0350 (4)
H12B	−0.0394	0.6885	0.0808	0.042*
C13B	−0.04531 (18)	0.54809 (16)	0.25991 (17)	0.0348 (4)
H13B	−0.1477	0.5640	0.2778	0.042*
C14B	0.03629 (18)	0.45028 (15)	0.35055 (15)	0.0312 (3)
H14B	−0.0085	0.3980	0.4296	0.037*
C15B	0.18638 (17)	0.43128 (14)	0.32170 (14)	0.0261 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0351 (6)	0.0327 (6)	0.0308 (6)	−0.0078 (5)	0.0006 (5)	−0.0045 (5)
O2A	0.0340 (6)	0.0307 (6)	0.0326 (6)	−0.0066 (5)	0.0002 (5)	−0.0046 (5)
N1A	0.0292 (7)	0.0200 (6)	0.0321 (7)	−0.0023 (5)	−0.0034 (5)	−0.0107 (5)
C1A	0.0345 (8)	0.0225 (7)	0.0280 (7)	−0.0073 (6)	0.0019 (6)	−0.0125 (6)
C2A	0.0340 (8)	0.0211 (7)	0.0348 (8)	−0.0053 (6)	−0.0007 (6)	−0.0140 (6)
C3A	0.0383 (9)	0.0215 (7)	0.0298 (8)	−0.0044 (6)	−0.0057 (6)	−0.0112 (6)
C4A	0.0304 (8)	0.0225 (7)	0.0225 (7)	−0.0036 (6)	−0.0023 (6)	−0.0056 (6)
C5A	0.0365 (9)	0.0259 (7)	0.0301 (8)	0.0000 (6)	−0.0014 (6)	−0.0086 (6)
C6A	0.0306 (8)	0.0379 (9)	0.0322 (8)	0.0020 (7)	−0.0019 (6)	−0.0077 (7)
C7A	0.0318 (8)	0.0391 (9)	0.0335 (9)	−0.0090 (7)	−0.0041 (7)	−0.0063 (7)
C8A	0.0357 (9)	0.0277 (8)	0.0279 (8)	−0.0094 (6)	−0.0038 (6)	−0.0061 (6)
C9A	0.0302 (8)	0.0232 (7)	0.0230 (7)	−0.0048 (6)	−0.0030 (6)	−0.0068 (6)
C10A	0.0330 (8)	0.0223 (7)	0.0225 (7)	−0.0047 (6)	−0.0022 (6)	−0.0077 (6)
C11A	0.0393 (9)	0.0248 (7)	0.0333 (8)	−0.0063 (6)	−0.0018 (7)	−0.0144 (7)
C12A	0.0401 (9)	0.0278 (8)	0.0394 (9)	0.0037 (7)	−0.0042 (7)	−0.0190 (7)
C13A	0.0293 (8)	0.0346 (8)	0.0383 (9)	0.0012 (7)	−0.0037 (7)	−0.0167 (7)
C14A	0.0317 (8)	0.0266 (7)	0.0329 (8)	−0.0058 (6)	−0.0032 (6)	−0.0115 (6)
C15A	0.0312 (8)	0.0209 (7)	0.0243 (7)	−0.0032 (6)	−0.0037 (6)	−0.0076 (6)
O1B	0.0383 (7)	0.0310 (6)	0.0559 (8)	−0.0018 (5)	−0.0064 (6)	−0.0197 (6)
O2B	0.0364 (7)	0.0296 (6)	0.0469 (7)	−0.0071 (5)	0.0021 (5)	−0.0158 (5)
N1B	0.0298 (7)	0.0238 (6)	0.0275 (7)	−0.0063 (5)	0.0000 (5)	−0.0088 (5)

C1B	0.0395 (9)	0.0207 (7)	0.0251 (7)	−0.0059 (6)	0.0003 (6)	−0.0029 (6)
C2B	0.0405 (9)	0.0264 (8)	0.0346 (9)	−0.0059 (7)	−0.0073 (7)	−0.0016 (7)
C3B	0.0406 (9)	0.0320 (8)	0.0257 (8)	−0.0101 (7)	−0.0022 (6)	−0.0087 (7)
C4B	0.0307 (8)	0.0273 (7)	0.0336 (8)	−0.0074 (6)	0.0014 (6)	−0.0179 (7)
C5B	0.0348 (9)	0.0350 (9)	0.0406 (9)	−0.0034 (7)	−0.0049 (7)	−0.0210 (8)
C6B	0.0285 (8)	0.0511 (11)	0.0543 (11)	−0.0040 (7)	−0.0025 (8)	−0.0343 (9)
C7B	0.0330 (9)	0.0562 (11)	0.0492 (11)	−0.0169 (8)	0.0106 (8)	−0.0340 (10)
C8B	0.0367 (9)	0.0392 (9)	0.0355 (9)	−0.0155 (7)	0.0083 (7)	−0.0205 (7)
C9B	0.0325 (8)	0.0261 (7)	0.0300 (8)	−0.0096 (6)	0.0021 (6)	−0.0168 (6)
C10B	0.0311 (8)	0.0219 (7)	0.0280 (7)	−0.0084 (6)	0.0027 (6)	−0.0135 (6)
C11B	0.0411 (9)	0.0228 (7)	0.0284 (8)	−0.0077 (6)	0.0009 (6)	−0.0089 (6)
C12B	0.0391 (9)	0.0264 (8)	0.0356 (9)	−0.0005 (6)	−0.0060 (7)	−0.0114 (7)
C13B	0.0287 (8)	0.0348 (8)	0.0417 (9)	−0.0033 (6)	0.0004 (7)	−0.0195 (7)
C14B	0.0317 (8)	0.0285 (8)	0.0316 (8)	−0.0109 (6)	0.0042 (6)	−0.0118 (7)
C15B	0.0320 (8)	0.0197 (7)	0.0277 (7)	−0.0057 (6)	−0.0003 (6)	−0.0116 (6)

Geometric parameters (Å, º)

O1A—H1A	0.8400	O1B—H1B	0.8400
O1A—C1A	1.3153 (19)	O1B—C1B	1.319 (2)
O2A—C1A	1.222 (2)	O2B—C1B	1.224 (2)
N1A—C3A	1.4520 (19)	N1B—C3B	1.4541 (19)
N1A—C4A	1.388 (2)	N1B—C4B	1.385 (2)
N1A—C15A	1.384 (2)	N1B—C15B	1.390 (2)
C1A—C2A	1.499 (2)	C1B—C2B	1.496 (2)
C2A—H2AA	0.9900	C2B—H2BA	0.9900
C2A—H2AB	0.9900	C2B—H2BB	0.9900
C2A—C3A	1.526 (2)	C2B—C3B	1.529 (2)
C3A—H3AA	0.9900	C3B—H3BA	0.9900
C3A—H3AB	0.9900	C3B—H3BB	0.9900
C4A—C5A	1.394 (2)	C4B—C5B	1.395 (2)
C4A—C9A	1.416 (2)	C4B—C9B	1.408 (2)
C5A—H5A	0.9500	C5B—H5B	0.9500
C5A—C6A	1.385 (3)	C5B—C6B	1.388 (3)
C6A—H6A	0.9500	C6B—H6B	0.9500
C6A—C7A	1.396 (3)	C6B—C7B	1.397 (3)
C7A—H7A	0.9500	C7B—H7B	0.9500
C7A—C8A	1.378 (2)	C7B—C8B	1.377 (3)
C8A—H8A	0.9500	C8B—H8B	0.9500
C8A—C9A	1.402 (2)	C8B—C9B	1.406 (2)
C9A—C10A	1.440 (2)	C9B—C10B	1.440 (2)
C10A—C11A	1.393 (2)	C10B—C11B	1.396 (2)
C10A—C15A	1.409 (2)	C10B—C15B	1.413 (2)
C11A—H11A	0.9500	C11B—H11B	0.9500
C11A—C12A	1.381 (2)	C11B—C12B	1.382 (2)
C12A—H12A	0.9500	C12B—H12B	0.9500
C12A—C13A	1.398 (2)	C12B—C13B	1.403 (2)
C13A—H13A	0.9500	C13B—H13B	0.9500

C13A—C14A	1.382 (2)	C13B—C14B	1.384 (2)
C14A—H14A	0.9500	C14B—H14B	0.9500
C14A—C15A	1.390 (2)	C14B—C15B	1.393 (2)
C1A—O1A—H1A	109.5	C1B—O1B—H1B	109.5
C4A—N1A—C3A	128.09 (13)	C4B—N1B—C3B	123.93 (14)
C15A—N1A—C3A	122.96 (13)	C4B—N1B—C15B	108.55 (13)
C15A—N1A—C4A	108.76 (13)	C15B—N1B—C3B	127.40 (13)
O1A—C1A—C2A	112.92 (14)	O1B—C1B—C2B	112.47 (15)
O2A—C1A—O1A	123.53 (15)	O2B—C1B—O1B	123.31 (16)
O2A—C1A—C2A	123.56 (14)	O2B—C1B—C2B	124.17 (16)
C1A—C2A—H2AA	108.9	C1B—C2B—H2BA	108.4
C1A—C2A—H2AB	108.9	C1B—C2B—H2BB	108.4
C1A—C2A—C3A	113.39 (13)	C1B—C2B—C3B	115.39 (14)
H2AA—C2A—H2AB	107.7	H2BA—C2B—H2BB	107.5
C3A—C2A—H2AA	108.9	C3B—C2B—H2BA	108.4
C3A—C2A—H2AB	108.9	C3B—C2B—H2BB	108.4
N1A—C3A—C2A	113.38 (13)	N1B—C3B—C2B	112.67 (14)
N1A—C3A—H3AA	108.9	N1B—C3B—H3BA	109.1
N1A—C3A—H3AB	108.9	N1B—C3B—H3BB	109.1
C2A—C3A—H3AA	108.9	C2B—C3B—H3BA	109.1
C2A—C3A—H3AB	108.9	C2B—C3B—H3BB	109.1
H3AA—C3A—H3AB	107.7	H3BA—C3B—H3BB	107.8
N1A—C4A—C5A	130.03 (15)	N1B—C4B—C5B	128.97 (16)
N1A—C4A—C9A	108.48 (13)	N1B—C4B—C9B	109.05 (14)
C5A—C4A—C9A	121.49 (14)	C5B—C4B—C9B	121.96 (15)
C4A—C5A—H5A	121.3	C4B—C5B—H5B	121.4
C6A—C5A—C4A	117.43 (16)	C6B—C5B—C4B	117.28 (17)
C6A—C5A—H5A	121.3	C6B—C5B—H5B	121.4
C5A—C6A—H6A	119.1	C5B—C6B—H6B	119.2
C5A—C6A—C7A	121.74 (16)	C5B—C6B—C7B	121.65 (17)
C7A—C6A—H6A	119.1	C7B—C6B—H6B	119.2
C6A—C7A—H7A	119.5	C6B—C7B—H7B	119.6
C8A—C7A—C6A	121.07 (16)	C8B—C7B—C6B	120.88 (16)
C8A—C7A—H7A	119.5	C8B—C7B—H7B	119.6
C7A—C8A—H8A	120.7	C7B—C8B—H8B	120.5
C7A—C8A—C9A	118.67 (16)	C7B—C8B—C9B	119.04 (17)
C9A—C8A—H8A	120.7	C9B—C8B—H8B	120.5
C4A—C9A—C10A	107.01 (13)	C4B—C9B—C10B	106.91 (13)
C8A—C9A—C4A	119.60 (15)	C8B—C9B—C4B	119.18 (16)
C8A—C9A—C10A	133.36 (15)	C8B—C9B—C10B	133.87 (16)
C11A—C10A—C9A	134.19 (15)	C11B—C10B—C9B	133.98 (14)
C11A—C10A—C15A	119.35 (15)	C11B—C10B—C15B	119.44 (14)
C15A—C10A—C9A	106.44 (13)	C15B—C10B—C9B	106.57 (14)
C10A—C11A—H11A	120.4	C10B—C11B—H11B	120.5
C12A—C11A—C10A	119.10 (15)	C12B—C11B—C10B	119.09 (15)
C12A—C11A—H11A	120.4	C12B—C11B—H11B	120.5
C11A—C12A—H12A	119.7	C11B—C12B—H12B	119.7

C11A—C12A—C13A	120.68 (15)	C11B—C12B—C13B	120.57 (16)
C13A—C12A—H12A	119.7	C13B—C12B—H12B	119.7
C12A—C13A—H13A	119.3	C12B—C13B—H13B	119.2
C14A—C13A—C12A	121.50 (16)	C14B—C13B—C12B	121.56 (15)
C14A—C13A—H13A	119.3	C14B—C13B—H13B	119.2
C13A—C14A—H14A	121.2	C13B—C14B—H14B	121.2
C13A—C14A—C15A	117.56 (15)	C13B—C14B—C15B	117.58 (15)
C15A—C14A—H14A	121.2	C15B—C14B—H14B	121.2
N1A—C15A—C10A	109.29 (14)	N1B—C15B—C10B	108.86 (13)
N1A—C15A—C14A	128.90 (15)	N1B—C15B—C14B	129.49 (14)
C14A—C15A—C10A	121.81 (15)	C14B—C15B—C10B	121.63 (14)
O1A—C1A—C2A—C3A	−169.33 (13)	O1B—C1B—C2B—C3B	167.86 (14)
O2A—C1A—C2A—C3A	10.8 (2)	O2B—C1B—C2B—C3B	−14.6 (2)
N1A—C4A—C5A—C6A	178.64 (16)	N1B—C4B—C5B—C6B	−176.93 (16)
N1A—C4A—C9A—C8A	−179.81 (14)	N1B—C4B—C9B—C8B	177.79 (14)
N1A—C4A—C9A—C10A	−1.30 (16)	N1B—C4B—C9B—C10B	−0.40 (17)
C1A—C2A—C3A—N1A	−85.68 (17)	C1B—C2B—C3B—N1B	−85.25 (18)
C3A—N1A—C4A—C5A	−2.3 (3)	C3B—N1B—C4B—C5B	0.9 (3)
C3A—N1A—C4A—C9A	176.60 (14)	C3B—N1B—C4B—C9B	−177.33 (14)
C3A—N1A—C15A—C10A	−176.56 (13)	C3B—N1B—C15B—C10B	178.26 (14)
C3A—N1A—C15A—C14A	2.7 (2)	C3B—N1B—C15B—C14B	−0.3 (3)
C4A—N1A—C3A—C2A	108.94 (17)	C4B—N1B—C3B—C2B	−76.71 (19)
C4A—N1A—C15A—C10A	−1.21 (17)	C4B—N1B—C15B—C10B	2.18 (17)
C4A—N1A—C15A—C14A	178.09 (16)	C4B—N1B—C15B—C14B	−176.35 (16)
C4A—C5A—C6A—C7A	0.7 (3)	C4B—C5B—C6B—C7B	−0.9 (3)
C4A—C9A—C10A—C11A	−177.58 (17)	C4B—C9B—C10B—C11B	−178.26 (17)
C4A—C9A—C10A—C15A	0.56 (16)	C4B—C9B—C10B—C15B	1.69 (17)
C5A—C4A—C9A—C8A	−0.8 (2)	C5B—C4B—C9B—C8B	−0.6 (2)
C5A—C4A—C9A—C10A	177.70 (14)	C5B—C4B—C9B—C10B	−178.80 (15)
C5A—C6A—C7A—C8A	−0.3 (3)	C5B—C6B—C7B—C8B	0.1 (3)
C6A—C7A—C8A—C9A	−0.6 (2)	C6B—C7B—C8B—C9B	0.4 (3)
C7A—C8A—C9A—C4A	1.2 (2)	C7B—C8B—C9B—C4B	−0.2 (2)
C7A—C8A—C9A—C10A	−176.89 (16)	C7B—C8B—C9B—C10B	177.41 (17)
C8A—C9A—C10A—C11A	0.6 (3)	C8B—C9B—C10B—C11B	3.9 (3)
C8A—C9A—C10A—C15A	178.78 (17)	C8B—C9B—C10B—C15B	−176.11 (17)
C9A—C4A—C5A—C6A	−0.1 (2)	C9B—C4B—C5B—C6B	1.1 (2)
C9A—C10A—C11A—C12A	178.20 (16)	C9B—C10B—C11B—C12B	−177.64 (17)
C9A—C10A—C15A—N1A	0.39 (17)	C9B—C10B—C15B—N1B	−2.39 (17)
C9A—C10A—C15A—C14A	−178.98 (14)	C9B—C10B—C15B—C14B	176.28 (14)
C10A—C11A—C12A—C13A	0.2 (3)	C10B—C11B—C12B—C13B	0.6 (3)
C11A—C10A—C15A—N1A	178.85 (13)	C11B—C10B—C15B—N1B	177.58 (14)
C11A—C10A—C15A—C14A	−0.5 (2)	C11B—C10B—C15B—C14B	−3.8 (2)
C11A—C12A—C13A—C14A	−0.3 (3)	C11B—C12B—C13B—C14B	−2.4 (3)
C12A—C13A—C14A—C15A	0.1 (3)	C12B—C13B—C14B—C15B	1.1 (3)
C13A—C14A—C15A—N1A	−178.88 (15)	C13B—C14B—C15B—N1B	−179.69 (16)
C13A—C14A—C15A—C10A	0.3 (2)	C13B—C14B—C15B—C10B	1.9 (2)
C15A—N1A—C3A—C2A	−76.66 (18)	C15B—N1B—C3B—C2B	107.77 (18)

C15A—N1A—C4A—C5A	−177.33 (15)	C15B—N1B—C4B—C5B	177.16 (16)
C15A—N1A—C4A—C9A	1.56 (17)	C15B—N1B—C4B—C9B	−1.09 (17)
C15A—C10A—C11A—C12A	0.2 (2)	C15B—C10B—C11B—C12B	2.4 (2)

Hydrogen-bond geometry (Å, º)

Cg2 and Cg9 are the centroids of the C4*A*–C9*A* ring of molecule *A*, and the C10*B*–C15*B* ring of molecule *B*, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*A*—H1*A*···O2*A*^{i}	0.84	1.79	2.6310 (17)	177
O1*B*—H1*B*···O2*B*^{ii}	0.84	1.85	2.6867 (18)	174
C2*A*—H2*AB*···*Cg*9	0.99	2.64	3.5319 (19)	150
C2*B*—H2*BB*···*Cg*2^{i}	0.99	2.94	3.805 (2)	147

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