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3,5-Bis[4-(diethylamino)benzylidene]-1,1-dimethyl-4-oxopiperidinium iodide: a prospective biophotonic material

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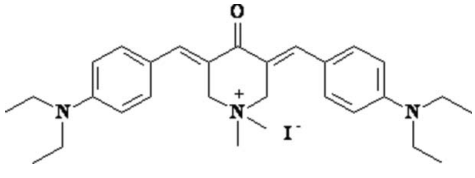
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.038; wR factor = 0.089; data-to-parameter ratio = 15.6.

In the title compound, $C_{29}H_{40}N_3O^+\cdot I^-$, the heterocyclic ring in the two independent molecules exhibits a sofa conformation, with the N atom deviating from the plane through the other ring atoms. The dihedral angles between the planar part of the heterocycle and the two almost planar fragments, which include the benzene rings and bridging atoms, are 29.21 (9)/5.43 (8) and 21.44 (10)/25.17 (10)° in the two independent molecules. Weak intermolecular C—H···O and C—H···I contacts link the cations and anions in the crystal structure.

Related literature

For related literature, see: Dimmock *et al.* (2001); Nesterov *et al.* (2003, 2007*a*,*b*); Sarkisov *et al.* (2005); Allen *et al.* (1987); Rowland & Taylor (1996).



Experimental

Crystal data

$C_{29}H_{40}N_3O^+\cdot I^-$
M_r = 573.54
Monoclinic, $P2_1/c$
a = 15.882 (3) Å
b = 25.123 (4) Å
c = 14.133 (3) Å
β = 100.882 (18)°
V = 5537.0 (18) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.18 mm^{-1}
T = 100 (2) K
0.18 × 0.12 × 0.08 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.815, T_{max} = 0.911
38649 measured reflections
9746 independent reflections
8748 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.089
S = 1.02
9746 reflections
625 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.94 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14A—H14A···O1A^{i}	0.99	2.44	3.407 (5)	167
C21A—H21A···O1A^{ii}	0.95	2.48	3.367 (4)	155
C29B—H29E···O1B^{iii}	0.98	2.59	3.491 (4)	152
C1A—H1AC···I2^{iv}	0.98	2.99	3.917 (3)	158
C1B—H1BA···I2^{v}	0.98	2.94	3.892 (3)	163

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL-NT* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL-NT*; molecular graphics: *SHELXTL-NT*; software used to prepare material for publication: *SHELXTL-NT*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2174).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–S19.
Bruker (2001). *SAINT-Plus.* Version 6.2. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2005). *APEX2*. Version 1.27. Bruker AXS Inc., Madison, Wisconsin, USA.
Dimmock, J. R., Padmanilayam, M. P., Puthucode, R. N., Nazarali, A. J., Motaganahalli, N. L., Zell, G. A., Quail, J. W., Oloo, E. O., Kraatz, H. B., Prisciak, J. S., Allen, T. M., Santos, C. L., Balzarini, J., De Clercq, E. & Manavathu, E. K. (2001). *J. Med. Chem.* **44**, 586–593.
Nesterov, V. N., Sarkisov, S. S., Curley, M. J. & Urbas, A. (2007*a*). *Acta Cryst.* E**63**, o1785–o1787.
Nesterov, V. N., Sarkisov, S. S., Curley, M. J. & Urbas, A. (2007*b*). *Acta Cryst.* E**63**, o3043–o3044.
Nesterov, V. N., Timofeeva, T. V., Sarkisov, S. S., Leyderman, A., Lee, C. Y.-C. & Antipin, M. Yu. (2003). *Acta Cryst.* C**59**, o605–o608.
Rowland, R. S. & Taylor, R. (1996). *J. Phys. Chem.* **100**, 7384–7391.
Sarkisov, S. S., Peterson, B. H., Curley, M. J., Nesterov, V. N., Timofeeva, T., Antipin, M., Radovanova, E. I., Leyderman, A. & Fleitz, P. (2005). *J. Nonlinear Opt. Phys. Mater.* **14**, 21–40.
Sheldrick, G. M. (2001). *SHELXTL-NT*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2003). *SADABS.* Version 2.03. Bruker AXS Inc., Madison, Wisconsin, USA.

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supplementary materials

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3,5-Bis[4-(diethylamino)benzylidene]-1,1-dimethyl-4-oxopiperidinium iodide: a prospective bio-photonic material

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Comment

As a continuation of our work on organic compounds containing a D-π-A-π-D motif (D = donor group, A = acceptor group) with nonlinear optical two-photon absorption (TPA) properties (Sarkisov *et al.*, 2005; Nesterov *et al.*, 2007*a*,b), we report here about the structure of the title organic salt (Fig. 1). Its TPA properties and fluorescence behavior had been published earlier (Sarkisov *et al.*, 2005). Such type of compound is well known and belongs to a group that has shown anticancer activity (Dimmock *et al.*, 2001).

The central heterocycle in two independent molecules (A and B) adopts a sofa conformation: atom N1A or N1B is out of the C2A/C3A/C4A/C5A/C6A or C2B/C3B/C4B/C5B/C6B plane (planar within 0.026 (2) and 0.011 (2), respectively) by −0.685 (2) or 0.725 (2) Å, respectively. The dihedral angles between the planar part of the central ring and the two almost flat side-chain fragments that include the aromatic ring and bridging atoms (C7A···C13A and C18A···C24A in A and C7B···C13B and C18B···C24B in B) are 29.21 (9), 5.43 (8)° and 21.44 (10), 25.17 (10) ° in A and B, respectively. Thus, both cations are slightly distorted from planarity. This might be partly due to the presence of short intramolecular contacts H2AB···H24A 1.93 Å and H6AB···H13A 2.09 Å in cation A and H2BA···H24B 2.10 Å, H6BA···H13B 2.09 Å and H12B···H16D 1.93 Å in cation B, that are shorter than the sum (2.2 Å) of the van der Waals radii of the H atoms (Rowland & Taylor, 1996). The cations have different orientations of the diethylamino substituents relative to the plane of the core: in A the three methyl groups are below the plane and one is above it, but in B two such groups are above and the others are below the one. Thus, it is possible to predict an existence the other polymorph modifications for the title compound with different orientations of such substituents (Nesterov *et al.*, 2003; Nesterov *et al.*, 2007*a*,b). Bond length distributions in the π-conjugated bridges and *p*-diethylaminophenyl fragments definitely show an alternation of single and double C—C bond lengths (Table 1) and are close to the standard conjugated values (Allen *et al.*, 1987).

There are weak intermolecular C—H···O and C—H···I contacts which link the cations and anions in the crystal (Fig. 2, Table 2).

Experimental

The title salt was obtained by the reaction of 3,5-bis[4-(diethylamino)benzylidene]-1-methyl-4-piperidone (Nesterov *et al.*, 2003) with CH_3I in 10 ml of ethanol. The precipitate was isolated and recrystallized from ethanol (melting point 505 K, yield 95%). Compound was characterized by ^1H and ^{13}C NMR spectroscopy.

Refinement

The H atoms were geometrically placed (C—H = 0.95–0.99 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C).

Figures

Fig. 1. : The asymmetric unit if the title compound showing 50% displacement ellipsoids (arbitrary spheres for the H atoms).

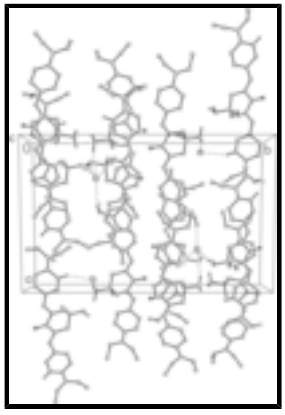


Fig. 2. : Projection of the crystal packing of the title compound along the *c* axis. Dashed lines denote intermolecular C—H···O and C—H···I contacts. The rest H atoms are omitted for clarity.

3,5-Bis[4-(diethylamino)benzylidene]-1,1-dimethyl-4-oxopiperidinium iodide

Crystal data

$C_{29}H_{40}N_3O^+\cdot I^-$	F_{000} = 2368
M_r = 573.54	D_x = 1.376 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3246 reflections
a = 15.882 (3) Å	θ = 3–26º
b = 25.123 (4) Å	μ = 1.18 mm^{-1}
c = 14.133 (3) Å	T = 100 (2) K
β = 100.882 (18)º	Plate, red
V = 5537.0 (18) Å^3	0.18 × 0.12 × 0.08 mm
Z = 8	

Data collection

Bruker SMART APEX II CCD diffractometer	9746 independent reflections
Radiation source: fine-focus sealed tube	8748 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.028
T = 100(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	h = −18→18
T_{min} = 0.815, T_{max} = 0.911	k = −29→29
38649 measured reflections	l = −15→16

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.038$	H-atom parameters constrained
$wR(F^2) = 0.089$	$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 12.931P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.002$
9746 reflections	$\Delta\rho_{max} = 0.94$ e Å^{-3}
625 parameters	$\Delta\rho_{min} = -0.59$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.262883 (13)	0.210152 (8)	0.151916 (15)	0.02940 (7)
I2	0.925132 (13)	0.223388 (8)	0.269180 (15)	0.02980 (7)
O1A	0.27250 (13)	0.02653 (8)	0.55043 (16)	0.0263 (5)
N1A	0.18568 (15)	0.16665 (9)	0.41795 (17)	0.0203 (5)
N2A	−0.21285 (17)	0.09166 (11)	0.6680 (2)	0.0322 (6)
N3A	0.67504 (16)	0.14195 (10)	0.3071 (2)	0.0272 (6)
C1A	0.1676 (2)	0.22418 (11)	0.3928 (2)	0.0243 (6)
H1AA	0.1922	0.2335	0.3364	0.036*
H1AB	0.1933	0.2466	0.4475	0.036*
H1AC	0.1055	0.2300	0.3783	0.036*
C2A	0.28133 (18)	0.15926 (12)	0.4367 (2)	0.0232 (6)
H2AA	0.3080	0.1854	0.4858	0.028*
H2AB	0.3029	0.1666	0.3767	0.028*
C3A	0.30808 (18)	0.10402 (11)	0.4713 (2)	0.0212 (6)
C4A	0.25282 (18)	0.07211 (11)	0.5224 (2)	0.0215 (6)
C5A	0.17140 (18)	0.09652 (11)	0.5381 (2)	0.0207 (6)
C6A	0.15162 (19)	0.15337 (11)	0.5086 (2)	0.0225 (6)
H6AA	0.1781	0.1774	0.5615	0.027*

H6AB	0.0888	0.1590	0.4968	0.027*
C7A	0.11637 (19)	0.06501 (12)	0.5752 (2)	0.0228 (6)
H7AA	0.1361	0.0295	0.5870	0.027*
C8A	0.03401 (18)	0.07478 (12)	0.6002 (2)	0.0222 (6)
C9A	−0.01971 (19)	0.03115 (12)	0.6069 (2)	0.0249 (6)
H9AA	0.0005	−0.0035	0.5957	0.030*
C10A	−0.0998 (2)	0.03595 (13)	0.6287 (2)	0.0282 (7)
H10A	−0.1339	0.0051	0.6308	0.034*
C11A	−0.1324 (2)	0.08644 (12)	0.6481 (2)	0.0256 (6)
C12A	−0.07684 (19)	0.13055 (12)	0.6475 (2)	0.0256 (6)
H12A	−0.0949	0.1648	0.6642	0.031*
C13A	0.00269 (19)	0.12486 (12)	0.6234 (2)	0.0243 (6)
H13A	0.0376	0.1555	0.6224	0.029*
C14A	−0.2752 (2)	0.04791 (14)	0.6505 (3)	0.0345 (8)
H14A	−0.2644	0.0268	0.5949	0.041*
H14B	−0.3336	0.0631	0.6332	0.041*
C15A	−0.2716 (2)	0.01140 (15)	0.7361 (3)	0.0399 (8)
H15A	−0.3130	−0.0176	0.7191	0.060*
H15B	−0.2857	0.0316	0.7904	0.060*
H15C	−0.2137	−0.0035	0.7542	0.060*
C16A	−0.2442 (2)	0.14281 (14)	0.6965 (3)	0.0341 (8)
H16A	−0.1958	0.1626	0.7354	0.041*
H16B	−0.2871	0.1363	0.7377	0.041*
C17A	−0.2847 (3)	0.17705 (16)	0.6113 (3)	0.0450 (9)
H17A	−0.3067	0.2100	0.6348	0.068*
H17B	−0.3320	0.1575	0.5716	0.068*
H17C	−0.2416	0.1857	0.5724	0.068*
C18A	0.38354 (19)	0.08157 (12)	0.4602 (2)	0.0237 (6)
H18A	0.3904	0.0461	0.4837	0.028*
C19A	0.45540 (19)	0.10021 (12)	0.4203 (2)	0.0237 (6)
C20A	0.52267 (19)	0.06425 (12)	0.4167 (2)	0.0262 (7)
H20A	0.5173	0.0289	0.4389	0.031*
C21A	0.5956 (2)	0.07732 (12)	0.3829 (2)	0.0277 (7)
H21A	0.6397	0.0516	0.3842	0.033*
C22A	0.60573 (19)	0.12870 (12)	0.3462 (2)	0.0254 (6)
C23A	0.5394 (2)	0.16564 (12)	0.3504 (3)	0.0308 (7)
H23A	0.5445	0.2009	0.3281	0.037*
C24A	0.4677 (2)	0.15174 (12)	0.3859 (2)	0.0299 (7)
H24A	0.4248	0.1779	0.3874	0.036*
C25A	0.7429 (2)	0.10379 (13)	0.3006 (3)	0.0312 (7)
H25A	0.7714	0.1143	0.2469	0.037*
H25B	0.7168	0.0683	0.2851	0.037*
C26A	0.8100 (2)	0.09969 (15)	0.3922 (3)	0.0431 (9)
H26A	0.8532	0.0732	0.3835	0.065*
H26B	0.7824	0.0888	0.4457	0.065*
H26C	0.8376	0.1344	0.4068	0.065*
C27A	0.6854 (2)	0.19618 (12)	0.2737 (2)	0.0304 (7)
H27A	0.6305	0.2080	0.2339	0.036*
H27B	0.7291	0.1960	0.2321	0.036*

C28A	0.7122 (2)	0.23591 (13)	0.3546 (3)	0.0347 (8)
H28A	0.7172	0.2714	0.3273	0.052*
H28B	0.7678	0.2254	0.3929	0.052*
H28C	0.6691	0.2367	0.3959	0.052*
C29A	0.14350 (19)	0.13286 (12)	0.3351 (2)	0.0252 (6)
H29A	0.1663	0.1422	0.2775	0.038*
H29B	0.0815	0.1391	0.3229	0.038*
H29C	0.1551	0.0952	0.3507	0.038*
O1B	0.93706 (14)	0.48758 (9)	0.38809 (17)	0.0322 (5)
N1B	1.00050 (16)	0.34183 (10)	0.50709 (18)	0.0232 (5)
N2B	1.39888 (17)	0.38884 (10)	0.2338 (2)	0.0306 (6)
N3B	0.51465 (17)	0.35744 (11)	0.5882 (2)	0.0305 (6)
C1B	1.0143 (2)	0.28396 (12)	0.5312 (2)	0.0267 (7)
H1BA	0.9860	0.2749	0.5850	0.040*
H1BB	1.0759	0.2768	0.5495	0.040*
H1BC	0.9900	0.2624	0.4749	0.040*
C2B	0.90571 (19)	0.35101 (12)	0.4763 (2)	0.0254 (6)
H2BA	0.8763	0.3407	0.5293	0.030*
H2BB	0.8834	0.3282	0.4200	0.030*
C3B	0.88609 (19)	0.40851 (12)	0.4502 (2)	0.0242 (6)
C4B	0.94958 (19)	0.44054 (12)	0.4086 (2)	0.0254 (6)
C5B	1.02852 (19)	0.41238 (12)	0.3927 (2)	0.0242 (6)
C6B	1.04330 (19)	0.35528 (12)	0.4236 (2)	0.0237 (6)
H6BA	1.1057	0.3487	0.4424	0.028*
H6BB	1.0206	0.3317	0.3686	0.028*
C7B	1.08469 (19)	0.43981 (12)	0.3505 (2)	0.0257 (6)
H7BA	1.0697	0.4760	0.3369	0.031*
C8B	1.16393 (19)	0.42324 (12)	0.3224 (2)	0.0242 (6)
C9B	1.2215 (2)	0.46305 (12)	0.3066 (2)	0.0267 (7)
H9BA	1.2065	0.4992	0.3145	0.032*
C10B	1.2985 (2)	0.45210 (12)	0.2803 (2)	0.0266 (7)
H10B	1.3364	0.4806	0.2738	0.032*
C11B	1.3228 (2)	0.39941 (12)	0.2625 (2)	0.0261 (6)
C12B	1.26324 (19)	0.35903 (12)	0.2741 (2)	0.0248 (6)
H12B	1.2758	0.3231	0.2612	0.030*
C13B	1.1873 (2)	0.37076 (12)	0.3039 (2)	0.0250 (6)
H13B	1.1497	0.3425	0.3122	0.030*
C14B	1.4516 (2)	0.43253 (13)	0.2093 (2)	0.0307 (7)
H14C	1.4136	0.4616	0.1795	0.037*
H14D	1.4847	0.4199	0.1610	0.037*
C15B	1.5135 (2)	0.45446 (15)	0.2957 (3)	0.0408 (8)
H15D	1.5422	0.4861	0.2763	0.061*
H15E	1.5564	0.4273	0.3203	0.061*
H15F	1.4817	0.4642	0.3463	0.061*
C16B	1.4219 (2)	0.33538 (13)	0.2071 (3)	0.0360 (8)
H16C	1.4032	0.3310	0.1366	0.043*
H16D	1.3900	0.3092	0.2390	0.043*
C17B	1.5168 (2)	0.32291 (16)	0.2335 (3)	0.0482 (10)
H17D	1.5262	0.2852	0.2210	0.072*

H17E	1.5373	0.3305	0.3020	0.072*
H17F	1.5482	0.3449	0.1946	0.072*
C18B	0.81378 (19)	0.43279 (12)	0.4639 (2)	0.0252 (6)
H18B	0.8117	0.4700	0.4515	0.030*
C19B	0.73842 (19)	0.41123 (12)	0.4947 (2)	0.0258 (6)
C20B	0.6822 (2)	0.44641 (13)	0.5288 (2)	0.0281 (7)
H20B	0.6947	0.4834	0.5307	0.034*
C21B	0.6096 (2)	0.42922 (13)	0.5596 (2)	0.0297 (7)
H21B	0.5749	0.4545	0.5843	0.036*
C22B	0.5856 (2)	0.37527 (13)	0.5553 (2)	0.0272 (7)
C23B	0.6386 (2)	0.34044 (13)	0.5153 (3)	0.0323 (7)
H23B	0.6231	0.3040	0.5074	0.039*
C24B	0.7127 (2)	0.35767 (13)	0.4873 (3)	0.0313 (7)
H24B	0.7474	0.3325	0.4623	0.038*
C25B	0.4591 (2)	0.39408 (14)	0.6285 (2)	0.0328 (7)
H25C	0.4955	0.4204	0.6694	0.039*
H25D	0.4274	0.3737	0.6705	0.039*
C26B	0.3950 (2)	0.42358 (15)	0.5541 (3)	0.0435 (9)
H26D	0.3631	0.4489	0.5864	0.065*
H26E	0.3551	0.3981	0.5171	0.065*
H26F	0.4255	0.4428	0.5104	0.065*
C27B	0.4833 (2)	0.30308 (14)	0.5693 (3)	0.0399 (8)
H27C	0.4472	0.2936	0.6167	0.048*
H27D	0.5330	0.2785	0.5793	0.048*
C28B	0.4323 (3)	0.29476 (18)	0.4698 (3)	0.0563 (11)
H28D	0.4150	0.2573	0.4617	0.085*
H28E	0.4674	0.3041	0.4222	0.085*
H28F	0.3811	0.3174	0.4604	0.085*
C29B	1.0362 (2)	0.37463 (13)	0.5939 (2)	0.0285 (7)
H29D	1.0055	0.3662	0.6461	0.043*
H29E	1.0291	0.4125	0.5777	0.043*
H29F	1.0972	0.3666	0.6148	0.043*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.02423 (12)	0.03144 (12)	0.03431 (13)	−0.00020 (8)	0.01009 (9)	0.00265 (8)
I2	0.02210 (12)	0.03461 (12)	0.03428 (13)	0.00125 (8)	0.00937 (9)	−0.00015 (8)
O1A	0.0246 (11)	0.0211 (11)	0.0346 (12)	0.0033 (8)	0.0096 (9)	0.0028 (9)
N1A	0.0173 (12)	0.0206 (12)	0.0236 (13)	0.0010 (9)	0.0058 (10)	0.0010 (10)
N2A	0.0226 (13)	0.0345 (15)	0.0417 (16)	−0.0011 (11)	0.0120 (12)	−0.0089 (12)
N3A	0.0203 (13)	0.0241 (13)	0.0396 (15)	0.0010 (10)	0.0114 (11)	0.0036 (11)
C1A	0.0227 (15)	0.0209 (15)	0.0304 (16)	0.0050 (12)	0.0081 (13)	0.0038 (12)
C2A	0.0160 (14)	0.0245 (15)	0.0297 (16)	0.0008 (11)	0.0055 (12)	0.0025 (12)
C3A	0.0187 (14)	0.0219 (14)	0.0234 (15)	0.0008 (11)	0.0047 (12)	−0.0010 (12)
C4A	0.0179 (14)	0.0233 (15)	0.0235 (15)	0.0025 (11)	0.0043 (12)	−0.0018 (12)
C5A	0.0222 (15)	0.0205 (14)	0.0199 (14)	0.0020 (11)	0.0054 (12)	−0.0026 (11)
C6A	0.0221 (15)	0.0225 (15)	0.0253 (15)	0.0027 (12)	0.0108 (12)	0.0010 (12)

C7A	0.0221 (15)	0.0220 (14)	0.0237 (15)	0.0018 (12)	0.0031 (12)	−0.0025 (12)
C8A	0.0204 (15)	0.0258 (15)	0.0206 (14)	0.0003 (12)	0.0049 (12)	0.0002 (12)
C9A	0.0257 (16)	0.0238 (15)	0.0265 (16)	−0.0003 (12)	0.0080 (13)	−0.0018 (12)
C10A	0.0255 (16)	0.0268 (16)	0.0341 (17)	−0.0039 (13)	0.0107 (14)	−0.0040 (13)
C11A	0.0246 (16)	0.0302 (16)	0.0229 (15)	0.0007 (13)	0.0069 (12)	−0.0019 (12)
C12A	0.0250 (16)	0.0251 (15)	0.0277 (16)	0.0032 (12)	0.0074 (13)	−0.0031 (12)
C13A	0.0256 (16)	0.0235 (15)	0.0252 (15)	−0.0014 (12)	0.0081 (13)	−0.0011 (12)
C14A	0.0239 (17)	0.043 (2)	0.0377 (19)	−0.0037 (14)	0.0096 (14)	−0.0109 (15)
C15A	0.0366 (19)	0.045 (2)	0.042 (2)	−0.0117 (16)	0.0152 (16)	−0.0104 (16)
C16A	0.0285 (17)	0.0376 (19)	0.0392 (19)	0.0019 (14)	0.0138 (15)	−0.0088 (15)
C17A	0.041 (2)	0.048 (2)	0.047 (2)	0.0117 (17)	0.0107 (17)	−0.0040 (18)
C18A	0.0225 (15)	0.0226 (15)	0.0259 (15)	0.0014 (12)	0.0047 (12)	−0.0014 (12)
C19A	0.0224 (15)	0.0218 (14)	0.0276 (16)	0.0019 (12)	0.0068 (12)	0.0016 (12)
C20A	0.0242 (16)	0.0211 (15)	0.0348 (17)	0.0008 (12)	0.0089 (13)	0.0040 (13)
C21A	0.0223 (16)	0.0238 (15)	0.0386 (18)	0.0042 (12)	0.0097 (13)	0.0002 (13)
C22A	0.0214 (15)	0.0234 (15)	0.0316 (17)	0.0005 (12)	0.0056 (13)	−0.0005 (12)
C23A	0.0248 (16)	0.0201 (15)	0.050 (2)	0.0005 (12)	0.0130 (15)	0.0035 (14)
C24A	0.0231 (16)	0.0213 (15)	0.048 (2)	0.0054 (12)	0.0120 (14)	0.0035 (14)
C25A	0.0259 (16)	0.0277 (16)	0.043 (2)	0.0006 (13)	0.0158 (15)	−0.0003 (14)
C26A	0.0295 (18)	0.0368 (19)	0.062 (2)	0.0044 (15)	0.0049 (17)	0.0130 (18)
C27A	0.0275 (17)	0.0266 (16)	0.0396 (19)	0.0006 (13)	0.0129 (14)	0.0042 (14)
C28A	0.0321 (18)	0.0306 (17)	0.046 (2)	−0.0027 (14)	0.0189 (16)	−0.0034 (15)
C29A	0.0230 (15)	0.0270 (16)	0.0244 (15)	0.0010 (12)	0.0010 (12)	−0.0016 (12)
O1B	0.0300 (12)	0.0249 (12)	0.0428 (14)	0.0029 (9)	0.0101 (10)	0.0034 (10)
N1B	0.0212 (12)	0.0240 (13)	0.0252 (13)	0.0021 (10)	0.0063 (10)	0.0014 (10)
N2B	0.0276 (14)	0.0228 (13)	0.0439 (17)	−0.0001 (11)	0.0131 (12)	−0.0011 (12)
N3B	0.0235 (14)	0.0306 (14)	0.0389 (16)	0.0004 (11)	0.0103 (12)	0.0000 (12)
C1B	0.0261 (16)	0.0246 (15)	0.0313 (17)	0.0042 (12)	0.0103 (13)	0.0048 (13)
C2B	0.0191 (15)	0.0278 (16)	0.0296 (16)	0.0014 (12)	0.0056 (12)	0.0007 (13)
C3B	0.0219 (15)	0.0250 (15)	0.0260 (16)	0.0009 (12)	0.0052 (12)	−0.0016 (12)
C4B	0.0230 (15)	0.0277 (16)	0.0255 (16)	0.0009 (12)	0.0051 (12)	−0.0022 (12)
C5B	0.0240 (15)	0.0255 (15)	0.0229 (15)	−0.0006 (12)	0.0036 (12)	−0.0006 (12)
C6B	0.0221 (15)	0.0256 (15)	0.0256 (15)	0.0005 (12)	0.0099 (12)	0.0024 (12)
C7B	0.0242 (16)	0.0256 (15)	0.0272 (16)	−0.0007 (12)	0.0046 (13)	−0.0010 (12)
C8B	0.0235 (15)	0.0259 (15)	0.0223 (15)	0.0007 (12)	0.0019 (12)	0.0017 (12)
C9B	0.0276 (16)	0.0204 (15)	0.0314 (17)	0.0007 (12)	0.0041 (13)	0.0016 (12)
C10B	0.0228 (15)	0.0243 (15)	0.0335 (17)	−0.0038 (12)	0.0069 (13)	0.0002 (13)
C11B	0.0245 (16)	0.0265 (15)	0.0277 (16)	−0.0011 (12)	0.0056 (13)	0.0009 (12)
C12B	0.0255 (16)	0.0220 (15)	0.0274 (16)	0.0002 (12)	0.0058 (13)	0.0007 (12)
C13B	0.0267 (16)	0.0245 (15)	0.0246 (15)	−0.0042 (12)	0.0068 (13)	0.0023 (12)
C14B	0.0274 (17)	0.0264 (16)	0.0406 (19)	−0.0003 (13)	0.0121 (14)	−0.0008 (14)
C15B	0.0305 (19)	0.040 (2)	0.053 (2)	−0.0031 (15)	0.0110 (17)	−0.0077 (17)
C16B	0.0326 (18)	0.0267 (17)	0.050 (2)	0.0021 (14)	0.0105 (16)	−0.0055 (15)
C17B	0.041 (2)	0.040 (2)	0.067 (3)	0.0084 (17)	0.0160 (19)	−0.0013 (19)
C18B	0.0228 (15)	0.0255 (15)	0.0263 (16)	−0.0007 (12)	0.0026 (12)	0.0013 (12)
C19B	0.0211 (15)	0.0277 (16)	0.0281 (16)	0.0013 (12)	0.0038 (12)	−0.0023 (13)
C20B	0.0252 (16)	0.0243 (15)	0.0342 (17)	0.0017 (12)	0.0038 (13)	−0.0018 (13)
C21B	0.0248 (16)	0.0273 (16)	0.0374 (18)	0.0048 (13)	0.0072 (14)	−0.0049 (14)
C22B	0.0241 (16)	0.0299 (16)	0.0265 (16)	0.0028 (13)	0.0022 (13)	−0.0002 (13)

C23B	0.0271 (17)	0.0251 (16)	0.046 (2)	−0.0008 (13)	0.0095 (15)	−0.0038 (14)
C24B	0.0237 (16)	0.0278 (16)	0.044 (2)	0.0020 (13)	0.0101 (14)	−0.0081 (14)
C25B	0.0308 (18)	0.0360 (18)	0.0348 (18)	0.0032 (14)	0.0144 (14)	0.0004 (14)
C26B	0.036 (2)	0.041 (2)	0.055 (2)	0.0114 (16)	0.0108 (17)	0.0025 (18)
C27B	0.0328 (19)	0.0329 (18)	0.059 (2)	−0.0006 (15)	0.0218 (17)	0.0029 (17)
C28B	0.053 (3)	0.050 (2)	0.066 (3)	−0.013 (2)	0.013 (2)	−0.020 (2)
C29B	0.0257 (16)	0.0339 (17)	0.0252 (16)	0.0019 (13)	0.0028 (13)	−0.0006 (13)

Geometric parameters (Å, °)

O1A—C4A	1.232 (4)	O1B—C4B	1.224 (4)
N1A—C29A	1.498 (4)	N1B—C29B	1.498 (4)
N1A—C1A	1.503 (4)	N1B—C1B	1.500 (4)
N1A—C2A	1.503 (4)	N1B—C2B	1.504 (4)
N1A—C6A	1.520 (4)	N1B—C6B	1.507 (4)
N2A—C11A	1.366 (4)	N2B—C11B	1.371 (4)
N2A—C16A	1.461 (4)	N2B—C16B	1.460 (4)
N2A—C14A	1.469 (4)	N2B—C14B	1.461 (4)
N3A—C22A	1.362 (4)	N3B—C22B	1.372 (4)
N3A—C25A	1.458 (4)	N3B—C27B	1.461 (4)
N3A—C27A	1.461 (4)	N3B—C25B	1.463 (4)
C1A—H1AA	0.9800	C1B—H1BA	0.9800
C1A—H1AB	0.9800	C1B—H1BB	0.9800
C1A—H1AC	0.9800	C1B—H1BC	0.9800
C2A—C3A	1.505 (4)	C2B—C3B	1.509 (4)
C2A—H2AA	0.9900	C2B—H2BA	0.9900
C2A—H2AB	0.9900	C2B—H2BB	0.9900
C3A—C18A	1.360 (4)	C3B—C18B	1.346 (4)
C3A—C4A	1.475 (4)	C3B—C4B	1.494 (4)
C4A—C5A	1.485 (4)	C4B—C5B	1.493 (4)
C5A—C7A	1.356 (4)	C5B—C7B	1.352 (4)
C5A—C6A	1.504 (4)	C5B—C6B	1.505 (4)
C6A—H6AA	0.9900	C6B—H6BA	0.9900
C6A—H6AB	0.9900	C6B—H6BB	0.9900
C7A—C8A	1.439 (4)	C7B—C8B	1.450 (4)
C7A—H7AA	0.9500	C7B—H7BA	0.9500
C8A—C9A	1.403 (4)	C8B—C9B	1.401 (4)
C8A—C13A	1.414 (4)	C8B—C13B	1.408 (4)
C9A—C10A	1.369 (4)	C9B—C10B	1.372 (4)
C9A—H9AA	0.9500	C9B—H9BA	0.9500
C10A—C11A	1.416 (4)	C10B—C11B	1.414 (4)
C10A—H10A	0.9500	C10B—H10B	0.9500
C11A—C12A	1.417 (4)	C11B—C12B	1.418 (4)
C12A—C13A	1.376 (4)	C12B—C13B	1.382 (4)
C12A—H12A	0.9500	C12B—H12B	0.9500
C13A—H13A	0.9500	C13B—H13B	0.9500
C14A—C15A	1.510 (5)	C14B—C15B	1.518 (5)
C14A—H14A	0.9900	C14B—H14C	0.9900
C14A—H14B	0.9900	C14B—H14D	0.9900

C15A—H15A	0.9800	C15B—H15D	0.9800
C15A—H15B	0.9800	C15B—H15E	0.9800
C15A—H15C	0.9800	C15B—H15F	0.9800
C16A—C17A	1.521 (5)	C16B—C17B	1.515 (5)
C16A—H16A	0.9900	C16B—H16C	0.9900
C16A—H16B	0.9900	C16B—H16D	0.9900
C17A—H17A	0.9800	C17B—H17D	0.9800
C17A—H17B	0.9800	C17B—H17E	0.9800
C17A—H17C	0.9800	C17B—H17F	0.9800
C18A—C19A	1.443 (4)	C18B—C19B	1.453 (4)
C18A—H18A	0.9500	C18B—H18B	0.9500
C19A—C20A	1.407 (4)	C19B—C24B	1.405 (4)
C19A—C24A	1.409 (4)	C19B—C20B	1.405 (4)
C20A—C21A	1.374 (4)	C20B—C21B	1.376 (5)
C20A—H20A	0.9500	C20B—H20B	0.9500
C21A—C22A	1.412 (4)	C21B—C22B	1.406 (4)
C21A—H21A	0.9500	C21B—H21B	0.9500
C22A—C23A	1.414 (4)	C22B—C23B	1.405 (4)
C23A—C24A	1.373 (4)	C23B—C24B	1.379 (5)
C23A—H23A	0.9500	C23B—H23B	0.9500
C24A—H24A	0.9500	C24B—H24B	0.9500
C25A—C26A	1.518 (5)	C25B—C26B	1.512 (5)
C25A—H25A	0.9900	C25B—H25C	0.9900
C25A—H25B	0.9900	C25B—H25D	0.9900
C26A—H26A	0.9800	C26B—H26D	0.9800
C26A—H26B	0.9800	C26B—H26E	0.9800
C26A—H26C	0.9800	C26B—H26F	0.9800
C27A—C28A	1.517 (5)	C27B—C28B	1.499 (6)
C27A—H27A	0.9900	C27B—H27C	0.9900
C27A—H27B	0.9900	C27B—H27D	0.9900
C28A—H28A	0.9800	C28B—H28D	0.9800
C28A—H28B	0.9800	C28B—H28E	0.9800
C28A—H28C	0.9800	C28B—H28F	0.9800
C29A—H29A	0.9800	C29B—H29D	0.9800
C29A—H29B	0.9800	C29B—H29E	0.9800
C29A—H29C	0.9800	C29B—H29F	0.9800
C29A—N1A—C1A	108.8 (2)	C29B—N1B—C1B	109.3 (2)
C29A—N1A—C2A	110.8 (2)	C29B—N1B—C2B	110.8 (2)
C1A—N1A—C2A	107.6 (2)	C1B—N1B—C2B	108.0 (2)
C29A—N1A—C6A	110.9 (2)	C29B—N1B—C6B	111.2 (2)
C1A—N1A—C6A	109.1 (2)	C1B—N1B—C6B	109.1 (2)
C2A—N1A—C6A	109.4 (2)	C2B—N1B—C6B	108.3 (2)
C11A—N2A—C16A	121.4 (3)	C11B—N2B—C16B	122.1 (3)
C11A—N2A—C14A	121.3 (3)	C11B—N2B—C14B	120.1 (3)
C16A—N2A—C14A	116.8 (3)	C16B—N2B—C14B	116.6 (3)
C22A—N3A—C25A	121.9 (3)	C22B—N3B—C27B	121.1 (3)
C22A—N3A—C27A	120.5 (3)	C22B—N3B—C25B	121.4 (3)
C25A—N3A—C27A	117.6 (2)	C27B—N3B—C25B	116.7 (3)
N1A—C1A—H1AA	109.5	N1B—C1B—H1BA	109.5

N1A—C1A—H1AB	109.5	N1B—C1B—H1BB	109.5
H1AA—C1A—H1AB	109.5	H1BA—C1B—H1BB	109.5
N1A—C1A—H1AC	109.5	N1B—C1B—H1BC	109.5
H1AA—C1A—H1AC	109.5	H1BA—C1B—H1BC	109.5
H1AB—C1A—H1AC	109.5	H1BB—C1B—H1BC	109.5
N1A—C2A—C3A	112.6 (2)	N1B—C2B—C3B	111.5 (2)
N1A—C2A—H2AA	109.1	N1B—C2B—H2BA	109.3
C3A—C2A—H2AA	109.1	C3B—C2B—H2BA	109.3
N1A—C2A—H2AB	109.1	N1B—C2B—H2BB	109.3
C3A—C2A—H2AB	109.1	C3B—C2B—H2BB	109.3
H2AA—C2A—H2AB	107.8	H2BA—C2B—H2BB	108.0
C18A—C3A—C4A	116.7 (3)	C18B—C3B—C4B	118.0 (3)
C18A—C3A—C2A	123.1 (3)	C18B—C3B—C2B	122.7 (3)
C4A—C3A—C2A	120.2 (2)	C4B—C3B—C2B	119.2 (3)
O1A—C4A—C3A	121.6 (3)	O1B—C4B—C5B	121.7 (3)
O1A—C4A—C5A	120.7 (3)	O1B—C4B—C3B	121.4 (3)
C3A—C4A—C5A	117.6 (2)	C5B—C4B—C3B	116.9 (3)
C7A—C5A—C4A	117.3 (3)	C7B—C5B—C4B	117.9 (3)
C7A—C5A—C6A	123.0 (3)	C7B—C5B—C6B	122.3 (3)
C4A—C5A—C6A	119.6 (2)	C4B—C5B—C6B	119.8 (3)
C5A—C6A—N1A	110.6 (2)	C5B—C6B—N1B	111.9 (2)
C5A—C6A—H6AA	109.5	C5B—C6B—H6BA	109.2
N1A—C6A—H6AA	109.5	N1B—C6B—H6BA	109.2
C5A—C6A—H6AB	109.5	C5B—C6B—H6BB	109.2
N1A—C6A—H6AB	109.5	N1B—C6B—H6BB	109.2
H6AA—C6A—H6AB	108.1	H6BA—C6B—H6BB	107.9
C5A—C7A—C8A	132.7 (3)	C5B—C7B—C8B	130.8 (3)
C5A—C7A—H7AA	113.7	C5B—C7B—H7BA	114.6
C8A—C7A—H7AA	113.7	C8B—C7B—H7BA	114.6
C9A—C8A—C13A	115.8 (3)	C9B—C8B—C13B	115.9 (3)
C9A—C8A—C7A	118.4 (3)	C9B—C8B—C7B	117.7 (3)
C13A—C8A—C7A	125.8 (3)	C13B—C8B—C7B	126.4 (3)
C10A—C9A—C8A	123.3 (3)	C10B—C9B—C8B	122.8 (3)
C10A—C9A—H9AA	118.4	C10B—C9B—H9BA	118.6
C8A—C9A—H9AA	118.4	C8B—C9B—H9BA	118.6
C9A—C10A—C11A	120.8 (3)	C9B—C10B—C11B	121.5 (3)
C9A—C10A—H10A	119.6	C9B—C10B—H10B	119.2
C11A—C10A—H10A	119.6	C11B—C10B—H10B	119.2
N2A—C11A—C10A	121.1 (3)	N2B—C11B—C10B	121.3 (3)
N2A—C11A—C12A	122.2 (3)	N2B—C11B—C12B	122.7 (3)
C10A—C11A—C12A	116.7 (3)	C10B—C11B—C12B	116.0 (3)
C13A—C12A—C11A	121.4 (3)	C13B—C12B—C11B	121.5 (3)
C13A—C12A—H12A	119.3	C13B—C12B—H12B	119.3
C11A—C12A—H12A	119.3	C11B—C12B—H12B	119.3
C12A—C13A—C8A	122.0 (3)	C12B—C13B—C8B	122.2 (3)
C12A—C13A—H13A	119.0	C12B—C13B—H13B	118.9
C8A—C13A—H13A	119.0	C8B—C13B—H13B	118.9
N2A—C14A—C15A	113.4 (3)	N2B—C14B—C15B	113.3 (3)
N2A—C14A—H14A	108.9	N2B—C14B—H14C	108.9

C15A—C14A—H14A	108.9	C15B—C14B—H14C	108.9
N2A—C14A—H14B	108.9	N2B—C14B—H14D	108.9
C15A—C14A—H14B	108.9	C15B—C14B—H14D	108.9
H14A—C14A—H14B	107.7	H14C—C14B—H14D	107.7
C14A—C15A—H15A	109.5	C14B—C15B—H15D	109.5
C14A—C15A—H15B	109.5	C14B—C15B—H15E	109.5
H15A—C15A—H15B	109.5	H15D—C15B—H15E	109.5
C14A—C15A—H15C	109.5	C14B—C15B—H15F	109.5
H15A—C15A—H15C	109.5	H15D—C15B—H15F	109.5
H15B—C15A—H15C	109.5	H15E—C15B—H15F	109.5
N2A—C16A—C17A	113.3 (3)	N2B—C16B—C17B	114.4 (3)
N2A—C16A—H16A	108.9	N2B—C16B—H16C	108.7
C17A—C16A—H16A	108.9	C17B—C16B—H16C	108.7
N2A—C16A—H16B	108.9	N2B—C16B—H16D	108.7
C17A—C16A—H16B	108.9	C17B—C16B—H16D	108.7
H16A—C16A—H16B	107.7	H16C—C16B—H16D	107.6
C16A—C17A—H17A	109.5	C16B—C17B—H17D	109.5
C16A—C17A—H17B	109.5	C16B—C17B—H17E	109.5
H17A—C17A—H17B	109.5	H17D—C17B—H17E	109.5
C16A—C17A—H17C	109.5	C16B—C17B—H17F	109.5
H17A—C17A—H17C	109.5	H17D—C17B—H17F	109.5
H17B—C17A—H17C	109.5	H17E—C17B—H17F	109.5
C3A—C18A—C19A	133.6 (3)	C3B—C18B—C19B	130.3 (3)
C3A—C18A—H18A	113.2	C3B—C18B—H18B	114.8
C19A—C18A—H18A	113.2	C19B—C18B—H18B	114.8
C20A—C19A—C24A	114.9 (3)	C24B—C19B—C20B	115.7 (3)
C20A—C19A—C18A	117.9 (3)	C24B—C19B—C18B	125.4 (3)
C24A—C19A—C18A	127.2 (3)	C20B—C19B—C18B	118.8 (3)
C21A—C20A—C19A	123.7 (3)	C21B—C20B—C19B	122.4 (3)
C21A—C20A—H20A	118.1	C21B—C20B—H20B	118.8
C19A—C20A—H20A	118.1	C19B—C20B—H20B	118.8
C20A—C21A—C22A	120.5 (3)	C20B—C21B—C22B	121.7 (3)
C20A—C21A—H21A	119.7	C20B—C21B—H21B	119.1
C22A—C21A—H21A	119.7	C22B—C21B—H21B	119.1
N3A—C22A—C21A	121.9 (3)	N3B—C22B—C23B	121.7 (3)
N3A—C22A—C23A	121.5 (3)	N3B—C22B—C21B	122.2 (3)
C21A—C22A—C23A	116.6 (3)	C23B—C22B—C21B	116.0 (3)
C24A—C23A—C22A	121.6 (3)	C24B—C23B—C22B	121.9 (3)
C24A—C23A—H23A	119.2	C24B—C23B—H23B	119.1
C22A—C23A—H23A	119.2	C22B—C23B—H23B	119.1
C23A—C24A—C19A	122.6 (3)	C23B—C24B—C19B	122.1 (3)
C23A—C24A—H24A	118.7	C23B—C24B—H24B	118.9
C19A—C24A—H24A	118.7	C19B—C24B—H24B	118.9
N3A—C25A—C26A	113.5 (3)	N3B—C25B—C26B	114.4 (3)
N3A—C25A—H25A	108.9	N3B—C25B—H25C	108.7
C26A—C25A—H25A	108.9	C26B—C25B—H25C	108.7
N3A—C25A—H25B	108.9	N3B—C25B—H25D	108.7
C26A—C25A—H25B	108.9	C26B—C25B—H25D	108.7
H25A—C25A—H25B	107.7	H25C—C25B—H25D	107.6

C25A—C26A—H26A	109.5	C25B—C26B—H26D	109.5
C25A—C26A—H26B	109.5	C25B—C26B—H26E	109.5
H26A—C26A—H26B	109.5	H26D—C26B—H26E	109.5
C25A—C26A—H26C	109.5	C25B—C26B—H26F	109.5
H26A—C26A—H26C	109.5	H26D—C26B—H26F	109.5
H26B—C26A—H26C	109.5	H26E—C26B—H26F	109.5
N3A—C27A—C28A	113.8 (3)	N3B—C27B—C28B	114.0 (3)
N3A—C27A—H27A	108.8	N3B—C27B—H27C	108.8
C28A—C27A—H27A	108.8	C28B—C27B—H27C	108.8
N3A—C27A—H27B	108.8	N3B—C27B—H27D	108.8
C28A—C27A—H27B	108.8	C28B—C27B—H27D	108.8
H27A—C27A—H27B	107.7	H27C—C27B—H27D	107.6
C27A—C28A—H28A	109.5	C27B—C28B—H28D	109.5
C27A—C28A—H28B	109.5	C27B—C28B—H28E	109.5
H28A—C28A—H28B	109.5	H28D—C28B—H28E	109.5
C27A—C28A—H28C	109.5	C27B—C28B—H28F	109.5
H28A—C28A—H28C	109.5	H28D—C28B—H28F	109.5
H28B—C28A—H28C	109.5	H28E—C28B—H28F	109.5
N1A—C29A—H29A	109.5	N1B—C29B—H29D	109.5
N1A—C29A—H29B	109.5	N1B—C29B—H29E	109.5
H29A—C29A—H29B	109.5	H29D—C29B—H29E	109.5
N1A—C29A—H29C	109.5	N1B—C29B—H29F	109.5
H29A—C29A—H29C	109.5	H29D—C29B—H29F	109.5
H29B—C29A—H29C	109.5	H29E—C29B—H29F	109.5
C29A—N1A—C2A—C3A	−66.2 (3)	C29B—N1B—C2B—C3B	60.5 (3)
C1A—N1A—C2A—C3A	174.9 (2)	C1B—N1B—C2B—C3B	−179.7 (2)
C6A—N1A—C2A—C3A	56.5 (3)	C6B—N1B—C2B—C3B	−61.7 (3)
N1A—C2A—C3A—C18A	155.5 (3)	N1B—C2B—C3B—C18B	−148.0 (3)
N1A—C2A—C3A—C4A	−26.4 (4)	N1B—C2B—C3B—C4B	31.0 (4)
C18A—C3A—C4A—O1A	−2.7 (4)	C18B—C3B—C4B—O1B	0.5 (5)
C2A—C3A—C4A—O1A	179.0 (3)	C2B—C3B—C4B—O1B	−178.6 (3)
C18A—C3A—C4A—C5A	178.1 (3)	C18B—C3B—C4B—C5B	−179.0 (3)
C2A—C3A—C4A—C5A	−0.1 (4)	C2B—C3B—C4B—C5B	1.9 (4)
O1A—C4A—C5A—C7A	−6.4 (4)	O1B—C4B—C5B—C7B	−3.0 (5)
C3A—C4A—C5A—C7A	172.7 (3)	C3B—C4B—C5B—C7B	176.6 (3)
O1A—C4A—C5A—C6A	176.2 (3)	O1B—C4B—C5B—C6B	176.9 (3)
C3A—C4A—C5A—C6A	−4.6 (4)	C3B—C4B—C5B—C6B	−3.5 (4)
C7A—C5A—C6A—N1A	−142.3 (3)	C7B—C5B—C6B—N1B	152.1 (3)
C4A—C5A—C6A—N1A	34.9 (4)	C4B—C5B—C6B—N1B	−27.8 (4)
C29A—N1A—C6A—C5A	62.1 (3)	C29B—N1B—C6B—C5B	−61.9 (3)
C1A—N1A—C6A—C5A	−178.0 (2)	C1B—N1B—C6B—C5B	177.4 (2)
C2A—N1A—C6A—C5A	−60.5 (3)	C2B—N1B—C6B—C5B	60.1 (3)
C4A—C5A—C7A—C8A	179.4 (3)	C4B—C5B—C7B—C8B	−177.3 (3)
C6A—C5A—C7A—C8A	−3.4 (5)	C6B—C5B—C7B—C8B	2.8 (5)
C5A—C7A—C8A—C9A	159.0 (3)	C5B—C7B—C8B—C9B	−161.4 (3)
C5A—C7A—C8A—C13A	−24.0 (5)	C5B—C7B—C8B—C13B	22.4 (5)
C13A—C8A—C9A—C10A	3.8 (5)	C13B—C8B—C9B—C10B	−3.8 (5)
C7A—C8A—C9A—C10A	−178.9 (3)	C7B—C8B—C9B—C10B	179.7 (3)
C8A—C9A—C10A—C11A	−1.4 (5)	C8B—C9B—C10B—C11B	3.3 (5)

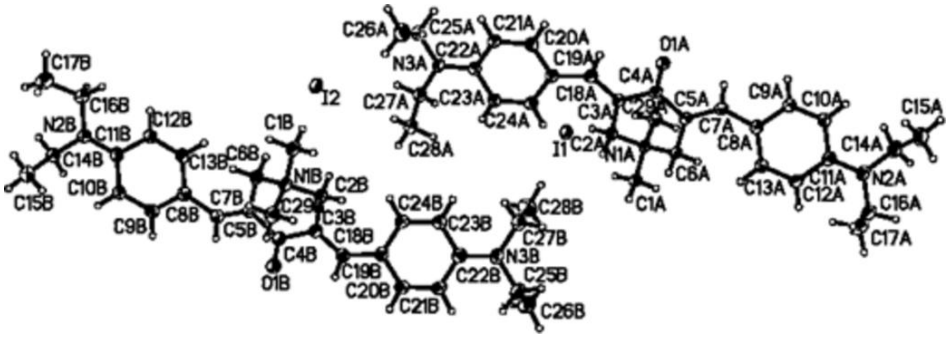
C16A—N2A—C11A—C10A	174.5 (3)	C16B—N2B—C11B—C10B	−174.6 (3)
C14A—N2A—C11A—C10A	−13.1 (5)	C14B—N2B—C11B—C10B	−7.6 (5)
C16A—N2A—C11A—C12A	−4.2 (5)	C16B—N2B—C11B—C12B	3.9 (5)
C14A—N2A—C11A—C12A	168.2 (3)	C14B—N2B—C11B—C12B	170.9 (3)
C9A—C10A—C11A—N2A	178.7 (3)	C9B—C10B—C11B—N2B	178.3 (3)
C9A—C10A—C11A—C12A	−2.5 (5)	C9B—C10B—C11B—C12B	−0.4 (5)
N2A—C11A—C12A—C13A	−177.3 (3)	N2B—C11B—C12B—C13B	179.5 (3)
C10A—C11A—C12A—C13A	3.9 (5)	C10B—C11B—C12B—C13B	−1.9 (4)
C11A—C12A—C13A—C8A	−1.5 (5)	C11B—C12B—C13B—C8B	1.3 (5)
C9A—C8A—C13A—C12A	−2.3 (4)	C9B—C8B—C13B—C12B	1.5 (4)
C7A—C8A—C13A—C12A	−179.4 (3)	C7B—C8B—C13B—C12B	177.7 (3)
C11A—N2A—C14A—C15A	90.4 (4)	C11B—N2B—C14B—C15B	87.5 (4)
C16A—N2A—C14A—C15A	−96.9 (4)	C16B—N2B—C14B—C15B	−104.7 (3)
C11A—N2A—C16A—C17A	86.9 (4)	C11B—N2B—C16B—C17B	−145.9 (3)
C14A—N2A—C16A—C17A	−85.9 (4)	C14B—N2B—C16B—C17B	46.7 (4)
C4A—C3A—C18A—C19A	−176.1 (3)	C4B—C3B—C18B—C19B	174.1 (3)
C2A—C3A—C18A—C19A	2.1 (5)	C2B—C3B—C18B—C19B	−6.8 (5)
C3A—C18A—C19A—C20A	−177.1 (3)	C3B—C18B—C19B—C24B	−22.0 (5)
C3A—C18A—C19A—C24A	4.7 (6)	C3B—C18B—C19B—C20B	162.7 (3)
C24A—C19A—C20A—C21A	0.2 (5)	C24B—C19B—C20B—C21B	4.4 (5)
C18A—C19A—C20A—C21A	−178.2 (3)	C18B—C19B—C20B—C21B	−179.8 (3)
C19A—C20A—C21A—C22A	−2.0 (5)	C19B—C20B—C21B—C22B	−2.4 (5)
C25A—N3A—C22A—C21A	0.2 (5)	C27B—N3B—C22B—C23B	−9.8 (5)
C27A—N3A—C22A—C21A	−177.2 (3)	C25B—N3B—C22B—C23B	−179.2 (3)
C25A—N3A—C22A—C23A	−178.6 (3)	C27B—N3B—C22B—C21B	170.2 (3)
C27A—N3A—C22A—C23A	3.9 (5)	C25B—N3B—C22B—C21B	0.9 (5)
C20A—C21A—C22A—N3A	−176.2 (3)	C20B—C21B—C22B—N3B	178.2 (3)
C20A—C21A—C22A—C23A	2.7 (5)	C20B—C21B—C22B—C23B	−1.7 (5)
N3A—C22A—C23A—C24A	177.2 (3)	N3B—C22B—C23B—C24B	−176.2 (3)
C21A—C22A—C23A—C24A	−1.7 (5)	C21B—C22B—C23B—C24B	3.7 (5)
C22A—C23A—C24A—C19A	0.0 (5)	C22B—C23B—C24B—C19B	−1.7 (5)
C20A—C19A—C24A—C23A	0.8 (5)	C20B—C19B—C24B—C23B	−2.4 (5)
C18A—C19A—C24A—C23A	179.1 (3)	C18B—C19B—C24B—C23B	−177.9 (3)
C22A—N3A—C25A—C26A	−83.9 (4)	C22B—N3B—C25B—C26B	80.9 (4)
C27A—N3A—C25A—C26A	93.6 (3)	C27B—N3B—C25B—C26B	−88.9 (4)
C22A—N3A—C27A—C28A	74.1 (4)	C22B—N3B—C27B—C28B	−79.0 (4)
C25A—N3A—C27A—C28A	−103.4 (3)	C25B—N3B—C27B—C28B	90.8 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14A—H14A···O1A^{i}	0.99	2.44	3.407 (5)	167
C21A—H21A···O1A^{ii}	0.95	2.48	3.367 (4)	155
C29B—H29E···O1B^{iii}	0.98	2.59	3.491 (4)	152
C1A—H1AC···I2^{iv}	0.98	2.99	3.917 (3)	158
C1B—H1BA···I2^{v}	0.98	2.94	3.892 (3)	163

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

Fig. 1


C26A
C25A
C21A
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N3A
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C17B
I2
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C23A
C18A
C5A
C9A
C10A
C15A
C16B
C3A
C29A
C24A
C7A
N2B
C12B
C1B
C28A
I1
C2A
N1A
C8A
C11B
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C19B
C22B
C25B
O1B
C20B
C21B
C26B

Fig. 2