Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{(*R*)-1,1′-Bis(1-naphthylmethyl)-3,3′-[1,1′-binaphthyl-2,2′-diyldi(oxyethylene)]di-1*H*-imidazol-2-yl}mercury(II) bis(hexafluoridophosphate) acetonitrile 3.5-solvate

Jin Lin[a] and Gui-Ying Dong[b]*

[a]College of Chemistry and Materials Science, Hebei Normal University, Shijiazhuang 050016, People's Republic of China, and [b]College of Chemical Engineering and Biotechnology, Hebei Polytechnic University, Tangshan 063009, People's Republic of China
Correspondence e-mail: tscghua@126.com

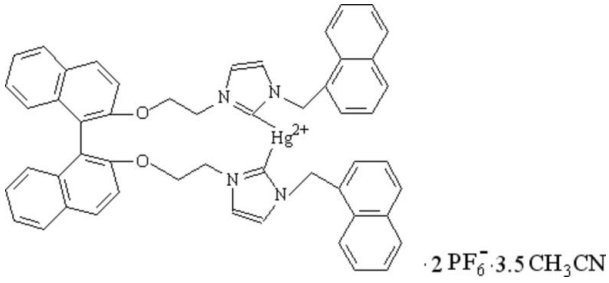
Received 30 May 2007; accepted 31 May 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.012 Å; disorder in solvent or counterion; R factor = 0.047; wR factor = 0.127; data-to-parameter ratio = 15.5.

In the title compound, $[Hg(C_{52}H_{42}N_4O_2)](PF_6)_2\cdot 3.5CH_3CN$, the linear coordination geometry of the Hg ion [C—Hg—C = 174.4 (2)°] is formed by two C atoms from the imidazole fragments [Hg—C = 2.072 (6) and 2.090 (6) Å]. The crystal packing exhibits weak intermolecular C—H···F and C—H···N hydrogen bonds.

Related literature

The related rhodium and iridium complexes of the carbene–naphthoxy ligands were applied to the catalytic asymmetric hydrosilylation of acetophenone with diphenylsilane; see: Chianese & Crabtree (2005); Scheele *et al.* (2006).



Experimental

Crystal data

$[Hg(C_{52}H_{42}N_4O_2)](PF_6)_2\cdot 3.5C_2H_3N$
M_r = 1389.12
Triclinic, $P\overline{1}$
a = 12.266 (4) Å
b = 14.908 (6) Å
c = 16.946 (6) Å
α = 94.448 (6)°
β = 107.027 (6)°
γ = 92.066 (7)°
V = 2948.4 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.75 mm^{-1}
T = 293 (2) K
0.20 × 0.14 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.634, T_{max} = 0.782
(expected range = 0.583–0.719)
17133 measured reflections
11938 independent reflections
8762 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.127
S = 1.04
11938 reflections
770 parameters
21 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.97 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C21—H21A···F11^{i}	0.97	2.54	3.257 (10)	131
C24—H24···F7^{i}	0.93	2.32	3.217 (12)	161
C38—H38B···F3^{ii}	0.97	2.54	3.423 (9)	151
C58—H58B···F8^{iii}	0.96	2.47	3.26 (2)	140
C26—H26A···N6^{iv}	0.97	2.58	3.320 (9)	133

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

The authors thank Hebei Normal University and Hebei Polytechnic University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2254).

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  doi:10.1107/S1600536807026682

supplementary materials

Acta Cryst. (2007). E**63**, m1802 [**doi:10.1107/S1600536807026682**]

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Comment

In the title compound, (I), the cation is a 15-membered macrocyclic metal complex of carbene-naphthoxy ligand adopting a *trans*-conformation. The short distance of 3.657 (4) Å between the centroids of C5—C10 and N3—C39—N4—C40—C41 rings shows a presence of intramolecular π···π interaction. The linear coordination geometry of the Hg ion is formed by two C atoms from the imidazole fragments [Hg—C 2.072 (6), 2.090 (6) Å, C—Hg—C 174.4 (2)°].

The crystal packing is stabilized by the weak C—H···F and C—H···N interactions (Table 1).

Experimental

The ligand (*R*)-2,2'-bis[imidazolium-3-oxyethyl-1-(1-menaphthyl)]-1,1'-binaphthyl bis(hexafluorophosphate) was prepared according to the reported procedure (Scheele *et al.*, 2006). A stirred acetonitrile solution (25 ml) of the corresponding diazolium salt (104.7 mg, 0.10 mmol) and anhydrous $Hg(OAc)_2$ (29.5 mg, 0.10 mmol) was heated at 353 K for 12 h, The remaining acetonitrile was then removed *in vacuo* to give a white solid which was washed with methanol to give the crude product. White single crystals of the title compound were obtained by recrystallization from acetonitile and ethyl ether (yield: 80%) Anal. Calcd. for $C_{118}H_{105}F_{24}Hg_2N_{15}O_4$: C, 51.01; H, 3.81; N, 7.56 Found: C, 50.99; H, 3.76; N 7.49.

Refinement

All H-atoms were geometrically positioned [C—H 0.93–0.97 Å] and refined as riding with U_{iso}(H) =1.2–1.5U_{eq}(C).

Figures

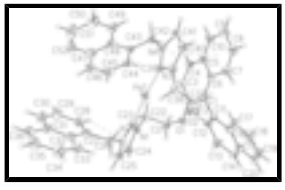


Fig. 1. The cation structure of the title compound, shown with 30% probability displacement ellipsoids. Dashed lines indicate intramolecular hydrogen bonds and π-π stacking interactions.

{(*R*)-1,1'-Bis(1-naphthylmethyl)-3,3'-[1,1'- diyldi(oxyethylene)]di-1*H*-imidazol-2-yl}mercury(II) bis(hexafluoridophosphate) acetonitrile 3.5-solvate

Crystal data

$[Hg(C_{52}H_{42}N_4O_2)](PF_6)_2\cdot 3.5C_2H_3N$	$Z = 2$
$M_r = 1389.12$	$F_{000} = 1386$

Triclinic, $P\bar{1}$	D_x = 1.565 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 12.266 (4) Å	Cell parameters from 923 reflections
b = 14.908 (6) Å	θ = 2.8–22.6º
c = 16.946 (6) Å	μ = 2.75 mm^{-1}
α = 94.448 (6)º	T = 293 (2) K
β = 107.027 (6)º	Block, white
γ = 92.066 (7)º	0.20 × 0.14 × 0.12 mm
V = 2948.4 (19) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	11938 independent reflections
Radiation source: fine-focus sealed tube	8762 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
T = 293(2) K	θ_{max} = 26.4º
phi and ω scans	θ_{min} = 1.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	h = −15→11
T_{min} = 0.634, T_{max} = 0.782	k = −18→16
17133 measured reflections	l = −20→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H-atom parameters constrained
$wR(F^2)$ = 0.127	$w = 1/[\sigma^2(F_o^2) + (0.0627P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.002
11938 reflections	$\Delta\rho_{max}$ = 0.97 e Å^{-3}
770 parameters	$\Delta\rho_{min}$ = −0.78 e Å^{-3}
21 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 calculat-

ing *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)
Hg1	0.84498 (2)	0.923454 (18)	0.734041 (15)	0.03985 (9)	
N1	0.8148 (4)	1.0221 (3)	0.8924 (3)	0.0415 (12)	
N2	0.9675 (4)	1.0740 (4)	0.8693 (3)	0.0410 (12)	
N3	0.9075 (4)	0.7732 (3)	0.6265 (3)	0.0403 (12)	
N4	0.7265 (4)	0.7915 (4)	0.5801 (3)	0.0436 (13)	
O1	0.7722 (4)	0.8275 (3)	0.9203 (3)	0.0497 (11)	
O2	0.9873 (4)	0.7644 (3)	0.8017 (3)	0.0461 (11)	
C1	0.7833 (5)	0.7046 (4)	0.8293 (4)	0.0392 (14)	
C2	0.7187 (5)	0.7712 (4)	0.8499 (4)	0.0407 (14)	
C3	0.6032 (5)	0.7774 (4)	0.8034 (4)	0.0465 (16)	
H3	0.5597	0.8206	0.8201	0.056*	
C4	0.5561 (5)	0.7204 (5)	0.7344 (4)	0.0488 (16)	
H4	0.4799	0.7244	0.7045	0.059*	
C5	0.6209 (6)	0.6547 (5)	0.7070 (4)	0.0462 (16)	
C6	0.7356 (5)	0.6464 (4)	0.7555 (4)	0.0400 (14)	
C7	0.7973 (6)	0.5790 (5)	0.7277 (4)	0.0530 (18)	
H7	0.8714	0.5704	0.7593	0.064*	
C8	0.7508 (7)	0.5266 (5)	0.6559 (5)	0.067 (2)	
H8	0.7941	0.4837	0.6386	0.081*	
C9	0.6381 (7)	0.5359 (6)	0.6071 (5)	0.069 (2)	
H9	0.6076	0.4994	0.5579	0.082*	
C10	0.5735 (6)	0.5983 (5)	0.6320 (5)	0.0598 (19)	
H10	0.4987	0.6040	0.6000	0.072*	
C11	0.8988 (5)	0.6914 (4)	0.8872 (4)	0.0402 (14)	
C12	0.9974 (5)	0.7190 (4)	0.8714 (4)	0.0406 (15)	
C13	1.1056 (6)	0.7054 (5)	0.9259 (4)	0.0514 (17)	
H13	1.1716	0.7256	0.9146	0.062*	
C14	1.1131 (6)	0.6621 (5)	0.9955 (4)	0.058 (2)	
H14	1.1846	0.6518	1.0305	0.070*	
C15	1.0162 (7)	0.6335 (5)	1.0147 (4)	0.0514 (18)	
C16	0.9066 (6)	0.6474 (5)	0.9608 (4)	0.0482 (16)	
C17	0.8098 (7)	0.6182 (5)	0.9819 (5)	0.065 (2)	
H17	0.7374	0.6275	0.9475	0.078*	
C18	0.8203 (10)	0.5758 (6)	1.0528 (6)	0.084 (3)	
H18	0.7554	0.5562	1.0659	0.101*	
C19	0.9286 (10)	0.5622 (6)	1.1051 (5)	0.082 (3)	
H19	0.9354	0.5337	1.1530	0.099*	
C20	1.0235 (8)	0.5898 (5)	1.0869 (5)	0.070 (2)	
H20	1.0948	0.5798	1.1225	0.084*	
C21	0.7127 (6)	0.9027 (4)	0.9414 (4)	0.0458 (16)	
H21A	0.7520	0.9273	0.9977	0.055*	
H21B	0.6363	0.8815	0.9397	0.055*	

C22	0.7044 (5)	0.9756 (4)	0.8850 (4)	0.0467 (16)
H22A	0.6711	0.9498	0.8283	0.056*
H22B	0.6534	1.0193	0.8970	0.056*
C23	0.8763 (5)	1.0159 (4)	0.8385 (4)	0.0414 (15)
C24	0.8692 (6)	1.0845 (5)	0.9582 (4)	0.0553 (18)
H24	0.8455	1.1004	1.0045	0.066*
C25	0.9630 (6)	1.1177 (5)	0.9423 (4)	0.0522 (18)
H25	1.0154	1.1623	0.9749	0.063*
C26	1.0481 (5)	1.1031 (5)	0.8264 (4)	0.0463 (16)
H26A	1.0560	1.0537	0.7881	0.056*
H26B	1.1223	1.1177	0.8667	0.056*
C27	1.0118 (5)	1.1836 (4)	0.7794 (4)	0.0431 (15)
C28	0.9035 (6)	1.2123 (5)	0.7634 (5)	0.061 (2)
H28	0.8509	1.1828	0.7840	0.074*
C29	0.8702 (7)	1.2868 (6)	0.7158 (6)	0.073 (2)
H29	0.7958	1.3048	0.7049	0.088*
C30	0.9450 (9)	1.3312 (6)	0.6865 (5)	0.075 (2)
H30	0.9222	1.3797	0.6556	0.089*
C31	1.0576 (7)	1.3048 (5)	0.7023 (4)	0.0586 (19)
C32	1.0923 (6)	1.2297 (5)	0.7483 (4)	0.0490 (17)
C33	1.2042 (6)	1.2028 (6)	0.7597 (5)	0.062 (2)
H33	1.2287	1.1532	0.7887	0.075*
C34	1.2777 (8)	1.2503 (7)	0.7277 (6)	0.081 (3)
H34	1.3513	1.2320	0.7348	0.097*
C35	1.2428 (10)	1.3252 (7)	0.6852 (6)	0.086 (3)
H35	1.2939	1.3570	0.6649	0.103*
C36	1.1366 (9)	1.3521 (6)	0.6729 (5)	0.073 (2)
H36	1.1150	1.4027	0.6446	0.088*
C37	1.0546 (5)	0.7325 (5)	0.7499 (4)	0.0491 (17)
H37A	1.0360	0.6688	0.7326	0.059*
H37B	1.1353	0.7407	0.7800	0.059*
C38	1.0277 (5)	0.7857 (5)	0.6761 (4)	0.0460 (16)
H38A	1.0462	0.8491	0.6946	0.055*
H38B	1.0753	0.7677	0.6416	0.055*
C39	0.8233 (5)	0.8233 (4)	0.6380 (3)	0.0370 (14)
C40	0.8621 (6)	0.7083 (5)	0.5621 (4)	0.0545 (18)
H40	0.9023	0.6647	0.5423	0.065*
C41	0.7516 (6)	0.7183 (5)	0.5329 (4)	0.0536 (18)
H41	0.7000	0.6832	0.4892	0.064*
C42	0.6119 (5)	0.8276 (4)	0.5654 (4)	0.0447 (15)
H42A	0.5731	0.8007	0.6008	0.054*
H42B	0.5672	0.8110	0.5083	0.054*
C43	0.6187 (5)	0.9279 (5)	0.5823 (4)	0.0463 (16)
C44	0.5870 (6)	0.9657 (6)	0.6479 (4)	0.059 (2)
H44	0.5616	0.9284	0.6812	0.070*
C45	0.5921 (7)	1.0592 (7)	0.6659 (6)	0.077 (3)
H45	0.5695	1.0835	0.7105	0.093*
C46	0.6290 (7)	1.1130 (6)	0.6194 (7)	0.079 (3)
H46	0.6345	1.1749	0.6334	0.095*

C47	0.6606 (6)	1.0797 (6)	0.5489 (6)	0.067 (2)	
C48	0.6555 (5)	0.9848 (5)	0.5302 (4)	0.0503 (17)	
C49	0.6852 (6)	0.9507 (6)	0.4588 (5)	0.061 (2)	
H49	0.6834	0.8887	0.4461	0.073*	
C50	0.7165 (7)	1.0083 (8)	0.4086 (6)	0.084 (3)	
H50	0.7366	0.9851	0.3626	0.100*	
C51	0.7181 (9)	1.1014 (9)	0.4262 (8)	0.100 (4)	
H51	0.7359	1.1397	0.3903	0.120*	
C52	0.6943 (8)	1.1366 (7)	0.4947 (8)	0.090 (3)	
H52	0.6999	1.1988	0.5068	0.108*	
P1	0.19960 (17)	0.60006 (14)	0.56869 (14)	0.0595 (5)	
P2	0.32712 (17)	0.93227 (15)	0.85090 (13)	0.0612 (5)	
F1	0.2784 (5)	0.6251 (4)	0.5131 (4)	0.0935 (16)	
F2	0.1375 (6)	0.5222 (4)	0.5022 (4)	0.135 (3)	
F3	0.1110 (4)	0.6682 (4)	0.5241 (3)	0.0961 (17)	
F4	0.2606 (5)	0.6805 (4)	0.6356 (3)	0.0995 (17)	
F5	0.2898 (5)	0.5351 (4)	0.6149 (5)	0.129 (2)	
F6	0.1198 (5)	0.5779 (4)	0.6244 (3)	0.0908 (16)	
F7	0.2254 (8)	0.9111 (6)	0.8835 (6)	0.183 (4)	
F8	0.4160 (12)	0.9258 (8)	0.9327 (7)	0.275 (7)	
F9	0.3290 (7)	0.8325 (5)	0.8279 (9)	0.225 (6)	
F10	0.2386 (6)	0.9440 (7)	0.7697 (4)	0.165 (3)	
F11	0.3235 (6)	1.0328 (4)	0.8804 (5)	0.132 (2)	
F12	0.4274 (6)	0.9544 (6)	0.8179 (7)	0.185 (4)	
N5	0.4918 (10)	0.6825 (9)	0.3671 (10)	0.156 (5)	
C53	0.4547 (12)	0.6419 (10)	0.3053 (12)	0.129 (5)	
C54	0.4075 (15)	0.5882 (11)	0.2256 (10)	0.182 (7)	
H54A	0.4682	0.5606	0.2095	0.273*	
H54B	0.3697	0.6266	0.1843	0.273*	
H54C	0.3537	0.5422	0.2306	0.273*	
N6	−0.0360 (7)	0.0136 (5)	0.6310 (4)	0.076 (2)	
C55	−0.0159 (7)	0.0671 (6)	0.5928 (5)	0.0584 (19)	
C56	0.0109 (8)	0.1352 (5)	0.5444 (5)	0.071 (2)	
H56A	0.0822	0.1669	0.5747	0.106*	
H56B	−0.0485	0.1768	0.5334	0.106*	
H56C	0.0169	0.1072	0.4930	0.106*	
N7	0.3716 (18)	0.7959 (13)	0.1389 (12)	0.183 (7)	
C57	0.4303 (18)	0.7870 (14)	0.1027 (12)	0.137 (7)	
C58	0.5033 (18)	0.7666 (15)	0.0536 (12)	0.211 (10)	
H58A	0.5739	0.7470	0.0879	0.316*	
H58B	0.5184	0.8194	0.0286	0.316*	
H58C	0.4671	0.7195	0.0110	0.316*	
N8	0.3182 (17)	0.5906 (14)	0.8172 (12)	0.116 (6)	0.50
C59	0.3992 (19)	0.5805 (17)	0.8650 (15)	0.127 (9)	0.50
C60	0.501 (2)	0.539 (2)	0.9171 (19)	0.198 (15)	0.50
H60A	0.5061	0.5507	0.9745	0.297*	0.50
H60B	0.5690	0.5636	0.9075	0.297*	0.50
H60C	0.4942	0.4747	0.9027	0.297*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.03965 (14)	0.04213 (15)	0.03645 (13)	0.00516 (9)	0.01044 (9)	−0.00233 (9)
N1	0.047 (3)	0.038 (3)	0.040 (3)	0.003 (2)	0.016 (2)	−0.004 (2)
N2	0.040 (3)	0.043 (3)	0.041 (3)	0.003 (2)	0.013 (2)	0.003 (2)
N3	0.045 (3)	0.043 (3)	0.036 (3)	0.008 (2)	0.015 (2)	0.000 (2)
N4	0.043 (3)	0.044 (3)	0.042 (3)	0.001 (2)	0.011 (2)	0.004 (2)
O1	0.048 (3)	0.044 (3)	0.052 (3)	0.009 (2)	0.010 (2)	−0.008 (2)
O2	0.038 (2)	0.057 (3)	0.047 (2)	0.013 (2)	0.016 (2)	0.008 (2)
C1	0.039 (3)	0.036 (3)	0.043 (3)	0.003 (3)	0.012 (3)	0.006 (3)
C2	0.042 (4)	0.037 (4)	0.043 (3)	−0.002 (3)	0.014 (3)	0.000 (3)
C3	0.037 (4)	0.043 (4)	0.062 (4)	0.003 (3)	0.019 (3)	0.001 (3)
C4	0.031 (3)	0.051 (4)	0.060 (4)	−0.002 (3)	0.010 (3)	0.002 (3)
C5	0.043 (4)	0.046 (4)	0.047 (4)	−0.004 (3)	0.011 (3)	0.003 (3)
C6	0.041 (4)	0.036 (4)	0.043 (3)	0.000 (3)	0.013 (3)	0.003 (3)
C7	0.047 (4)	0.052 (4)	0.056 (4)	0.013 (3)	0.011 (3)	−0.007 (3)
C8	0.067 (5)	0.060 (5)	0.068 (5)	0.021 (4)	0.012 (4)	−0.012 (4)
C9	0.074 (6)	0.061 (5)	0.060 (5)	0.006 (4)	0.006 (4)	−0.012 (4)
C10	0.053 (4)	0.059 (5)	0.057 (4)	0.002 (4)	0.004 (3)	−0.006 (4)
C11	0.040 (4)	0.037 (4)	0.041 (3)	0.007 (3)	0.008 (3)	0.000 (3)
C12	0.039 (4)	0.041 (4)	0.036 (3)	0.010 (3)	0.004 (3)	−0.002 (3)
C13	0.039 (4)	0.056 (4)	0.053 (4)	0.003 (3)	0.006 (3)	−0.004 (3)
C14	0.056 (5)	0.053 (5)	0.047 (4)	0.013 (4)	−0.013 (3)	0.007 (3)
C15	0.071 (5)	0.037 (4)	0.038 (3)	0.011 (3)	0.005 (3)	−0.002 (3)
C16	0.055 (4)	0.042 (4)	0.044 (4)	0.006 (3)	0.012 (3)	−0.001 (3)
C17	0.066 (5)	0.063 (5)	0.069 (5)	0.009 (4)	0.023 (4)	0.019 (4)
C18	0.118 (8)	0.069 (6)	0.082 (6)	0.007 (5)	0.050 (6)	0.024 (5)
C19	0.129 (9)	0.062 (6)	0.053 (5)	0.014 (6)	0.017 (5)	0.024 (4)
C20	0.092 (7)	0.052 (5)	0.054 (5)	0.008 (4)	0.002 (4)	0.011 (4)
C21	0.052 (4)	0.045 (4)	0.045 (4)	0.001 (3)	0.024 (3)	−0.003 (3)
C22	0.044 (4)	0.045 (4)	0.055 (4)	0.003 (3)	0.021 (3)	0.000 (3)
C23	0.042 (4)	0.039 (4)	0.042 (3)	0.006 (3)	0.010 (3)	0.001 (3)
C24	0.065 (5)	0.054 (4)	0.046 (4)	−0.003 (4)	0.019 (3)	−0.014 (3)
C25	0.056 (4)	0.045 (4)	0.049 (4)	−0.002 (3)	0.010 (3)	−0.010 (3)
C26	0.039 (4)	0.051 (4)	0.048 (4)	0.001 (3)	0.013 (3)	0.007 (3)
C27	0.042 (4)	0.038 (4)	0.042 (3)	0.001 (3)	0.003 (3)	−0.004 (3)
C28	0.052 (4)	0.054 (5)	0.078 (5)	0.012 (3)	0.016 (4)	0.011 (4)
C29	0.060 (5)	0.063 (6)	0.087 (6)	0.025 (4)	0.006 (5)	0.010 (5)
C30	0.097 (7)	0.058 (5)	0.065 (5)	0.024 (5)	0.014 (5)	0.015 (4)
C31	0.083 (6)	0.049 (4)	0.043 (4)	0.004 (4)	0.018 (4)	0.005 (3)
C32	0.052 (4)	0.047 (4)	0.042 (4)	0.004 (3)	0.005 (3)	0.000 (3)
C33	0.058 (5)	0.071 (5)	0.060 (5)	−0.002 (4)	0.020 (4)	0.013 (4)
C34	0.065 (6)	0.093 (7)	0.091 (6)	−0.004 (5)	0.028 (5)	0.027 (6)
C35	0.108 (8)	0.081 (7)	0.075 (6)	−0.031 (6)	0.041 (6)	0.010 (5)
C36	0.099 (7)	0.059 (5)	0.063 (5)	−0.004 (5)	0.022 (5)	0.014 (4)
C37	0.037 (4)	0.062 (5)	0.049 (4)	0.009 (3)	0.016 (3)	−0.004 (3)

C38	0.038 (4)	0.053 (4)	0.052 (4)	0.008 (3)	0.021 (3)	0.002 (3)
C39	0.039 (3)	0.039 (4)	0.034 (3)	0.000 (3)	0.012 (3)	0.004 (3)
C40	0.062 (5)	0.053 (4)	0.050 (4)	0.008 (4)	0.021 (4)	−0.006 (3)
C41	0.066 (5)	0.047 (4)	0.042 (4)	−0.002 (3)	0.012 (3)	−0.011 (3)
C42	0.036 (3)	0.049 (4)	0.046 (4)	0.003 (3)	0.006 (3)	0.012 (3)
C43	0.035 (3)	0.050 (4)	0.044 (4)	0.005 (3)	−0.002 (3)	0.002 (3)
C44	0.052 (4)	0.073 (6)	0.046 (4)	0.018 (4)	0.005 (3)	0.008 (4)
C45	0.062 (5)	0.090 (7)	0.068 (6)	0.021 (5)	0.004 (4)	−0.018 (5)
C46	0.056 (5)	0.053 (5)	0.104 (7)	0.016 (4)	−0.010 (5)	−0.018 (5)
C47	0.038 (4)	0.056 (5)	0.091 (6)	0.001 (3)	−0.010 (4)	0.012 (5)
C48	0.031 (3)	0.053 (4)	0.057 (4)	−0.001 (3)	−0.003 (3)	0.012 (3)
C49	0.049 (4)	0.073 (5)	0.060 (5)	0.006 (4)	0.009 (4)	0.022 (4)
C50	0.066 (6)	0.102 (8)	0.089 (7)	0.010 (5)	0.027 (5)	0.035 (6)
C51	0.073 (7)	0.100 (9)	0.128 (10)	−0.010 (6)	0.023 (7)	0.052 (8)
C52	0.054 (5)	0.061 (6)	0.137 (10)	−0.006 (4)	−0.007 (6)	0.034 (6)
P1	0.0561 (12)	0.0521 (12)	0.0762 (13)	0.0048 (9)	0.0300 (10)	0.0009 (10)
P2	0.0511 (12)	0.0636 (14)	0.0654 (12)	0.0107 (10)	0.0131 (10)	−0.0023 (10)
F1	0.094 (4)	0.086 (4)	0.126 (4)	0.011 (3)	0.070 (3)	0.016 (3)
F2	0.135 (5)	0.115 (5)	0.160 (6)	−0.048 (4)	0.080 (5)	−0.074 (5)
F3	0.081 (4)	0.128 (5)	0.087 (3)	0.045 (3)	0.029 (3)	0.023 (3)
F4	0.103 (4)	0.087 (4)	0.092 (4)	−0.021 (3)	0.013 (3)	−0.014 (3)
F5	0.114 (5)	0.111 (5)	0.196 (7)	0.061 (4)	0.076 (5)	0.082 (5)
F6	0.103 (4)	0.087 (4)	0.107 (4)	0.001 (3)	0.069 (3)	0.008 (3)
F7	0.224 (9)	0.172 (8)	0.223 (9)	−0.023 (6)	0.179 (8)	0.016 (7)
F8	0.303 (14)	0.206 (11)	0.186 (10)	0.014 (10)	−0.140 (10)	0.059 (8)
F9	0.128 (6)	0.073 (5)	0.454 (17)	−0.001 (4)	0.080 (8)	−0.077 (7)
F10	0.130 (6)	0.259 (11)	0.078 (4)	−0.013 (6)	−0.009 (4)	0.013 (5)
F11	0.114 (5)	0.092 (5)	0.180 (7)	0.020 (4)	0.037 (5)	−0.027 (5)
F12	0.088 (5)	0.175 (8)	0.314 (12)	−0.024 (5)	0.116 (7)	−0.058 (8)
N5	0.100 (8)	0.114 (10)	0.226 (16)	0.006 (7)	0.017 (9)	−0.032 (10)
C53	0.093 (10)	0.097 (11)	0.197 (17)	−0.009 (7)	0.049 (11)	−0.004 (10)
C54	0.212 (18)	0.165 (16)	0.160 (15)	−0.069 (13)	0.060 (13)	−0.012 (13)
N6	0.097 (6)	0.062 (5)	0.068 (4)	−0.013 (4)	0.025 (4)	0.008 (4)
C55	0.060 (5)	0.059 (5)	0.052 (4)	−0.004 (4)	0.016 (4)	−0.007 (4)
C56	0.095 (6)	0.058 (5)	0.064 (5)	−0.004 (4)	0.029 (5)	0.014 (4)
N7	0.20 (2)	0.141 (13)	0.184 (17)	0.008 (13)	0.030 (13)	−0.007 (12)
C57	0.149 (19)	0.131 (15)	0.113 (14)	−0.009 (13)	0.008 (11)	0.038 (12)
C58	0.21 (2)	0.26 (3)	0.147 (16)	−0.010 (18)	0.014 (15)	0.083 (17)
N8	0.114 (9)	0.120 (10)	0.112 (9)	0.023 (8)	0.023 (8)	0.022 (8)
C59	0.127 (12)	0.134 (12)	0.128 (12)	−0.015 (9)	0.050 (9)	0.013 (9)
C60	0.201 (17)	0.205 (18)	0.195 (17)	−0.002 (10)	0.071 (10)	0.025 (10)

Geometric parameters (Å, °)

Hg1—C39	2.072 (6)	C31—C36	1.405 (12)
Hg1—C23	2.090 (6)	C31—C32	1.420 (10)
N1—C23	1.345 (8)	C32—C33	1.407 (10)
N1—C24	1.383 (8)	C33—C34	1.381 (11)
N1—C22	1.466 (8)	C33—H33	0.9300

N2—C23	1.338 (8)	C34—C35	1.388 (13)
N2—C25	1.369 (8)	C34—H34	0.9300
N2—C26	1.461 (8)	C35—C36	1.339 (13)
N3—C39	1.346 (8)	C35—H35	0.9300
N3—C40	1.372 (8)	C36—H36	0.9300
N3—C38	1.465 (8)	C37—C38	1.494 (9)
N4—C39	1.342 (7)	C37—H37A	0.9700
N4—C41	1.400 (8)	C37—H37B	0.9700
N4—C42	1.482 (8)	C38—H38A	0.9700
O1—C2	1.380 (7)	C38—H38B	0.9700
O1—C21	1.437 (7)	C40—C41	1.318 (10)
O2—C12	1.382 (7)	C40—H40	0.9300
O2—C37	1.437 (7)	C41—H41	0.9300
C1—C2	1.379 (9)	C42—C43	1.494 (9)
C1—C6	1.423 (8)	C42—H42A	0.9700
C1—C11	1.498 (8)	C42—H42B	0.9700
C2—C3	1.416 (9)	C43—C44	1.369 (10)
C3—C4	1.355 (9)	C43—C48	1.424 (10)
C3—H3	0.9300	C44—C45	1.399 (12)
C4—C5	1.417 (9)	C44—H44	0.9300
C4—H4	0.9300	C45—C46	1.323 (13)
C5—C6	1.421 (9)	C45—H45	0.9300
C5—C10	1.424 (9)	C46—C47	1.421 (13)
C6—C7	1.413 (9)	C46—H46	0.9300
C7—C8	1.352 (10)	C47—C48	1.420 (10)
C7—H7	0.9300	C47—C52	1.433 (14)
C8—C9	1.405 (10)	C48—C49	1.425 (10)
C8—H8	0.9300	C49—C50	1.375 (12)
C9—C10	1.363 (10)	C49—H49	0.9300
C9—H9	0.9300	C50—C51	1.396 (15)
C10—H10	0.9300	C50—H50	0.9300
C11—C12	1.369 (9)	C51—C52	1.350 (15)
C11—C16	1.433 (9)	C51—H51	0.9300
C12—C13	1.410 (9)	C52—H52	0.9300
C13—C14	1.369 (10)	P1—F2	1.558 (6)
C13—H13	0.9300	P1—F5	1.570 (6)
C14—C15	1.383 (11)	P1—F3	1.582 (5)
C14—H14	0.9300	P1—F4	1.584 (5)
C15—C20	1.413 (10)	P1—F1	1.589 (5)
C15—C16	1.419 (9)	P1—F6	1.589 (5)
C16—C17	1.402 (10)	P2—F8	1.504 (8)
C17—C18	1.376 (11)	P2—F10	1.510 (7)
C17—H17	0.9300	P2—F9	1.510 (7)
C18—C19	1.396 (13)	P2—F12	1.529 (7)
C18—H18	0.9300	P2—F7	1.538 (7)
C19—C20	1.345 (13)	P2—F11	1.549 (6)
C19—H19	0.9300	N5—C53	1.127 (18)
C20—H20	0.9300	C53—C54	1.46 (2)
C21—C22	1.489 (9)	C54—H54A	0.9600

C21—H21A	0.9700	C54—H54B	0.9600
C21—H21B	0.9700	C54—H54C	0.9600
C22—H22A	0.9700	N6—C55	1.129 (10)
C22—H22B	0.9700	C55—C56	1.439 (11)
C24—C25	1.342 (10)	C56—H56A	0.9600
C24—H24	0.9300	C56—H56B	0.9600
C25—H25	0.9300	C56—H56C	0.9600
C26—C27	1.501 (9)	N7—C57	1.08 (2)
C26—H26A	0.9700	C57—C58	1.42 (2)
C26—H26B	0.9700	C58—H58A	0.9600
C27—C28	1.367 (9)	C58—H58B	0.9600
C27—C32	1.427 (10)	C58—H58C	0.9600
C28—C29	1.425 (11)	N8—C59	1.107 (9)
C28—H28	0.9300	C59—C60	1.493 (9)
C29—C30	1.342 (12)	C60—H60A	0.9600
C29—H29	0.9300	C60—H60B	0.9600
C30—C31	1.404 (12)	C60—H60C	0.9600
C30—H30	0.9300		
C39—Hg1—C23	174.4 (2)	C33—C34—H34	119.6
C23—N1—C24	109.4 (5)	C35—C34—H34	119.6
C23—N1—C22	128.0 (5)	C36—C35—C34	120.8 (9)
C24—N1—C22	122.6 (5)	C36—C35—H35	119.6
C23—N2—C25	109.7 (6)	C34—C35—H35	119.6
C23—N2—C26	126.8 (5)	C35—C36—C31	120.7 (9)
C25—N2—C26	122.3 (6)	C35—C36—H36	119.7
C39—N3—C40	109.0 (5)	C31—C36—H36	119.7
C39—N3—C38	125.2 (5)	O2—C37—C38	107.5 (5)
C40—N3—C38	125.8 (5)	O2—C37—H37A	110.2
C39—N4—C41	108.4 (6)	C38—C37—H37A	110.2
C39—N4—C42	127.0 (5)	O2—C37—H37B	110.2
C41—N4—C42	124.6 (5)	C38—C37—H37B	110.2
C2—O1—C21	118.4 (5)	H37A—C37—H37B	108.5
C12—O2—C37	115.3 (5)	N3—C38—C37	112.7 (5)
C2—C1—C6	118.9 (6)	N3—C38—H38A	109.1
C2—C1—C11	119.5 (5)	C37—C38—H38A	109.1
C6—C1—C11	121.4 (5)	N3—C38—H38B	109.1
C1—C2—O1	115.8 (5)	C37—C38—H38B	109.1
C1—C2—C3	121.2 (6)	H38A—C38—H38B	107.8
O1—C2—C3	122.9 (6)	N4—C39—N3	107.1 (5)
C4—C3—C2	120.0 (6)	N4—C39—Hg1	128.6 (5)
C4—C3—H3	120.0	N3—C39—Hg1	124.1 (4)
C2—C3—H3	120.0	C41—C40—N3	108.3 (6)
C3—C4—C5	121.1 (6)	C41—C40—H40	125.8
C3—C4—H4	119.4	N3—C40—H40	125.8
C5—C4—H4	119.4	C40—C41—N4	107.2 (6)
C4—C5—C6	118.8 (6)	C40—C41—H41	126.4
C4—C5—C10	121.2 (6)	N4—C41—H41	126.4
C6—C5—C10	120.0 (6)	N4—C42—C43	112.0 (5)
C7—C6—C5	117.5 (6)	N4—C42—H42A	109.2

C7—C6—C1	122.8 (6)	C43—C42—H42A	109.2
C5—C6—C1	119.7 (6)	N4—C42—H42B	109.2
C8—C7—C6	121.4 (6)	C43—C42—H42B	109.2
C8—C7—H7	119.3	H42A—C42—H42B	107.9
C6—C7—H7	119.3	C44—C43—C48	119.4 (7)
C7—C8—C9	121.1 (7)	C44—C43—C42	119.7 (7)
C7—C8—H8	119.4	C48—C43—C42	120.9 (6)
C9—C8—H8	119.4	C43—C44—C45	121.6 (8)
C10—C9—C8	120.1 (7)	C43—C44—H44	119.2
C10—C9—H9	120.0	C45—C44—H44	119.2
C8—C9—H9	120.0	C46—C45—C44	119.8 (9)
C9—C10—C5	119.9 (7)	C46—C45—H45	120.1
C9—C10—H10	120.1	C44—C45—H45	120.1
C5—C10—H10	120.1	C45—C46—C47	122.4 (9)
C12—C11—C16	118.9 (6)	C45—C46—H46	118.8
C12—C11—C1	122.0 (6)	C47—C46—H46	118.8
C16—C11—C1	119.2 (6)	C48—C47—C46	118.0 (8)
C11—C12—O2	117.7 (5)	C48—C47—C52	118.5 (9)
C11—C12—C13	121.5 (6)	C46—C47—C52	123.5 (9)
O2—C12—C13	120.8 (6)	C47—C48—C43	118.8 (7)
C14—C13—C12	119.6 (7)	C47—C48—C49	118.5 (7)
C14—C13—H13	120.2	C43—C48—C49	122.7 (7)
C12—C13—H13	120.2	C50—C49—C48	120.7 (9)
C13—C14—C15	121.2 (6)	C50—C49—H49	119.6
C13—C14—H14	119.4	C48—C49—H49	119.6
C15—C14—H14	119.4	C49—C50—C51	120.4 (10)
C14—C15—C20	121.4 (7)	C49—C50—H50	119.8
C14—C15—C16	119.8 (6)	C51—C50—H50	119.8
C20—C15—C16	118.9 (8)	C52—C51—C50	120.8 (10)
C17—C16—C15	118.6 (7)	C52—C51—H51	119.6
C17—C16—C11	122.4 (6)	C50—C51—H51	119.6
C15—C16—C11	119.1 (6)	C51—C52—C47	121.1 (10)
C18—C17—C16	120.9 (8)	C51—C52—H52	119.5
C18—C17—H17	119.5	C47—C52—H52	119.5
C16—C17—H17	119.5	F2—P1—F5	91.3 (4)
C17—C18—C19	119.8 (9)	F2—P1—F3	90.5 (4)
C17—C18—H18	120.1	F5—P1—F3	178.1 (4)
C19—C18—H18	120.1	F2—P1—F4	178.8 (4)
C20—C19—C18	120.9 (8)	F5—P1—F4	89.9 (4)
C20—C19—H19	119.5	F3—P1—F4	88.3 (3)
C18—C19—H19	119.5	F2—P1—F1	90.0 (3)
C19—C20—C15	120.9 (8)	F5—P1—F1	90.5 (3)
C19—C20—H20	119.5	F3—P1—F1	89.3 (3)
C15—C20—H20	119.5	F4—P1—F1	90.2 (3)
O1—C21—C22	113.2 (5)	F2—P1—F6	90.9 (3)
O1—C21—H21A	108.9	F5—P1—F6	90.8 (3)
C22—C21—H21A	108.9	F3—P1—F6	89.4 (3)
O1—C21—H21B	108.9	F4—P1—F6	88.8 (3)
C22—C21—H21B	108.9	F1—P1—F6	178.4 (3)

H21A—C21—H21B	107.8	F8—P2—F10	177.0 (6)
N1—C22—C21	113.5 (6)	F8—P2—F9	91.0 (7)
N1—C22—H22A	108.9	F10—P2—F9	91.9 (6)
C21—C22—H22A	108.9	F8—P2—F12	85.9 (7)
N1—C22—H22B	108.9	F10—P2—F12	93.5 (5)
C21—C22—H22B	108.9	F9—P2—F12	92.3 (5)
H22A—C22—H22B	107.7	F8—P2—F7	94.6 (8)
N2—C23—N1	106.7 (5)	F10—P2—F7	85.9 (5)
N2—C23—Hg1	126.6 (5)	F9—P2—F7	88.3 (5)
N1—C23—Hg1	126.4 (5)	F12—P2—F7	179.2 (6)
C25—C24—N1	106.6 (6)	F8—P2—F11	86.5 (6)
C25—C24—H24	126.7	F10—P2—F11	90.6 (5)
N1—C24—H24	126.7	F9—P2—F11	175.8 (6)
C24—C25—N2	107.6 (6)	F12—P2—F11	90.9 (4)
C24—C25—H25	126.2	F7—P2—F11	88.5 (4)
N2—C25—H25	126.2	N5—C53—C54	179 (2)
N2—C26—C27	113.0 (5)	C53—C54—H54A	109.5
N2—C26—H26A	109.0	C53—C54—H54B	109.5
C27—C26—H26A	109.0	H54A—C54—H54B	109.5
N2—C26—H26B	109.0	C53—C54—H54C	109.5
C27—C26—H26B	109.0	H54A—C54—H54C	109.5
H26A—C26—H26B	107.8	H54B—C54—H54C	109.5
C28—C27—C32	119.3 (7)	N6—C55—C56	179.5 (10)
C28—C27—C26	122.1 (6)	C55—C56—H56A	109.5
C32—C27—C26	118.6 (6)	C55—C56—H56B	109.5
C27—C28—C29	120.8 (8)	H56A—C56—H56B	109.5
C27—C28—H28	119.6	C55—C56—H56C	109.5
C29—C28—H28	119.6	H56A—C56—H56C	109.5
C30—C29—C28	120.6 (8)	H56B—C56—H56C	109.5
C30—C29—H29	119.7	N7—C57—C58	174 (3)
C28—C29—H29	119.7	C57—C58—H58A	109.5
C29—C30—C31	120.4 (8)	C57—C58—H58B	109.5
C29—C30—H30	119.8	H58A—C58—H58B	109.5
C31—C30—H30	119.8	C57—C58—H58C	109.5
C30—C31—C36	120.5 (8)	H58A—C58—H58C	109.5
C30—C31—C32	120.0 (7)	H58B—C58—H58C	109.5
C36—C31—C32	119.5 (8)	N8—C59—C60	163 (3)
C33—C32—C31	118.3 (7)	C59—C60—H60A	109.5
C33—C32—C27	122.8 (7)	C59—C60—H60B	109.5
C31—C32—C27	118.8 (7)	H60A—C60—H60B	109.5
C34—C33—C32	119.8 (8)	C59—C60—H60C	109.5
C34—C33—H33	120.1	H60A—C60—H60C	109.5
C32—C33—H33	120.1	H60B—C60—H60C	109.5
C33—C34—C35	120.7 (9)		
C6—C1—C2—O1	−177.3 (5)	N1—C24—C25—N2	−2.0 (8)
C11—C1—C2—O1	6.3 (9)	C23—N2—C25—C24	1.7 (8)
C6—C1—C2—C3	5.8 (9)	C26—N2—C25—C24	169.9 (6)
C11—C1—C2—C3	−170.6 (6)	C23—N2—C26—C27	88.2 (8)
C21—O1—C2—C1	175.1 (6)	C25—N2—C26—C27	−77.9 (7)

C21—O1—C2—C3	−8.0 (9)	N2—C26—C27—C28	−14.1 (9)
C1—C2—C3—C4	−3.8 (10)	N2—C26—C27—C32	167.9 (5)
O1—C2—C3—C4	179.5 (6)	C32—C27—C28—C29	0.6 (11)
C2—C3—C4—C5	−0.8 (10)	C26—C27—C28—C29	−177.5 (7)
C3—C4—C5—C6	3.0 (10)	C27—C28—C29—C30	−1.0 (13)
C3—C4—C5—C10	−176.3 (7)	C28—C29—C30—C31	0.1 (13)
C4—C5—C6—C7	178.6 (6)	C29—C30—C31—C36	−179.0 (8)
C10—C5—C6—C7	−2.1 (10)	C29—C30—C31—C32	1.1 (12)
C4—C5—C6—C1	−0.9 (9)	C30—C31—C32—C33	177.2 (7)
C10—C5—C6—C1	178.4 (6)	C36—C31—C32—C33	−2.7 (10)
C2—C1—C6—C7	177.1 (7)	C30—C31—C32—C27	−1.5 (10)
C11—C1—C6—C7	−6.5 (10)	C36—C31—C32—C27	178.6 (7)
C2—C1—C6—C5	−3.4 (9)	C28—C27—C32—C33	−178.0 (7)
C11—C1—C6—C5	172.9 (6)	C26—C27—C32—C33	0.2 (10)
C5—C6—C7—C8	2.6 (11)	C28—C27—C32—C31	0.6 (10)
C1—C6—C7—C8	−177.9 (7)	C26—C27—C32—C31	178.8 (6)
C6—C7—C8—C9	−1.5 (13)	C31—C32—C33—C34	1.2 (11)
C7—C8—C9—C10	−0.2 (14)	C27—C32—C33—C34	179.8 (7)
C8—C9—C10—C5	0.7 (13)	C32—C33—C34—C35	0.8 (13)
C4—C5—C10—C9	179.8 (8)	C33—C34—C35—C36	−1.2 (15)
C6—C5—C10—C9	0.5 (11)	C34—C35—C36—C31	−0.4 (14)
C2—C1—C11—C12	−104.9 (7)	C30—C31—C36—C35	−177.5 (8)
C6—C1—C11—C12	78.8 (8)	C32—C31—C36—C35	2.4 (12)
C2—C1—C11—C16	76.1 (8)	C12—O2—C37—C38	176.9 (5)
C6—C1—C11—C16	−100.2 (7)	C39—N3—C38—C37	89.3 (7)
C16—C11—C12—O2	−177.6 (5)	C40—N3—C38—C37	−89.5 (7)
C1—C11—C12—O2	3.4 (9)	O2—C37—C38—N3	−61.9 (7)
C16—C11—C12—C13	−0.2 (9)	C41—N4—C39—N3	1.6 (7)
C1—C11—C12—C13	−179.3 (6)	C42—N4—C39—N3	−177.0 (6)
C37—O2—C12—C11	−131.8 (6)	C41—N4—C39—Hg1	−174.4 (5)
C37—O2—C12—C13	50.9 (8)	C42—N4—C39—Hg1	7.0 (9)
C11—C12—C13—C14	1.2 (10)	C40—N3—C39—N4	−1.5 (7)
O2—C12—C13—C14	178.4 (6)	C38—N3—C39—N4	179.5 (5)
C12—C13—C14—C15	−1.7 (11)	C40—N3—C39—Hg1	174.7 (5)
C13—C14—C15—C20	−179.3 (7)	C38—N3—C39—Hg1	−4.3 (8)
C13—C14—C15—C16	1.3 (11)	C23—Hg1—C39—N4	132 (2)
C14—C15—C16—C17	−179.7 (7)	C23—Hg1—C39—N3	−43 (3)
C20—C15—C16—C17	0.8 (10)	C39—N3—C40—C41	0.9 (8)
C14—C15—C16—C11	−0.3 (10)	C38—N3—C40—C41	179.9 (6)
C20—C15—C16—C11	−179.7 (6)	N3—C40—C41—N4	0.1 (8)
C12—C11—C16—C17	179.2 (6)	C39—N4—C41—C40	−1.0 (8)
C1—C11—C16—C17	−1.7 (10)	C42—N4—C41—C40	177.6 (6)
C12—C11—C16—C15	−0.2 (9)	C39—N4—C42—C43	34.2 (9)
C1—C11—C16—C15	178.8 (6)	C41—N4—C42—C43	−144.1 (6)
C15—C16—C17—C18	−0.9 (11)	N4—C42—C43—C44	−112.5 (7)
C11—C16—C17—C18	179.7 (7)	N4—C42—C43—C48	68.8 (7)
C16—C17—C18—C19	0.6 (13)	C48—C43—C44—C45	−1.3 (10)
C17—C18—C19—C20	−0.2 (14)	C42—C43—C44—C45	180.0 (6)
C18—C19—C20—C15	0.2 (13)	C43—C44—C45—C46	−0.5 (12)

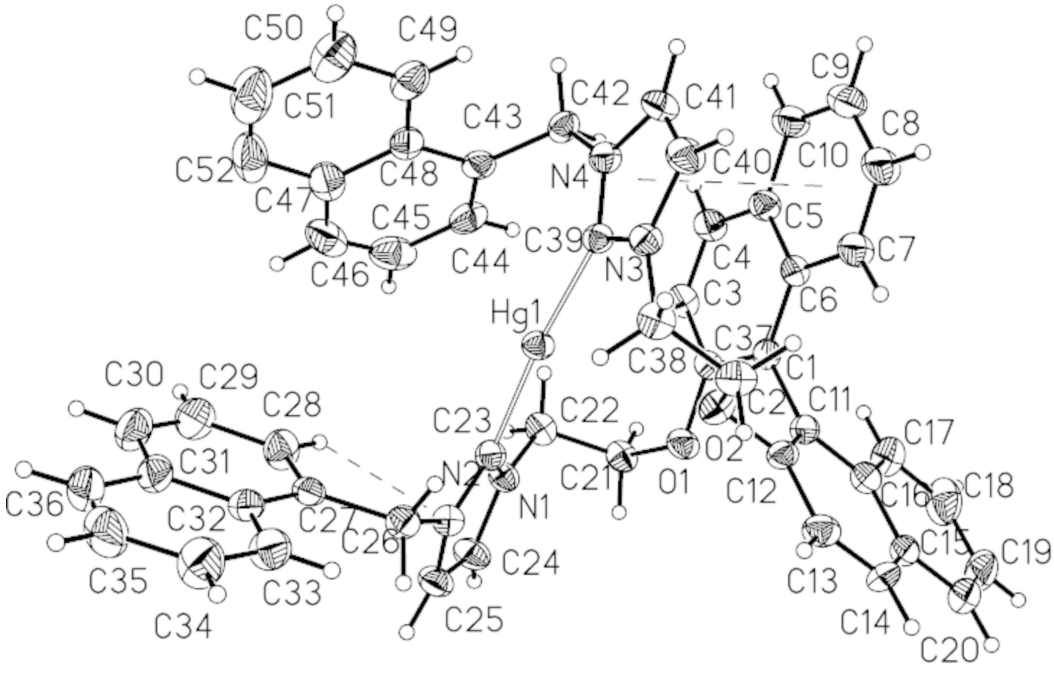
C14—C15—C20—C19	180.0 (8)	C44—C45—C46—C47	2.3 (13)
C16—C15—C20—C19	−0.6 (11)	C45—C46—C47—C48	−2.2 (12)
C2—O1—C21—C22	−71.7 (7)	C45—C46—C47—C52	176.1 (8)
C23—N1—C22—C21	107.3 (7)	C46—C47—C48—C43	0.3 (9)
C24—N1—C22—C21	−75.7 (8)	C52—C47—C48—C43	−178.1 (6)
O1—C21—C22—N1	−67.6 (7)	C46—C47—C48—C49	179.0 (6)
C25—N2—C23—N1	−0.7 (7)	C52—C47—C48—C49	0.6 (10)
C26—N2—C23—N1	−168.2 (6)	C44—C43—C48—C47	1.3 (9)
C25—N2—C23—Hg1	−174.5 (5)	C42—C43—C48—C47	−180.0 (6)
C26—N2—C23—Hg1	18.0 (9)	C44—C43—C48—C49	−177.3 (6)
C24—N1—C23—N2	−0.5 (7)	C42—C43—C48—C49	1.5 (9)
C22—N1—C23—N2	176.8 (6)	C47—C48—C49—C50	−0.9 (10)
C24—N1—C23—Hg1	173.3 (5)	C43—C48—C49—C50	177.7 (7)
C22—N1—C23—Hg1	−9.4 (9)	C48—C49—C50—C51	−0.9 (13)
C39—Hg1—C23—N2	86 (3)	C49—C50—C51—C52	3.1 (15)
C39—Hg1—C23—N1	−87 (3)	C50—C51—C52—C47	−3.4 (15)
C23—N1—C24—C25	1.6 (8)	C48—C47—C52—C51	1.6 (13)
C22—N1—C24—C25	−176.0 (6)	C46—C47—C52—C51	−176.7 (9)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C21—H21A···F11^{i}	0.97	2.54	3.257 (10)	131
C24—H24···F7^{i}	0.93	2.32	3.217 (12)	161
C38—H38B···F3^{ii}	0.97	2.54	3.423 (9)	151
C58—H58B···F8^{iii}	0.96	2.47	3.26 (2)	140
C26—H26A···N6^{iv}	0.97	2.58	3.320 (9)	133

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

Fig. 1


C50
C49
C51
C43
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C9
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C52
C48
N4
C40
C10
C47
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C5
C7
C46
C44
N3
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C21
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C36
C32
C27
N1
O1
C12
C16
C18
C26
C24
C15
C19
C35
C33
C13
C34
C25
C14
C20