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Key indicators

 Single-crystal X-ray study
 $T = 293$ K
 Mean $\sigma(\text{C}-\text{C}) = 0.011$ Å
 R factor = 0.049
 wR factor = 0.092
 Data-to-parameter ratio = 18.0

 For details of how these key indicators were
 automatically derived from the article, see
<http://journals.iucr.org/e>.

Bis[2-(2-methylphenylimino)phenyl]mercury(II)

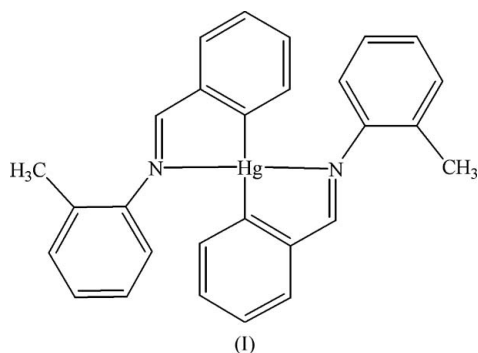
 The structure of the cyclomercurated 2-phenyliminophenyl title compound, $[\text{Hg}(\text{C}_{14}\text{H}_{12}\text{N})_2]$, shows that the mercury coordination is essentially square planar

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Comment

The structure of the title compound, (I), is shown in Fig. 1. Organomercurials are often used as transmetallation reagents in the synthesis of organometallic complexes (Roper & Wright, 1977). Several years ago we reported a synthetic route for the preparation of a range of functionalized 1-mercurio-2-phenyliminophenyls (Flower *et al.*, 2002) and from the structural data obtained concurred with a previous report of Batsanov (1998) that the van der Waals radius of mercury is in the range 2.0–2.2 Å, rather than the often quoted value of 1.55 Å (Bondi, 1964). Here, and in the following paper (Flower & Pritchard, 2006), we report two additional structures of this type of compound. All of the bond lengths and angles in the two structures are as expected. The Hg–N distances in (I) and bis-2-(2-isopropylphenyliminophenyl)-mercury, (II), range from 2.787 (10) to 2.850 (10) Å and are comfortably within the sum of the van der Waals radii (3.5–3.7 Å), if the van der Waals radius of Hg is considered to be 2.0–2.2 Å, indicating significant Hg–N interactions. This gives rise to an overall distorted square-planar geometry at Hg in both cases. Other examples of square planar Hg^{II} complexes are known (Balasubramani *et al.*, 2005; Haid *et al.*, 2003; Cheng *et al.*, 1994).



Experimental

Caution: preparation of an organomercurial. Organomercurials are extremely toxic. To $\text{Hg}(\text{C}_6\text{H}_4\text{-2-CHO})_2$ (1 g, 2.4 mmol) dissolved in ethanol (10 ml) containing *p*-toluenesulfonic acid (10 mg, 0.05 mmol) was added 2-methylaniline (0.56 g, 6 mmol) and the solution was refluxed for 5 h, during which time white crystals of (I) precipitated.

The crystalline material was collected by filtration, washed with water and dried in a desiccator. Yield 0.93 g, 68%. An analytically pure sample was obtained through recrystallization from hot ethanol, and crystals suitable for the diffraction study were grown by dissolving approximately 10 mg of (I) in CH₂Cl₂ (0.2 ml) in a small vial (1 × 5 cm), layering ethanol (5 ml) on top and leaving the vial to stand for 24 h. Elemental analysis C₂₈H₂₄HgN₂ requires: C 57.56, H 4.11, N 4.76%; found: C 57.79, H 4.22, N 4.91%.

Crystal data

[Hg(C ₁₄ H ₁₂ N) ₂]	Z = 4
M _r = 589.08	D _x = 1.736 Mg m ⁻³
Monoclinic, P2 ₁ /c	Mo Kα radiation
a = 11.9925 (3) Å	μ = 6.85 mm ⁻¹
b = 11.3864 (3) Å	T = 293 (2) K
c = 16.6542 (5) Å	Plate, yellow
β = 97.6730 (10)°	0.2 × 0.15 × 0.05 mm
V = 2253.79 (11) Å ³	

Data collection

Nonius KappaCCD diffractometer	14711 measured reflections
φ and ω scans	5084 independent reflections
Absorption correction: multi-scan (SORTAV; Blessing, 1995)	3476 reflections with I > 2σ(I)
T _{min} = 0.254, T _{max} = 0.707	R _{int} = 0.086
	θ _{max} = 27.4°

Refinement

Refinement on F ²	w = 1/[σ ² (F _o ²) + (0.0284P) ² + 5.7069P]
R[F ² > 2σ(F ²)] = 0.050	where P = (F _o ² + 2F _c ²)/3
wR(F ²) = 0.092	(Δ/σ) _{max} = 0.001
S = 1.02	Δρ _{max} = 1.54 e Å ⁻³
5084 reflections	Δρ _{min} = -1.64 e Å ⁻³
283 parameters	Extinction correction: SHELXL97
H-atom parameters constrained	Extinction coefficient: 0.00103 (15)

H atoms were positioned geometrically and treated as riding, with C—H = 0.93 and 0.96 Å, and with U_{iso}(H) values of 1.2 and 1.5 times U_{eq}(C). The highest residual peak is located 1.03 Å from Hg1 and deepest hole is located 0.92 Å from Hg1.

Data collection: COLLECT (Nonius, 2000); cell refinement: SCALEPACK (Otwinowski & Minor, 1997); data reduction: SCALEPACK and DENZO (Otwinowski & Minor, 1997);

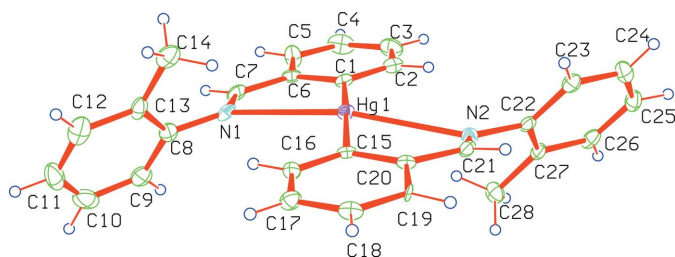


Figure 1

The molecular structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are shown at the 30% probability level.

program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

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supporting information

Acta Cryst. (2006). E62, m1467–m1468 [https://doi.org/10.1107/S1600536806020149]

Bis[2-(2-methylphenylimino)phenyl]mercury(II)

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(I)

Crystal data

[Hg(C₁₄H₁₂N)₂]
M_r = 589.08
 Monoclinic, *P*2₁/*c*
 Hall symbol: -*P* 2ybc
a = 11.9925 (3) Å
b = 11.3864 (3) Å
c = 16.6542 (5) Å
 β = 97.673 (1)°
V = 2253.79 (11) Å³
Z = 4

F(000) = 1144
D_x = 1.736 Mg m⁻³
 Mo *K*α radiation, λ = 0.71073 Å
 Cell parameters from 13603 reflections
 θ = 1.0–27.5°
 μ = 6.85 mm⁻¹
T = 293 K
 Plate, yellow
 0.2 × 0.15 × 0.05 mm

Data collection

Nonius KappaCCD
 diffractometer
 Radiation source: Enraf–Nonius FR590
 Graphite monochromator
 Detector resolution: 9 pixels mm⁻¹
 CCD rotation images, thick slices scans
 Absorption correction: multi-scan
 (SORTAV; Blessing, 1995)
T_{min} = 0.254, *T_{max}* = 0.707

14711 measured reflections
 5084 independent reflections
 3476 reflections with *I* > 2σ(*I*)
R_{int} = 0.086
 θ_{\max} = 27.4°, θ_{\min} = 3.2°
h = -15→15
k = -14→14
l = -21→19

Refinement

Refinement on *F*²
 Least-squares matrix: full
R[*F*² > 2σ(*F*²)] = 0.050
wR(*F*²) = 0.092
S = 1.02
 5084 reflections
 283 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods
 Secondary atom site location: difference Fourier
 map

Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0284P)^2 + 5.7069P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 1.54 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -1.64 \text{ e } \text{Å}^{-3}$
 Extinction correction: SHELXL97,
 $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.00103 (15)

Special details

Experimental. ¹H NMR (CDCl₃, 200 MHz): δ 8.50 (s, CH, *J*_{H_{Hg}} = 10.41 Hz), 7.65–7.06 (m, 14H, aryl-H), 6.73 (d, 2H, aryl-H, *J*_{H_H} = 7.07 Hz), 2.15 (s, 3H, CH₃). ¹³C {¹H} NMR (CDCl₃, 100 MHz): δ 167.5, 164.6, 151.2, 143.9, 139.1, 133.4, 131.9, 131.3, 130.0, 127.3, 126.6, 125.4, 118.4, 18.3.

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Hg1	0.51462 (2)	0.41352 (2)	0.389990 (15)	0.02255 (12)
C1	0.4516 (6)	0.3315 (6)	0.4861 (4)	0.0235 (16)
C2	0.3449 (7)	0.3543 (6)	0.5050 (4)	0.0320 (18)
H2	0.301	0.4099	0.4746	0.038*
C3	0.3004 (7)	0.2977 (7)	0.5676 (5)	0.042 (2)
H3	0.2278	0.3145	0.5779	0.05*
C4	0.3658 (8)	0.2160 (7)	0.6143 (5)	0.045 (2)
H4	0.3371	0.1761	0.6558	0.054*
C5	0.4737 (7)	0.1950 (7)	0.5985 (4)	0.037 (2)
H5	0.519	0.1438	0.632	0.044*
C6	0.5164 (6)	0.2467 (6)	0.5351 (4)	0.0256 (16)
C7	0.6273 (7)	0.2110 (6)	0.5197 (4)	0.0285 (18)
H7	0.6633	0.1526	0.5525	0.034*
C8	0.7850 (7)	0.2068 (6)	0.4513 (4)	0.0297 (18)
C9	0.7969 (8)	0.0870 (7)	0.4347 (4)	0.040 (2)
H9	0.7365	0.0362	0.4361	0.048*
C10	0.8987 (10)	0.0445 (9)	0.4162 (5)	0.059 (3)
H10	0.9066	-0.0341	0.403	0.07*
C11	0.9875 (9)	0.1205 (10)	0.4176 (5)	0.062 (3)
H11	1.0564	0.0917	0.4064	0.075*
C12	0.9784 (7)	0.2378 (9)	0.4351 (5)	0.050 (2)
H12	1.0404	0.287	0.4359	0.06*
C13	0.8744 (6)	0.2830 (7)	0.4517 (4)	0.0333 (19)
C14	0.8630 (7)	0.4101 (7)	0.4717 (5)	0.041 (2)
H14A	0.7925	0.4393	0.4451	0.062*
H14B	0.9236	0.4536	0.4537	0.062*
H14C	0.8655	0.419	0.5292	0.062*
C15	0.5770 (6)	0.4864 (5)	0.2894 (4)	0.0203 (15)
C16	0.6826 (6)	0.4634 (6)	0.2706 (4)	0.0281 (17)
H16	0.7288	0.413	0.3041	0.034*
C17	0.7238 (7)	0.5116 (6)	0.2042 (4)	0.0308 (18)
H17	0.7955	0.4926	0.1929	0.037*
C18	0.6569 (6)	0.5882 (6)	0.1549 (4)	0.0285 (17)
H18	0.6842	0.6242	0.1114	0.034*
C19	0.5489 (5)	0.6109 (5)	0.1710 (4)	0.0146 (13)
H19	0.5022	0.6585	0.1356	0.018*

C20	0.5089 (6)	0.5652 (5)	0.2377 (4)	0.0215 (15)
C21	0.3909 (6)	0.5915 (6)	0.2481 (4)	0.0231 (15)
H21	0.3547	0.6528	0.2182	0.028*
C22	0.2222 (6)	0.5675 (6)	0.3016 (4)	0.0240 (16)
C23	0.1905 (6)	0.6849 (6)	0.3109 (4)	0.0290 (17)
H23	0.2438	0.7443	0.3115	0.035*
C24	0.0817 (7)	0.7121 (6)	0.3190 (4)	0.0346 (19)
H24	0.0612	0.7899	0.326	0.041*
C25	0.0029 (7)	0.6249 (7)	0.3169 (4)	0.0347 (19)
H25	-0.0716	0.6439	0.321	0.042*
C26	0.0332 (6)	0.5085 (7)	0.3087 (4)	0.0315 (18)
H26	-0.0211	0.4501	0.3085	0.038*
C27	0.1438 (6)	0.4775 (6)	0.3007 (4)	0.0249 (16)
C28	0.1756 (6)	0.3514 (6)	0.2904 (5)	0.0342 (19)
H28A	0.1868	0.3378	0.2352	0.051*
H28B	0.1164	0.3014	0.304	0.051*
H28C	0.2438	0.3343	0.3255	0.051*
N1	0.6795 (5)	0.2533 (5)	0.4645 (3)	0.0272 (13)
N2	0.3364 (5)	0.5348 (5)	0.2958 (3)	0.0230 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.02761 (18)	0.02238 (15)	0.01747 (16)	-0.00002 (15)	0.00228 (10)	0.00166 (12)
C1	0.025 (4)	0.025 (4)	0.019 (4)	-0.007 (3)	0.000 (3)	-0.005 (3)
C2	0.038 (5)	0.032 (4)	0.025 (4)	-0.004 (4)	0.001 (4)	-0.005 (3)
C3	0.043 (6)	0.048 (5)	0.039 (5)	-0.005 (4)	0.020 (4)	-0.008 (4)
C4	0.066 (7)	0.034 (5)	0.041 (5)	-0.017 (5)	0.023 (5)	0.001 (4)
C5	0.037 (5)	0.054 (5)	0.022 (4)	0.016 (4)	0.015 (4)	0.016 (4)
C6	0.036 (4)	0.030 (4)	0.011 (3)	-0.004 (4)	0.006 (3)	-0.003 (3)
C7	0.041 (5)	0.025 (4)	0.017 (4)	0.000 (3)	-0.009 (3)	0.006 (3)
C8	0.033 (5)	0.037 (4)	0.019 (4)	0.005 (4)	0.003 (3)	0.006 (3)
C9	0.049 (6)	0.047 (5)	0.022 (4)	0.009 (5)	-0.004 (4)	0.005 (4)
C10	0.084 (8)	0.064 (6)	0.026 (5)	0.029 (6)	0.000 (5)	-0.005 (4)
C11	0.060 (7)	0.093 (8)	0.033 (5)	0.047 (7)	0.006 (5)	0.011 (5)
C12	0.038 (5)	0.082 (7)	0.031 (5)	0.001 (5)	0.008 (4)	0.019 (5)
C13	0.024 (4)	0.057 (5)	0.019 (4)	0.006 (4)	0.001 (3)	0.010 (3)
C14	0.037 (5)	0.057 (5)	0.028 (4)	-0.008 (5)	0.004 (4)	0.004 (4)
C15	0.028 (4)	0.020 (3)	0.013 (3)	-0.005 (3)	0.003 (3)	-0.004 (3)
C16	0.030 (5)	0.032 (4)	0.022 (4)	0.008 (4)	0.001 (3)	-0.003 (3)
C17	0.032 (5)	0.037 (4)	0.022 (4)	-0.002 (4)	0.003 (4)	0.000 (3)
C18	0.039 (5)	0.023 (3)	0.026 (4)	-0.009 (4)	0.010 (3)	-0.002 (3)
C19	0.009 (3)	0.019 (3)	0.014 (3)	0.004 (3)	-0.004 (3)	0.007 (3)
C20	0.028 (4)	0.021 (3)	0.016 (3)	-0.003 (3)	0.005 (3)	-0.003 (3)
C21	0.025 (4)	0.023 (3)	0.019 (3)	0.000 (3)	-0.005 (3)	0.001 (3)
C22	0.024 (4)	0.033 (4)	0.013 (3)	0.002 (3)	-0.002 (3)	0.000 (3)
C23	0.031 (5)	0.035 (4)	0.020 (4)	-0.001 (4)	0.001 (3)	0.004 (3)
C24	0.036 (5)	0.030 (4)	0.038 (5)	0.008 (4)	0.008 (4)	0.005 (3)

C25	0.023 (4)	0.051 (5)	0.029 (4)	0.008 (4)	0.004 (4)	0.004 (4)
C26	0.021 (4)	0.048 (5)	0.024 (4)	-0.007 (4)	-0.001 (3)	0.002 (3)
C27	0.020 (4)	0.028 (4)	0.024 (4)	-0.001 (3)	-0.004 (3)	-0.001 (3)
C28	0.024 (5)	0.036 (4)	0.044 (5)	-0.001 (4)	0.011 (4)	-0.001 (4)
N1	0.027 (3)	0.037 (3)	0.015 (3)	-0.006 (3)	-0.005 (3)	0.006 (3)
N2	0.023 (3)	0.023 (3)	0.024 (3)	-0.001 (3)	0.003 (3)	-0.002 (2)

Geometric parameters (Å, °)

Hg1—C1	2.080 (7)	C14—H14C	0.96
Hg1—C15	2.095 (6)	C15—C16	1.370 (9)
C1—C2	1.382 (10)	C15—C20	1.423 (9)
C1—C6	1.427 (10)	C16—C17	1.383 (9)
C2—C3	1.390 (10)	C16—H16	0.93
C2—H2	0.93	C17—C18	1.379 (10)
C3—C4	1.387 (11)	C17—H17	0.93
C3—H3	0.93	C18—C19	1.381 (9)
C4—C5	1.376 (11)	C18—H18	0.93
C4—H4	0.93	C19—C20	1.371 (8)
C5—C6	1.367 (9)	C19—H19	0.93
C5—H5	0.93	C20—C21	1.480 (9)
C6—C7	1.446 (10)	C21—N2	1.270 (8)
C7—N1	1.274 (8)	C21—H21	0.93
C7—H7	0.93	C22—C27	1.388 (9)
C8—C13	1.379 (10)	C22—C23	1.404 (9)
C8—C9	1.403 (10)	C22—N2	1.435 (8)
C8—N1	1.415 (9)	C23—C24	1.365 (10)
C9—C10	1.386 (12)	C23—H23	0.93
C9—H9	0.93	C24—C25	1.368 (10)
C10—C11	1.370 (14)	C24—H24	0.93
C10—H10	0.93	C25—C26	1.386 (10)
C11—C12	1.374 (13)	C25—H25	0.93
C11—H11	0.93	C26—C27	1.397 (10)
C12—C13	1.410 (10)	C26—H26	0.93
C12—H12	0.93	C27—C28	1.502 (10)
C13—C14	1.496 (10)	C28—H28A	0.96
C14—H14A	0.96	C28—H28B	0.96
C14—H14B	0.96	C28—H28C	0.96
C1—Hg1—C15	176.5 (2)	C16—C15—Hg1	123.1 (5)
C2—C1—C6	116.5 (6)	C20—C15—Hg1	119.7 (5)
C2—C1—Hg1	122.3 (5)	C15—C16—C17	123.1 (7)
C6—C1—Hg1	121.2 (5)	C15—C16—H16	118.5
C1—C2—C3	122.9 (7)	C17—C16—H16	118.5
C1—C2—H2	118.5	C18—C17—C16	119.0 (7)
C3—C2—H2	118.5	C18—C17—H17	120.5
C4—C3—C2	119.1 (8)	C16—C17—H17	120.5
C4—C3—H3	120.5	C17—C18—C19	119.3 (6)

C2—C3—H3	120.5	C17—C18—H18	120.4
C5—C4—C3	119.0 (7)	C19—C18—H18	120.4
C5—C4—H4	120.5	C20—C19—C18	121.6 (6)
C3—C4—H4	120.5	C20—C19—H19	119.2
C6—C5—C4	122.2 (7)	C18—C19—H19	119.2
C6—C5—H5	118.9	C19—C20—C15	119.7 (6)
C4—C5—H5	118.9	C19—C20—C21	117.5 (6)
C5—C6—C1	120.1 (7)	C15—C20—C21	122.5 (6)
C5—C6—C7	117.7 (6)	N2—C21—C20	123.4 (6)
C1—C6—C7	122.2 (6)	N2—C21—H21	118.3
N1—C7—C6	125.0 (6)	C20—C21—H21	118.3
N1—C7—H7	117.5	C27—C22—C23	120.7 (7)
C6—C7—H7	117.5	C27—C22—N2	117.3 (6)
C13—C8—C9	120.8 (7)	C23—C22—N2	121.9 (6)
C13—C8—N1	118.4 (6)	C24—C23—C22	120.2 (7)
C9—C8—N1	120.7 (7)	C24—C23—H23	119.9
C10—C9—C8	120.0 (9)	C22—C23—H23	119.9
C10—C9—H9	120	C23—C24—C25	119.9 (7)
C8—C9—H9	120	C23—C24—H24	120
C11—C10—C9	118.8 (9)	C25—C24—H24	120
C11—C10—H10	120.6	C24—C25—C26	120.5 (7)
C9—C10—H10	120.6	C24—C25—H25	119.8
C10—C11—C12	122.3 (9)	C26—C25—H25	119.8
C10—C11—H11	118.9	C25—C26—C27	121.0 (7)
C12—C11—H11	118.9	C25—C26—H26	119.5
C11—C12—C13	119.6 (9)	C27—C26—H26	119.5
C11—C12—H12	120.2	C22—C27—C26	117.6 (6)
C13—C12—H12	120.2	C22—C27—C28	121.7 (6)
C8—C13—C12	118.5 (8)	C26—C27—C28	120.7 (6)
C8—C13—C14	121.0 (7)	C27—C28—H28A	109.5
C12—C13—C14	120.4 (8)	C27—C28—H28B	109.5
C13—C14—H14A	109.5	H28A—C28—H28B	109.5
C13—C14—H14B	109.5	C27—C28—H28C	109.5
H14A—C14—H14B	109.5	H28A—C28—H28C	109.5
C13—C14—H14C	109.5	H28B—C28—H28C	109.5
H14A—C14—H14C	109.5	C7—N1—C8	120.4 (6)
H14B—C14—H14C	109.5	C21—N2—C22	119.0 (6)
C16—C15—C20	117.1 (6)		
C6—C1—C2—C3	-0.8 (10)	C16—C17—C18—C19	-2.8 (10)
Hg1—C1—C2—C3	178.1 (6)	C17—C18—C19—C20	4.3 (10)
C1—C2—C3—C4	1.1 (11)	C18—C19—C20—C15	-4.0 (10)
C2—C3—C4—C5	1.3 (12)	C18—C19—C20—C21	-178.1 (6)
C3—C4—C5—C6	-4.0 (12)	C16—C15—C20—C19	2.2 (9)
C4—C5—C6—C1	4.2 (12)	Hg1—C15—C20—C19	-178.7 (5)
C4—C5—C6—C7	-174.8 (7)	C16—C15—C20—C21	176.0 (6)
C2—C1—C6—C5	-1.8 (10)	Hg1—C15—C20—C21	-4.9 (8)
Hg1—C1—C6—C5	179.3 (6)	C19—C20—C21—N2	163.7 (6)

C2—C1—C6—C7	177.3 (6)	C15—C20—C21—N2	-10.2 (10)
Hg1—C1—C6—C7	-1.7 (9)	C27—C22—C23—C24	-0.1 (10)
C5—C6—C7—N1	-178.0 (7)	N2—C22—C23—C24	-177.7 (6)
C1—C6—C7—N1	3.0 (11)	C22—C23—C24—C25	-1.0 (11)
C13—C8—C9—C10	-1.8 (11)	C23—C24—C25—C26	1.7 (11)
N1—C8—C9—C10	175.3 (6)	C24—C25—C26—C27	-1.4 (11)
C8—C9—C10—C11	2.5 (12)	C23—C22—C27—C26	0.4 (10)
C9—C10—C11—C12	-1.5 (13)	N2—C22—C27—C26	178.1 (6)
C10—C11—C12—C13	-0.4 (13)	C23—C22—C27—C28	179.7 (6)
C9—C8—C13—C12	-0.1 (10)	N2—C22—C27—C28	-2.6 (10)
N1—C8—C13—C12	-177.3 (6)	C25—C26—C27—C22	0.3 (10)
C9—C8—C13—C14	-178.2 (7)	C25—C26—C27—C28	-179.0 (7)
N1—C8—C13—C14	4.6 (10)	C6—C7—N1—C8	-176.0 (6)
C11—C12—C13—C8	1.2 (11)	C13—C8—N1—C7	-126.5 (7)
C11—C12—C13—C14	179.3 (7)	C9—C8—N1—C7	56.3 (9)
C20—C15—C16—C17	-0.9 (10)	C20—C21—N2—C22	179.9 (6)
Hg1—C15—C16—C17	-180.0 (5)	C27—C22—N2—C21	135.0 (7)
C15—C16—C17—C18	1.2 (11)	C23—C22—N2—C21	-47.3 (9)
