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9-Ethyl-3,6-bis(2-thienyl)carbazole

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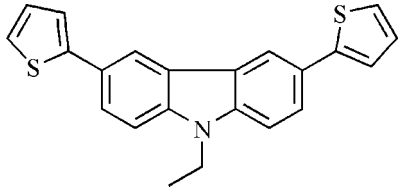
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.064; wR factor = 0.201; data-to-parameter ratio = 17.3.

The asymmetric unit of the title compound, $C_{22}H_{17}NS_2$, contains three crystallographically independent molecules. In the crystal structure, molecules are stacked through C—H···π interactions, with H···centroid distances ranging from 2.69 to 3.18 Å. Weak H···S interactions (2.91 Å) also contribute to the stabilization of the crystal structure. Four thiophene rings are disordered over two positions each; site occupancy factors range from 0.26 to 0.75.

Related literature

For bond length data, see: Allen *et al.* (1987). For related literature, see: Horowitz *et al.* (1989); Mi *et al.* (2003).



Experimental

Crystal data

$C_{22}H_{17}NS_2$
M_r = 359.51
Triclinic, $P\overline{1}$
a = 13.826 (5) Å
b = 14.436 (5) Å
c = 15.525 (5) Å
α = 70.674 (5)°
β = 69.206 (5)°
γ = 87.850 (5)°
V = 2722.3 (16) Å^3
Z = 6
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 298 (2) K
0.50 × 0.50 × 0.28 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.866, T_{max} = 0.922
25041 measured reflections
12368 independent reflections
8498 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.202
S = 1.03
12368 reflections
716 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2250).

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supplementary materials

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9-Ethyl-3,6-bis(2-thienyl)carbazole

P. Wang, Y. Ju, S. Y. Tang, J. Y. Wu and H. P. Zhou

Comment

The derivatives of thiophene have been studied so far mainly for their semiconductor and charge-transport properties such as high-field-effect charge mobility (Horowitz *et al.*, 1989). The derivatives of carbazole complexes are being explored for a multitude of optoelectronic and photocatalytic applications, including organic light emitting diodes (OLEDs) (Mi *et al.*, 2003). The two derivatives both have excellent optical-electronic properties. A new molecule was designed and synthesized combining the two derivatives in order to get a new compound with excellent electrochemical properties. We herein report its crystal structure.

The asymmetric unit of the title compound, (I), contains three crystallographically independent molecules (Fig. 1). The bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987).

When the crystal structure was solved,the atoms C10, C20, C54, C64, H10, H20, H54, H64, S1, S2, S5 and S6 were found to be disordered. So, for instance, the position of C10 atom may be occupied by S1 atom. It could be elucidated that the thiophene ring is linked to the benzene ring by a single bond, which spins so fast that the configuration is turn from one to another. In fact, it may not be possible to separate S atoms from C atoms, and that is the reason why the the C—S bonds are longer than C═C bonds, but shorter than normal C—S single bonds. The dihedral angles between the planar thiophen and benzene rings are between 1.71 (3)–27.17 (3) °.

In the crystal structure, the molecules are stacked through C—H···π interactions with H···centroid distances in the range 2.69–3.18 Å. Weak H···S interactions also contribute to the stabilization of the crystal structure, *e.g.* H56···S2 = 2.91 Å.

Experimental

For the preparation of the title compound, (I), a mixture of 9-ethyl-3,6 -diiodo-carbazole (0.44 g, 1 mmol), sodium carbonate (0.42 g, 4 mmol) and 2-thiophenyl boronic acid (0.32 g, 2.5 mmol) was heated at 333 K with DMF (20 ml) and water (10 ml) as solvents. Then, the mixture was heated for 0.5 h, palladium acetate (0.0076 g, 0.05 mmol) was added to the mixture with the temperature up to 353 K for 3 h. Then, it was cooled and poured into water (1000 ml). The precipitated yellow solid was filtered off and washed with water, dried over anhydrous magnesium sulfate, and eluted with petroleum ether/ethyl acetate (15:1). The product was obtained as yellow solid (yield; 0.2 g, 56%). Single crystals of (I) were grown by slow evaporation of a dichloromethane/ethyl acetate (1:1) solution.

Refinement

When the crystal structure was solved,the atoms C10, C20, C54, C64, H10, H20, H54, H64, S1, S2, S5 and S6 were found to be disordered. During refinement with isotropic thermal parameters, the occupancies of disordered H atoms were refined as H10 = 0.742 (4), H10' = 0.258 (4), H20 = 0.548 (4), H20' = 0.452 (4), H54 = 0.694 (4), H54' = 0.306 (4), H64 = 0.310 (5) and H64' = 0.690 (5). The remaining site occupancy factors were also refined as C10 = 0.724 (4), C10' = 0.258 (4), C20

= 0.548 (4), C20' = 0.452 (4), C54 = 0.694 (4), C54' = 0.306 (4), C64 = 0.310 (5), C64' = 0.690 (5), S1 = 0.742 (4), S1' = 0.258 (4), S2 = 0.548 (4), S2' = 0.452 (4), S5 = 0.694 (4), S5' = 0.306 (4), S6 = 0.310 (5) and S6' = 0.690 (5) during anisotropic refinement. H11, H12, H21, H22, H55, H56, H65 and H66 atoms were located in difference syntheses and refined isotropically [C—H = 0.86 (4)–1.09 (5) Å and U_{iso}(H) = 0.096 (12)–0.132 (18) Å^2]. The remaining H atoms were positioned geometrically with C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H and x = 1.2 for all other H atoms.

Figures

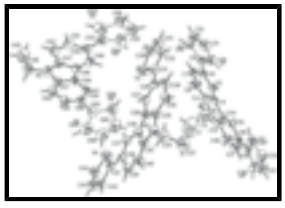

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

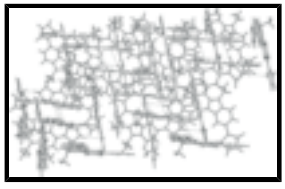

Fig. 2. A packing diagram of (I). The interactions are shown as dashed lines.

9-Ethyl-3,6-bis(2-thienyl)carbazole

Crystal data

$C_{22}H_{17}NS_2$	Z = 6
M_r = 359.51	F_{000} = 1128
Triclinic, $P\overline{1}$	D_x = 1.316 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71069 Å
a = 13.826 (5) Å	Cell parameters from 12368 reflections
b = 14.436 (5) Å	θ = 1.5–27.7º
c = 15.525 (5) Å	μ = 0.30 mm^{-1}
α = 70.674 (5)º	T = 298 (2) K
β = 69.206 (5)º	Plate, yellow
γ = 87.850 (5)º	0.50 × 0.50 × 0.28 mm
V = 2722.3 (16) Å^3	

Data collection

Bruker APEX II CCD area-detector diffractometer	12368 independent reflections
Radiation source: fine-focus sealed tube	8498 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.019
T = 298(2) K	θ_{max} = 27.7º
φ and ω scans	θ_{min} = 1.5º

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.866, T_{max} = 0.922
25041 measured reflections

h = −16→18
k = −18→18
l = −20→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.202
S = 1.03
12368 reflections
716 parameters
1 restraint
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0912P)^2 + 1.7033P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.012
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}
Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0022 (7)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.71244 (10)	0.73415 (7)	−0.10946 (9)	0.0812 (4)	0.742 (4)
S1'	0.61263 (17)	0.59080 (15)	−0.12592 (16)	0.0828 (8)	0.258 (4)
S2	0.51077 (10)	0.03050 (9)	0.11620 (10)	0.0719 (5)	0.548 (4)
S2'	0.58974 (13)	−0.10133 (10)	0.23914 (13)	0.0822 (6)	0.452 (4)
S3	0.80073 (9)	0.72853 (8)	0.19477 (7)	0.0992 (4)	
S4	0.57467 (7)	0.42975 (8)	0.71323 (7)	0.0831 (3)	
S5	1.19353 (8)	0.99255 (10)	0.17451 (9)	0.0808 (5)	0.694 (4)
S5'	1.04342 (18)	0.90629 (16)	0.14985 (16)	0.0941 (9)	0.306 (4)
S6	0.39927 (16)	0.64444 (17)	0.67458 (19)	0.0977 (9)	0.310 (5)
S6'	0.49871 (12)	0.65660 (11)	0.48471 (11)	0.0940 (6)	0.690 (5)
N1	0.8483 (2)	0.31631 (19)	0.1567 (2)	0.0810 (9)	

N2	1.04847 (17)	0.38998 (17)	0.42305 (17)	0.0573 (5)	
N3	0.7489 (2)	1.01317 (19)	0.53198 (19)	0.0673 (6)	
C1	0.8887 (4)	0.3126 (4)	0.2850 (6)	0.143 (2)	
H1A	0.8568	0.3730	0.2842	0.214*	
H1B	0.9368	0.3050	0.3183	0.214*	
H1C	0.8361	0.2581	0.3186	0.214*	
C2	0.9394 (6)	0.3151 (3)	0.1930 (4)	0.128 (2)	
H2A	0.9770	0.2573	0.1913	0.154*	
H2B	0.9873	0.3739	0.1547	0.154*	
C3	0.8148 (2)	0.3983 (2)	0.1017 (2)	0.0633 (7)	
C4	0.73899 (19)	0.36810 (18)	0.07278 (17)	0.0471 (5)	
C5	0.69553 (19)	0.43772 (18)	0.01479 (18)	0.0477 (5)	
H5	0.6458	0.4179	−0.0046	0.057*	
C6	0.7267 (2)	0.53743 (18)	−0.01424 (19)	0.0528 (6)	
C7	0.8000 (3)	0.5648 (2)	0.0185 (2)	0.0682 (8)	
H7	0.8189	0.6315	0.0011	0.082*	
C8	0.8451 (3)	0.4974 (2)	0.0750 (3)	0.0755 (9)	
H8	0.8944	0.5176	0.0948	0.091*	
C9	0.6841 (2)	0.61193 (19)	−0.0791 (2)	0.0585 (7)	
C10	0.61263 (17)	0.59080 (15)	−0.12592 (16)	0.0828 (8)	0.742 (4)
H10	0.5870	0.5300	−0.1213	0.099*	0.742 (4)
C10'	0.71244 (10)	0.73415 (7)	−0.10946 (9)	0.0812 (4)	0.258 (4)
H10'	0.7537	0.7701	−0.0934	0.097*	0.258 (4)
C11	0.5931 (3)	0.6909 (3)	−0.1812 (3)	0.0905 (12)	
H11	0.550 (3)	0.698 (3)	−0.216 (3)	0.105 (14)*	
C12	0.6414 (3)	0.7662 (3)	−0.1768 (3)	0.0944 (13)	
H12	0.636 (3)	0.839 (3)	−0.206 (3)	0.114 (14)*	
C13	0.7929 (2)	0.2335 (2)	0.1665 (2)	0.0606 (7)	
C14	0.72440 (19)	0.26127 (18)	0.11561 (17)	0.0465 (5)	
C15	0.65954 (18)	0.18905 (17)	0.11686 (17)	0.0440 (5)	
H15	0.6138	0.2068	0.0835	0.053*	
C16	0.66299 (18)	0.09035 (17)	0.16788 (18)	0.0460 (5)	
C17	0.7337 (2)	0.0654 (2)	0.2172 (2)	0.0619 (7)	
H17	0.7364	−0.0006	0.2509	0.074*	
C18	0.7985 (3)	0.1348 (2)	0.2172 (3)	0.0745 (9)	
H18	0.8447	0.1169	0.2499	0.089*	
C19	0.59496 (19)	0.01153 (18)	0.17285 (18)	0.0487 (5)	
C20	0.58974 (13)	−0.10133 (10)	0.23914 (13)	0.0822 (6)	0.548 (4)
H20	0.6243	−0.1315	0.2813	0.099*	0.548 (4)
C20'	0.51077 (10)	0.03050 (9)	0.11620 (10)	0.0719 (5)	0.452 (4)
H20'	0.4935	0.0877	0.0770	0.086*	0.452 (4)
C21	0.5085 (3)	−0.1447 (3)	0.2107 (3)	0.0852 (11)	
H21	0.491 (3)	−0.208 (3)	0.237 (3)	0.096 (12)*	
C22	0.4697 (3)	−0.0816 (3)	0.1512 (3)	0.0828 (10)	
H22	0.416 (4)	−0.097 (3)	0.130 (3)	0.128 (16)*	
C23	1.1401 (3)	0.2518 (3)	0.3855 (3)	0.0884 (11)	
H23A	1.0839	0.2050	0.4348	0.133*	
H23B	1.2045	0.2223	0.3790	0.133*	
H23C	1.1301	0.2713	0.3240	0.133*	

C24	1.1428 (2)	0.3390 (2)	0.4140 (2)	0.0667 (8)
H24A	1.1528	0.3188	0.4761	0.080*
H24B	1.2018	0.3845	0.3654	0.080*
C25	1.0308 (2)	0.46353 (19)	0.34844 (19)	0.0521 (6)
C26	0.93146 (19)	0.49525 (18)	0.38463 (18)	0.0469 (5)
C27	0.8959 (2)	0.56896 (18)	0.32279 (18)	0.0484 (5)
H27	0.8307	0.5904	0.3471	0.058*
C28	0.9580 (2)	0.61119 (19)	0.22376 (18)	0.0517 (6)
C29	1.0566 (2)	0.5771 (2)	0.1899 (2)	0.0614 (7)
H29	1.0979	0.6046	0.1239	0.074*
C30	1.0940 (2)	0.5054 (2)	0.2497 (2)	0.0601 (7)
H30	1.1597	0.4849	0.2254	0.072*
C31	0.9213 (2)	0.6882 (2)	0.1564 (2)	0.0593 (7)
C32	0.9754 (3)	0.7401 (2)	0.0557 (2)	0.0681 (8)
H32	1.0422	0.7301	0.0195	0.082*
C33	0.9120 (4)	0.8099 (3)	0.0179 (3)	0.0912 (12)
H33	0.9342	0.8512	−0.0471	0.109*
C34	0.8199 (4)	0.8116 (3)	0.0819 (3)	0.1027 (13)
H34	0.7708	0.8535	0.0671	0.123*
C35	0.9612 (2)	0.37190 (19)	0.5078 (2)	0.0524 (6)
C36	0.88737 (19)	0.43696 (17)	0.48713 (18)	0.0469 (5)
C37	0.79393 (19)	0.43471 (18)	0.56199 (18)	0.0480 (5)
H37	0.7453	0.4779	0.5489	0.058*
C38	0.7725 (2)	0.36834 (18)	0.65638 (18)	0.0492 (5)
C39	0.8477 (2)	0.30319 (19)	0.6736 (2)	0.0573 (6)
H39	0.8336	0.2582	0.7364	0.069*
C40	0.9404 (2)	0.3039 (2)	0.6014 (2)	0.0592 (7)
H40	0.9884	0.2598	0.6145	0.071*
C41	0.6749 (2)	0.36582 (18)	0.73637 (19)	0.0517 (6)
C42	0.6492 (2)	0.31051 (18)	0.84272 (17)	0.0502 (6)
H42	0.6917	0.2717	0.8723	0.060*
C43	0.5429 (3)	0.3306 (3)	0.8902 (2)	0.0728 (8)
H43	0.5082	0.3032	0.9576	0.087*
C44	0.4976 (3)	0.3902 (3)	0.8324 (2)	0.0763 (9)
H44	0.4305	0.4080	0.8557	0.092*
C45	0.7056 (5)	1.1735 (3)	0.5483 (4)	0.1303 (19)
H45A	0.7553	1.2076	0.4841	0.195*
H45B	0.6989	1.2121	0.5896	0.195*
H45C	0.6395	1.1636	0.5438	0.195*
C46	0.7408 (3)	1.0782 (3)	0.5898 (3)	0.0829 (10)
H46A	0.6925	1.0459	0.6561	0.100*
H46B	0.8081	1.0886	0.5930	0.100*
C47	0.8363 (2)	1.0072 (2)	0.4559 (2)	0.0573 (6)
C48	0.8150 (2)	0.93445 (18)	0.42109 (18)	0.0495 (6)
C49	0.8915 (2)	0.91588 (18)	0.34354 (18)	0.0494 (6)
H49	0.8782	0.8673	0.3210	0.059*
C50	0.9881 (2)	0.96989 (18)	0.2995 (2)	0.0526 (6)
C51	1.0070 (2)	1.0402 (2)	0.3377 (2)	0.0637 (7)
H51	1.0722	1.0749	0.3097	0.076*

C52	0.9331 (3)	1.0597 (2)	0.4145 (2)	0.0663 (7)	
H52	0.9475	1.1068	0.4381	0.080*	
C53	1.0670 (2)	0.95582 (19)	0.2127 (2)	0.0568 (6)	
C54	1.04342 (18)	0.90629 (16)	0.14985 (16)	0.0941 (9)	0.694 (4)
H54	0.9801	0.8786	0.1571	0.113*	0.694 (4)
C54'	1.19353 (8)	0.99255 (10)	0.17451 (9)	0.0808 (5)	0.306 (4)
H54'	1.2312	1.0228	0.1986	0.097*	0.306 (4)
C55	1.1501 (3)	0.9132 (3)	0.0715 (3)	0.0892 (11)	
H55	1.152 (4)	0.889 (3)	0.021 (3)	0.120 (16)*	
C56	1.2267 (3)	0.9560 (3)	0.0796 (3)	0.0928 (13)	
H56	1.290 (4)	0.964 (3)	0.040 (3)	0.117 (15)*	
C57	0.6711 (2)	0.9463 (2)	0.5461 (2)	0.0598 (7)	
C58	0.7091 (2)	0.89398 (19)	0.48028 (19)	0.0518 (6)	
C59	0.6470 (2)	0.8165 (2)	0.48735 (19)	0.0541 (6)	
H59	0.6725	0.7808	0.4452	0.065*	
C60	0.5466 (2)	0.7918 (2)	0.5575 (2)	0.0583 (6)	
C61	0.5089 (3)	0.8504 (2)	0.6172 (2)	0.0700 (8)	
H61	0.4405	0.8369	0.6612	0.084*	
C62	0.5689 (3)	0.9260 (2)	0.6129 (2)	0.0733 (9)	
H62	0.5422	0.9631	0.6535	0.088*	
C63	0.4823 (2)	0.7047 (2)	0.5730 (2)	0.0635 (7)	
C64	0.49871 (12)	0.65660 (11)	0.48471 (11)	0.0940 (6)	0.310 (5)
H64	0.5439	0.6736	0.4199	0.113*	0.310 (5)
C64'	0.39927 (16)	0.64444 (17)	0.67458 (19)	0.0977 (9)	0.690 (5)
H64'	0.3796	0.6542	0.7346	0.117*	0.690 (5)
C65	0.4048 (3)	0.5678 (4)	0.5558 (4)	0.1007 (14)	
H65	0.396 (4)	0.522 (4)	0.533 (4)	0.132 (18)*	
C66	0.3597 (3)	0.5652 (3)	0.6472 (4)	0.0968 (12)	
H66	0.300 (4)	0.511 (3)	0.708 (3)	0.119 (14)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0917 (8)	0.0497 (5)	0.0826 (8)	0.0056 (5)	−0.0222 (6)	−0.0080 (5)
S1'	0.0875 (15)	0.0686 (12)	0.0853 (15)	0.0189 (10)	−0.0396 (12)	−0.0098 (10)
S2	0.0766 (8)	0.0641 (7)	0.0823 (9)	0.0009 (6)	−0.0368 (7)	−0.0249 (6)
S2'	0.0918 (11)	0.0548 (8)	0.1083 (13)	0.0041 (7)	−0.0453 (10)	−0.0280 (8)
S3	0.0994 (7)	0.0981 (7)	0.0698 (6)	0.0341 (6)	−0.0243 (5)	−0.0001 (5)
S4	0.0743 (5)	0.0946 (6)	0.0649 (5)	0.0193 (5)	−0.0127 (4)	−0.0226 (5)
S5	0.0552 (6)	0.1086 (10)	0.0667 (7)	0.0035 (6)	−0.0151 (5)	−0.0223 (6)
S5'	0.0909 (15)	0.0976 (15)	0.0767 (14)	0.0044 (11)	0.0012 (10)	−0.0421 (11)
S6	0.0665 (12)	0.1033 (16)	0.1164 (19)	−0.0115 (10)	−0.0153 (11)	−0.0462 (14)
S6'	0.0980 (10)	0.1008 (10)	0.0908 (10)	−0.0029 (7)	−0.0298 (8)	−0.0455 (8)
N1	0.100 (2)	0.0581 (14)	0.096 (2)	−0.0127 (14)	−0.0713 (18)	−0.0002 (14)
N2	0.0479 (12)	0.0613 (13)	0.0558 (13)	0.0112 (10)	−0.0150 (10)	−0.0159 (11)
N3	0.0773 (17)	0.0634 (14)	0.0626 (15)	0.0079 (12)	−0.0161 (13)	−0.0334 (12)
C1	0.108 (4)	0.122 (4)	0.229 (8)	0.020 (3)	−0.071 (5)	−0.088 (5)
C2	0.232 (7)	0.069 (2)	0.107 (4)	−0.016 (3)	−0.104 (4)	−0.008 (2)

C3	0.0728 (18)	0.0553 (15)	0.0615 (17)	−0.0086 (13)	−0.0344 (15)	−0.0069 (13)
C4	0.0490 (13)	0.0483 (12)	0.0397 (12)	−0.0006 (10)	−0.0135 (10)	−0.0117 (10)
C5	0.0477 (13)	0.0481 (12)	0.0424 (13)	0.0032 (10)	−0.0128 (10)	−0.0131 (10)
C6	0.0539 (14)	0.0476 (13)	0.0456 (14)	0.0026 (11)	−0.0084 (11)	−0.0120 (11)
C7	0.082 (2)	0.0468 (14)	0.0695 (19)	−0.0109 (14)	−0.0268 (16)	−0.0117 (13)
C8	0.093 (2)	0.0573 (17)	0.081 (2)	−0.0144 (16)	−0.0485 (19)	−0.0084 (15)
C9	0.0576 (15)	0.0487 (14)	0.0520 (15)	0.0082 (11)	−0.0066 (12)	−0.0103 (11)
C10	0.0875 (15)	0.0686 (12)	0.0853 (15)	0.0189 (10)	−0.0396 (12)	−0.0098 (10)
C10'	0.0917 (8)	0.0497 (5)	0.0826 (8)	0.0056 (5)	−0.0222 (6)	−0.0080 (5)
C11	0.082 (2)	0.093 (3)	0.085 (3)	0.026 (2)	−0.035 (2)	−0.012 (2)
C12	0.093 (3)	0.058 (2)	0.090 (3)	0.0197 (19)	−0.007 (2)	−0.0029 (18)
C13	0.0649 (17)	0.0555 (15)	0.0635 (17)	−0.0030 (13)	−0.0355 (14)	−0.0088 (13)
C14	0.0479 (13)	0.0483 (12)	0.0405 (12)	0.0022 (10)	−0.0160 (10)	−0.0115 (10)
C15	0.0438 (12)	0.0499 (12)	0.0385 (12)	0.0071 (10)	−0.0147 (10)	−0.0159 (10)
C16	0.0450 (12)	0.0479 (12)	0.0424 (13)	0.0061 (10)	−0.0131 (10)	−0.0154 (10)
C17	0.0703 (18)	0.0480 (14)	0.0668 (18)	0.0039 (12)	−0.0374 (15)	−0.0053 (12)
C18	0.084 (2)	0.0582 (16)	0.090 (2)	0.0009 (15)	−0.061 (2)	−0.0032 (15)
C19	0.0469 (13)	0.0530 (13)	0.0459 (13)	0.0079 (10)	−0.0117 (11)	−0.0225 (11)
C20	0.0918 (11)	0.0548 (8)	0.1083 (13)	0.0041 (7)	−0.0453 (10)	−0.0280 (8)
C20'	0.0766 (8)	0.0641 (7)	0.0823 (9)	0.0009 (6)	−0.0368 (7)	−0.0249 (6)
C21	0.105 (3)	0.0528 (18)	0.100 (3)	−0.0048 (18)	−0.039 (2)	−0.0255 (19)
C22	0.073 (2)	0.096 (3)	0.096 (3)	0.0035 (19)	−0.035 (2)	−0.049 (2)
C23	0.092 (3)	0.095 (3)	0.100 (3)	0.037 (2)	−0.050 (2)	−0.047 (2)
C24	0.0520 (16)	0.0754 (19)	0.0690 (19)	0.0160 (14)	−0.0199 (14)	−0.0233 (15)
C25	0.0475 (13)	0.0551 (14)	0.0517 (14)	0.0045 (11)	−0.0149 (11)	−0.0190 (12)
C26	0.0454 (12)	0.0482 (12)	0.0445 (13)	0.0001 (10)	−0.0128 (10)	−0.0160 (10)
C27	0.0482 (13)	0.0483 (13)	0.0450 (13)	0.0021 (10)	−0.0130 (11)	−0.0152 (10)
C28	0.0579 (15)	0.0502 (13)	0.0433 (13)	−0.0039 (11)	−0.0153 (11)	−0.0138 (11)
C29	0.0596 (16)	0.0674 (17)	0.0428 (14)	−0.0038 (13)	−0.0042 (12)	−0.0151 (12)
C30	0.0475 (14)	0.0715 (17)	0.0536 (16)	0.0044 (12)	−0.0074 (12)	−0.0232 (13)
C31	0.0751 (18)	0.0517 (14)	0.0453 (14)	−0.0013 (13)	−0.0175 (13)	−0.0132 (11)
C32	0.097 (2)	0.0541 (15)	0.0468 (15)	−0.0025 (15)	−0.0254 (15)	−0.0082 (12)
C33	0.140 (4)	0.069 (2)	0.0528 (19)	0.002 (2)	−0.036 (2)	−0.0034 (16)
C34	0.133 (4)	0.088 (3)	0.073 (3)	0.032 (3)	−0.045 (3)	−0.004 (2)
C35	0.0509 (14)	0.0525 (14)	0.0516 (14)	0.0056 (11)	−0.0177 (12)	−0.0161 (11)
C36	0.0484 (13)	0.0445 (12)	0.0455 (13)	0.0031 (10)	−0.0167 (11)	−0.0129 (10)
C37	0.0476 (13)	0.0472 (12)	0.0475 (14)	0.0041 (10)	−0.0171 (11)	−0.0142 (10)
C38	0.0531 (14)	0.0454 (12)	0.0456 (13)	0.0003 (10)	−0.0152 (11)	−0.0136 (10)
C39	0.0646 (17)	0.0505 (14)	0.0485 (15)	0.0039 (12)	−0.0192 (13)	−0.0076 (11)
C40	0.0600 (16)	0.0544 (14)	0.0585 (16)	0.0122 (12)	−0.0236 (14)	−0.0118 (12)
C41	0.0572 (15)	0.0488 (13)	0.0457 (14)	−0.0021 (11)	−0.0146 (12)	−0.0155 (11)
C42	0.0479 (13)	0.0521 (13)	0.0372 (12)	−0.0123 (10)	0.0043 (10)	−0.0181 (10)
C43	0.079 (2)	0.077 (2)	0.0494 (16)	−0.0069 (16)	−0.0092 (15)	−0.0192 (15)
C44	0.0642 (19)	0.090 (2)	0.064 (2)	0.0040 (17)	−0.0041 (16)	−0.0340 (18)
C45	0.182 (5)	0.090 (3)	0.126 (4)	0.045 (3)	−0.050 (4)	−0.056 (3)
C46	0.093 (3)	0.086 (2)	0.077 (2)	0.0097 (19)	−0.0221 (19)	−0.0463 (19)
C47	0.0650 (17)	0.0531 (14)	0.0547 (16)	0.0120 (12)	−0.0210 (13)	−0.0211 (12)
C48	0.0535 (14)	0.0480 (13)	0.0461 (13)	0.0116 (11)	−0.0178 (11)	−0.0160 (10)
C49	0.0527 (14)	0.0465 (12)	0.0485 (14)	0.0115 (10)	−0.0195 (11)	−0.0152 (11)

C50	0.0529 (14)	0.0468 (13)	0.0551 (15)	0.0123 (11)	−0.0222 (12)	−0.0115 (11)
C51	0.0577 (16)	0.0584 (16)	0.0730 (19)	0.0055 (13)	−0.0238 (15)	−0.0198 (14)
C52	0.076 (2)	0.0588 (16)	0.0719 (19)	0.0060 (14)	−0.0304 (16)	−0.0277 (15)
C53	0.0527 (15)	0.0508 (14)	0.0543 (15)	0.0103 (11)	−0.0148 (12)	−0.0078 (12)
C54	0.0909 (15)	0.0976 (15)	0.0767 (14)	0.0044 (11)	0.0012 (10)	−0.0421 (11)
C54'	0.0552 (6)	0.1086 (10)	0.0667 (7)	0.0035 (6)	−0.0151 (5)	−0.0223 (6)
C55	0.081 (3)	0.099 (3)	0.069 (2)	0.010 (2)	−0.0033 (19)	−0.032 (2)
C56	0.064 (2)	0.114 (3)	0.063 (2)	0.018 (2)	−0.0053 (18)	−0.005 (2)
C57	0.0699 (18)	0.0585 (15)	0.0491 (15)	0.0123 (13)	−0.0157 (13)	−0.0230 (12)
C58	0.0575 (15)	0.0518 (13)	0.0449 (13)	0.0135 (11)	−0.0174 (12)	−0.0172 (11)
C59	0.0560 (15)	0.0610 (15)	0.0468 (14)	0.0122 (12)	−0.0160 (12)	−0.0237 (12)
C60	0.0567 (15)	0.0647 (16)	0.0497 (15)	0.0094 (12)	−0.0156 (12)	−0.0193 (12)
C61	0.0643 (18)	0.077 (2)	0.0550 (17)	0.0066 (15)	−0.0028 (14)	−0.0262 (15)
C62	0.078 (2)	0.076 (2)	0.0568 (18)	0.0126 (16)	−0.0044 (15)	−0.0338 (15)
C63	0.0533 (15)	0.0745 (18)	0.0644 (18)	0.0110 (13)	−0.0226 (14)	−0.0252 (15)
C64	0.0980 (10)	0.1008 (10)	0.0908 (10)	−0.0029 (7)	−0.0298 (8)	−0.0455 (8)
C64'	0.0665 (12)	0.1033 (16)	0.1164 (19)	−0.0115 (10)	−0.0153 (11)	−0.0462 (14)
C65	0.077 (3)	0.115 (3)	0.135 (4)	0.007 (2)	−0.043 (3)	−0.069 (3)
C66	0.060 (2)	0.107 (3)	0.115 (4)	−0.005 (2)	−0.019 (2)	−0.040 (3)

Geometric parameters (Å, °)

S1—C9	1.691 (3)	C29—H29	0.9300
S1—C12	1.627 (5)	C30—H30	0.9300
S1'—C9	1.509 (4)	C31—C32	1.415 (4)
S1'—C11	1.487 (4)	C31—S3	1.710 (3)
S2—C19	1.658 (3)	C32—C33	1.427 (5)
S2—C22	1.583 (4)	C32—H32	0.9300
S2'—C19	1.602 (3)	C33—C34	1.313 (6)
S2'—C21	1.561 (4)	C33—H33	0.9300
S5—C53	1.679 (3)	C34—S3	1.698 (4)
S5—C56	1.637 (5)	C34—H34	0.9300
S5'—C53	1.509 (4)	C35—N2	1.387 (3)
S5'—C55	1.523 (4)	C35—C40	1.392 (4)
S6—C63	1.564 (4)	C35—C36	1.410 (3)
S6—C66	1.526 (5)	C36—C37	1.390 (3)
S6'—C63	1.677 (3)	C37—C38	1.392 (3)
S6'—C65	1.649 (5)	C37—H37	0.9300
C1—C2	1.338 (8)	C38—C39	1.412 (4)
C1—H1A	0.9600	C38—C41	1.466 (4)
C1—H1B	0.9600	C39—C40	1.370 (4)
C1—H1C	0.9600	C39—H39	0.9300
C2—N1	1.550 (6)	C40—H40	0.9300
C2—H2A	0.9700	C41—C42	1.491 (4)
C2—H2B	0.9700	C41—S4	1.714 (3)
C3—N1	1.384 (4)	C42—C43	1.459 (4)
C3—C8	1.387 (4)	C42—H42	0.9300
C3—C4	1.410 (4)	C43—C44	1.336 (5)
C4—C5	1.386 (3)	C43—H43	0.9300

C4—C14	1.453 (3)	C44—S4	1.683 (3)
C5—C6	1.393 (3)	C44—H44	0.9300
C5—H5	0.9300	C45—C46	1.460 (6)
C6—C7	1.404 (4)	C45—H45A	0.9600
C6—C9	1.474 (4)	C45—H45B	0.9600
C7—C8	1.372 (4)	C45—H45C	0.9600
C7—H7	0.9300	C46—N3	1.475 (4)
C8—H8	0.9300	C46—H46A	0.9700
C9—C10	1.509 (4)	C46—H46B	0.9700
C9—C10'	1.691 (3)	C47—N3	1.381 (4)
C10—C11	1.487 (4)	C47—C52	1.386 (4)
C10—H10	0.9300	C47—C48	1.412 (4)
C10'—H10'	0.9300	C48—C49	1.389 (4)
C11—C12	1.329 (6)	C48—C58	1.443 (4)
C11—H11	0.92 (4)	C49—C50	1.391 (4)
C12—C10'	1.627 (5)	C49—H49	0.9300
C12—H12	1.01 (4)	C50—C51	1.406 (4)
C13—N1	1.380 (4)	C50—C53	1.473 (4)
C13—C18	1.395 (4)	C51—C52	1.371 (4)
C13—C14	1.405 (3)	C51—H51	0.9300
C14—C15	1.391 (3)	C52—H52	0.9300
C15—C16	1.391 (3)	C53—C54	1.508 (4)
C15—H15	0.9300	C53—C54'	1.678 (3)
C16—C17	1.413 (4)	C54—C55	1.523 (4)
C16—C19	1.468 (3)	C54—H54	0.9300
C17—C18	1.369 (4)	C54'—H54'	0.9300
C17—H17	0.9300	C55—C56	1.309 (6)
C18—H18	0.9300	C55—H55	0.95 (5)
C19—C20	1.602 (3)	C56—C54'	1.636 (5)
C19—C20'	1.657 (3)	C56—H56	0.86 (5)
C20—C21	1.561 (4)	C57—N3	1.382 (4)
C20—H20	0.9300	C57—C62	1.395 (4)
C20'—H20'	0.9300	C57—C58	1.411 (4)
C21—C22	1.315 (6)	C58—C59	1.386 (4)
C21—H21	0.86 (4)	C59—C60	1.396 (4)
C22—C20'	1.582 (4)	C59—H59	0.9300
C22—H22	0.97 (5)	C60—C61	1.410 (4)
C23—C24	1.472 (5)	C60—C63	1.470 (4)
C23—H23A	0.9600	C61—C62	1.366 (5)
C23—H23B	0.9600	C61—H61	0.9300
C23—H23C	0.9600	C62—H62	0.9300
C24—N2	1.459 (3)	C63—C64'	1.563 (4)
C24—H24A	0.9700	C63—C64	1.676 (3)
C24—H24B	0.9700	C64—C65	1.649 (5)
C25—N2	1.377 (3)	C64—H64	0.9300
C25—C30	1.398 (4)	C64'—H64'	0.9300
C25—C26	1.409 (3)	C65—C66	1.320 (7)
C26—C27	1.384 (3)	C65—H65	0.87 (5)
C26—C36	1.441 (3)	C66—C64'	1.524 (5)

C27—C28	1.398 (4)	C66—H66	1.09 (5)
C27—H27	0.9300	C10'—H10'	0.9300
C28—C29	1.410 (4)	C20'—H20'	0.9300
C28—C31	1.467 (4)	C54'—H54'	0.9300
C29—C30	1.367 (4)	C64'—H64'	0.9300

C12—S1—C9	C32—C31—C28
C9—S1'—H10	C32—C31—S3
C11—S1'—C9	C28—C31—S3
C11—S1'—H10	C31—C32—C33
C22—S2—C19	C31—C32—H32
C21—S2'—C19	C33—C32—H32
C21—S2'—H20	C34—C33—C32
C19—S2'—H20	C34—C33—H33
C34—S3—C31	C32—C33—H33
C44—S4—C41	C33—C34—S3
C56—S5—C53	C33—C34—H34
C53—S5'—C55	S3—C34—H34
C53—S5—H54	N2—C35—C40
C66—S6—C63	N2—C35—C36
C63—S6'—H64	C40—C35—C36
C65—S6'—H64	C37—C36—C35
C65—S6'—C63	C37—C36—C26
C13—N1—C3	C35—C36—C26
C13—N1—C2	C36—C37—C38
C3—N1—C2	C36—C37—H37
C25—N2—C35	C38—C37—H37
C25—N2—C24	C37—C38—C39
C35—N2—C24	C37—C38—C41
C47—N3—C57	C39—C38—C41
C47—N3—C46	C40—C39—C38
C57—N3—C46	C40—C39—H39
C2—C1—H1A	C38—C39—H39
C2—C1—H1B	C39—C40—C35
H1A—C1—H1B	C39—C40—H40
C2—C1—H1C	C35—C40—H40
H1A—C1—H1C	C38—C41—C42
H1B—C1—H1C	C38—C41—S4
C1—C2—N1	C42—C41—S4
C1—C2—H2A	C43—C42—C41
N1—C2—H2A	C43—C42—H42
C1—C2—H2B	C41—C42—H42
N1—C2—H2B	C44—C43—C42
H2A—C2—H2B	C44—C43—H43
N1—C3—C8	C42—C43—H43
N1—C3—C4	C43—C44—S4
C8—C3—C4	C43—C44—H44
C5—C4—C3	S4—C44—H44
C5—C4—C14	C46—C45—H45A
C3—C4—C14	C46—C45—H45B

C4—C5—C6
C4—C5—H5
C6—C5—H5
C5—C6—C7
C5—C6—C9
C7—C6—C9
C8—C7—C6
C8—C7—H7
C6—C7—H7
C7—C8—C3
C7—C8—H8
C3—C8—H8
C6—C9—S1
C10—C9—S1
C6—C9—C10
C6—C9—C10'
C10—C9—C10'
C11—C10—C9
C11—C10—H10
C9—C10—H10
C12—C11—S1'
S1'—C11—H11
C12—C11—C10
C12—C11—H11
C10—C11—H11
S1—C12—H12
C11—C12—S1
C11—C12—C10'
C11—C12—H12
C10'—C12—H12
N1—C13—C18
N1—C13—C14
C18—C13—C14
C15—C14—C13
C15—C14—C4
C13—C14—C4
C16—C15—C14
C16—C15—H15
C14—C15—H15
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C15—C16—C19
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C18—C17—C16
C18—C17—H17
C16—C17—H17
C17—C18—C13
C17—C18—H18
C13—C18—H18
C16—C19—S2'
H45A—C45—H45B
C46—C45—H45C
H45A—C45—H45C
H45B—C45—H45C
C45—C46—N3
C45—C46—H46A
N3—C46—H46A
C45—C46—H46B
N3—C46—H46B
H46A—C46—H46B
N3—C47—C52
N3—C47—C48
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C47—C52—H52
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C56—C55—S5'
S5'—C55—H55
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C56—C55—H55
C54—C55—H55
S5—C56—H56
C55—C56—S5
C55—C56—C54'
C55—C56—H56
C54'—C56—H56
N3—C57—C62
N3—C57—C58

C16—C19—S2		C62—C57—C58	
C20—C19—S2		C59—C58—C57	
C16—C19—C20		C59—C58—C48	
C16—C19—C20'		C57—C58—C48	
C20—C19—C20'		C58—C59—C60	
C21—C20—C19		C58—C59—H59	
C21—C20—H20		C60—C59—H59	
C19—C20—H20		C59—C60—C61	
C22—C21—S2'		C59—C60—C63	
S2'—C21—H21		C61—C60—C63	
C22—C21—C20		C62—C61—C60	
C22—C21—H21		C62—C61—H61	
C20—C21—H21		C60—C61—H61	
S2—C22—H22		C61—C62—C57	
C21—C22—S2		C61—C62—H62	
C21—C22—C20'		C57—C62—H62	
C21—C22—H22		S6—C63—C64	
C20'—C22—H22		C60—C63—S6	
C24—C23—H23A		C60—C63—S6'	
C24—C23—H23B		C60—C63—C64'	
H23A—C23—H23B		C60—C63—C64	
C24—C23—H23C		C64'—C63—C64	
H23A—C23—H23C		C65—C64—C63	
H23B—C23—H23C		C65—C64—H64	
N2—C24—C23		C63—C64—H64	
N2—C24—H24A		C66—C65—C64	
C23—C24—H24A		C66—C65—H65	
N2—C24—H24B		C64—C65—H65	
C23—C24—H24B		S6—C66—H66	
H24A—C24—H24B		C65—C66—S6	
N2—C25—C30		C65—C66—C64'	
N2—C25—C26		C65—C66—H66	
C30—C25—C26		C64'—C66—H66	
C27—C26—C25		C12—C10'—C9	
C27—C26—C36		C12—C10'—H10'	
C25—C26—C36		C9—C10'—H10'	
C26—C27—C28		C22—C20'—C19	
C26—C27—H27		C22—C20'—H20'	
C28—C27—H27		C19—C20'—H20'	
C27—C28—C29		C56—C54'—C53	
C27—C28—C31		C56—C54'—H54'	
C29—C28—C31		C53—C54'—H54'	
C30—C29—C28		C66—C64'—C63	
C30—C29—H29		C66—C64'—H64'	
C28—C29—H29		C63—C64'—H64'	
C29—C30—C25		C66—C65—S6'	
C29—C30—H30		S6'—C65—H65	
C25—C30—H30			
N1—C3—C4—C5	−178.5 (3)	C52—C47—C48—C49	−0.7 (4)

C8—C3—C4—C5	1.6 (5)	N3—C47—C48—C58	−0.5 (3)
N1—C3—C4—C14	1.6 (3)	C52—C47—C48—C58	179.3 (3)
C8—C3—C4—C14	−178.3 (3)	C47—C48—C49—C50	−1.0 (4)
C3—C4—C5—C6	−0.3 (4)	C58—C48—C49—C50	178.9 (3)
C14—C4—C5—C6	179.5 (3)	C48—C49—C50—C51	2.3 (4)
C4—C5—C6—C7	−1.6 (4)	C48—C49—C50—C53	−175.5 (2)
C4—C5—C6—C9	177.6 (2)	C49—C50—C51—C52	−2.0 (4)
C5—C6—C7—C8	2.3 (5)	C53—C50—C51—C52	175.8 (3)
C9—C6—C7—C8	−176.8 (3)	C50—C51—C52—C47	0.3 (5)
C6—C7—C8—C3	−1.1 (5)	N3—C47—C52—C51	−179.1 (3)
N1—C3—C8—C7	179.3 (4)	C48—C47—C52—C51	1.1 (4)
C4—C3—C8—C7	−0.9 (5)	C49—C50—C53—C54	16.8 (4)
C5—C6—C9—C10	−4.9 (4)	C51—C50—C53—C54	−160.9 (2)
C7—C6—C9—C10	174.2 (3)	C49—C50—C53—C54'	−162.4 (2)
C5—C6—C9—C10'	175.3 (2)	C51—C50—C53—C54'	19.9 (4)
C7—C6—C9—C10'	−5.6 (4)	C50—C53—C54—C55	179.1 (3)
C6—C9—C10—C11	179.0 (3)	C54'—C53—C54—C55	−1.6 (3)
C10'—C9—C10—C11	−1.1 (3)	C53—C54—C55—C56	0.4 (4)
C9—C10—C11—C12	1.2 (4)	C54—C55—C56—C54'	1.1 (5)
C10—C11—C12—C10'	−0.9 (5)	N3—C57—C58—C59	174.1 (2)
N1—C13—C14—C15	−179.1 (3)	C62—C57—C58—C59	−5.2 (4)
C18—C13—C14—C15	0.9 (4)	N3—C57—C58—C48	−2.0 (3)
N1—C13—C14—C4	−0.4 (3)	C62—C57—C58—C48	178.7 (3)
C18—C13—C14—C4	179.7 (3)	C49—C48—C58—C59	6.3 (5)
C5—C4—C14—C15	−2.1 (5)	C47—C48—C58—C59	−173.8 (3)
C3—C4—C14—C15	177.7 (3)	C49—C48—C58—C57	−178.4 (3)
C5—C4—C14—C13	179.4 (3)	C47—C48—C58—C57	1.5 (3)
C3—C4—C14—C13	−0.8 (3)	C57—C58—C59—C60	1.6 (4)
C13—C14—C15—C16	−0.2 (4)	C48—C58—C59—C60	176.4 (3)
C4—C14—C15—C16	−178.5 (3)	C58—C59—C60—C61	2.8 (4)
C14—C15—C16—C17	−0.5 (4)	C58—C59—C60—C63	−174.3 (3)
C14—C15—C16—C19	178.9 (2)	C59—C60—C61—C62	−4.0 (5)
C15—C16—C17—C18	0.5 (5)	C63—C60—C61—C62	173.2 (3)
C19—C16—C17—C18	−179.0 (3)	C60—C61—C62—C57	0.5 (5)
C16—C17—C18—C13	0.3 (5)	N3—C57—C62—C61	−175.1 (3)
N1—C13—C18—C17	179.0 (4)	C58—C57—C62—C61	4.1 (5)
C14—C13—C18—C17	−1.0 (5)	C59—C60—C63—C64'	149.2 (3)
C15—C16—C19—C20	−174.1 (2)	C61—C60—C63—C64'	−27.9 (4)
C17—C16—C19—C20	5.4 (3)	C59—C60—C63—C64	−25.9 (4)
C15—C16—C19—C20'	2.1 (3)	C61—C60—C63—C64	156.9 (3)
C17—C16—C19—C20'	−178.4 (2)	C60—C63—C64—C65	179.5 (3)
C16—C19—C20—C21	−178.9 (2)	C64'—C63—C64—C65	4.0 (3)
C20'—C19—C20—C21	4.6 (2)	C63—C64—C65—C66	−2.7 (4)
C19—C20—C21—C22	−2.9 (4)	C64—C65—C66—C64'	0.5 (6)
C20—C21—C22—C20'	0.0 (5)	C11—C12—C10'—C9	0.1 (3)
N2—C25—C26—C27	−179.8 (2)	C6—C9—C10'—C12	−179.5 (3)
C30—C25—C26—C27	−0.6 (4)	C10—C9—C10'—C12	0.6 (2)
N2—C25—C26—C36	0.0 (3)	C21—C22—C20'—C19	2.7 (3)
C30—C25—C26—C36	179.2 (2)	C16—C19—C20'—C22	179.0 (2)

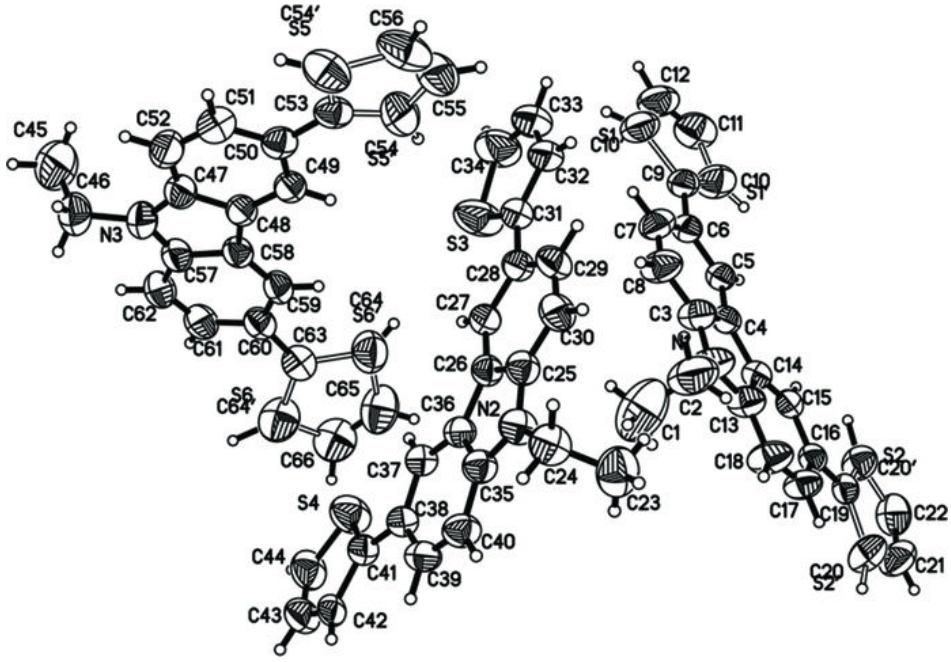
C25—C26—C27—C28	0.9 (4)	C20—C19—C20'—C22	−4.5 (2)
C36—C26—C27—C28	−178.9 (3)	C55—C56—C54'—C53	−1.9 (4)
C26—C27—C28—C29	−0.3 (4)	C50—C53—C54'—C56	−178.6 (2)
C26—C27—C28—C31	178.9 (2)	C54—C53—C54'—C56	2.1 (2)
C27—C28—C29—C30	−0.6 (4)	C65—C66—C64'—C63	2.1 (5)
C31—C28—C29—C30	−179.8 (3)	C60—C63—C64'—C66	−179.5 (3)
C28—C29—C30—C25	0.9 (4)	C64—C63—C64'—C66	−4.0 (3)
N2—C25—C30—C29	178.8 (3)	C18—C13—N1—C3	−178.7 (4)
C26—C25—C30—C29	−0.3 (4)	C14—C13—N1—C3	1.4 (4)
C27—C28—C31—C32	177.9 (3)	C18—C13—N1—C2	6.8 (6)
C29—C28—C31—C32	−2.9 (4)	C14—C13—N1—C2	−173.1 (4)
C27—C28—C31—S3	−1.1 (4)	C8—C3—N1—C13	178.0 (4)
C29—C28—C31—S3	178.2 (2)	C4—C3—N1—C13	−1.9 (4)
C28—C31—C32—C33	−179.0 (3)	C8—C3—N1—C2	−7.6 (7)
S3—C31—C32—C33	0.0 (3)	C4—C3—N1—C2	172.5 (4)
C31—C32—C33—C34	−0.1 (5)	C1—C2—N1—C13	−88.4 (5)
C32—C33—C34—S3	0.1 (5)	C1—C2—N1—C3	98.1 (5)
N2—C35—C36—C37	−178.2 (2)	C30—C25—N2—C35	−178.3 (3)
C40—C35—C36—C37	1.8 (4)	C26—C25—N2—C35	0.8 (3)
N2—C35—C36—C26	1.3 (3)	C30—C25—N2—C24	1.1 (5)
C40—C35—C36—C26	−178.7 (2)	C26—C25—N2—C24	−179.8 (2)
C27—C26—C36—C37	−1.6 (5)	C40—C35—N2—C25	178.6 (3)
C25—C26—C36—C37	178.6 (3)	C36—C35—N2—C25	−1.3 (3)
C27—C26—C36—C35	179.0 (3)	C40—C35—N2—C24	−0.8 (5)
C25—C26—C36—C35	−0.8 (3)	C36—C35—N2—C24	179.2 (2)
C35—C36—C37—C38	−0.7 (4)	C23—C24—N2—C25	−88.5 (4)
C26—C36—C37—C38	180.0 (3)	C23—C24—N2—C35	90.8 (4)
C36—C37—C38—C39	−0.5 (4)	C52—C47—N3—C57	179.4 (3)
C36—C37—C38—C41	179.3 (2)	C48—C47—N3—C57	−0.7 (3)
C37—C38—C39—C40	0.6 (4)	C52—C47—N3—C46	−1.8 (5)
C41—C38—C39—C40	−179.2 (3)	C48—C47—N3—C46	178.0 (3)
C38—C39—C40—C35	0.5 (4)	C62—C57—N3—C47	−179.0 (3)
N2—C35—C40—C39	178.3 (3)	C58—C57—N3—C47	1.7 (3)
C36—C35—C40—C39	−1.7 (4)	C62—C57—N3—C46	2.2 (5)
C37—C38—C41—C42	−169.6 (2)	C58—C57—N3—C46	−177.0 (3)
C39—C38—C41—C42	10.2 (4)	C45—C46—N3—C47	90.8 (5)
C37—C38—C41—S4	10.8 (3)	C45—C46—N3—C57	−90.7 (5)
C39—C38—C41—S4	−169.4 (2)	C33—C34—S3—C31	0.0 (4)
C38—C41—C42—C43	−178.7 (2)	C32—C31—S3—C34	0.0 (3)
S4—C41—C42—C43	0.9 (3)	C28—C31—S3—C34	179.1 (3)
C41—C42—C43—C44	−1.0 (4)	C43—C44—S4—C41	0.0 (3)
C42—C43—C44—S4	0.7 (4)	C38—C41—S4—C44	179.1 (2)
N3—C47—C48—C49	179.4 (2)	C42—C41—S4—C44	−0.6 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C29—H29···S2^{i}	0.93	2.69	3.096 (3)	107

Symmetry codes: (i) −*x*, −*y*, −*z*.

Fig. 1


C54'
S5
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C53
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C50
S5
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C46
C47
C49
C34
C32
C11
S1
C10
C9
C10
S1
C48
C31
C7
C6
N3
C58
S3
C28
C29
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C57
C8
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C65
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C64'
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C20'
C35
C23
S4
C38
C17
C19
C22
C40
C44
C41
C39
C20
S2
C21
C43
C42

Fig. 2