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

Kevin R. Flower* and Robin G. Pritchard

School of Chemistry, University of Manchester, Sackville Street, Manchester, England

Correspondence e-mail: k.r.flower@manchester.ac.uk

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The structure of the centrosymmetric cyclomercurated 2-phenyliminophenyl title compound, $[Hg(C_{16}H_{16}N)_2]$, has been determined at 120 (2) K. The coordination geometry at the Hg atom is essentially square planar.

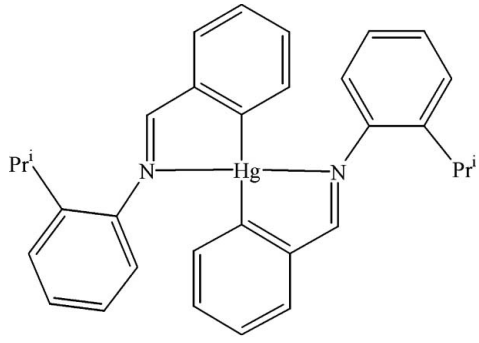
Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.005 Å
R factor = 0.023
wR factor = 0.058
Data-to-parameter ratio = 19.0

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

Comment

The stucture of the centrosymmetric title compound, (I), is shown below. For a discussion of the structure, together with that of a similar complex, see Flower & Pritchard (2006).



(I)

Experimental

Caution: **preparation of an organomercurial. . Organomercurials are extremely toxic.** Compound (I) was prepared by the method previously described (Flower & Pritchard, 2006) (yield 1.12 g, 75%). Elemental analysis $C_{32}H_{32}N_2Hg$ requires: C 59.58, H 4.99, N 4.4%; found: C 59.54, H 5.01, N 4.41%.

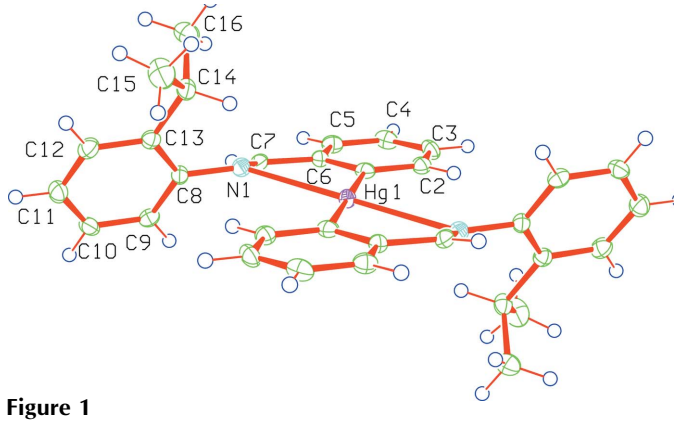


Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Unlabelled atoms are related to labelled atoms by $2-x$, $-y$, $2-z$. Displacement ellipsoids are shown at the 30% probability level.

Crystal data

$[Hg(C_{16}H_{16}N)_2]$	$Z = 2$
$M_r = 645.19$	$D_x = 1.582$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 12.585$ (3) Å	$\mu = 5.70$ mm^{-1}
$b = 8.2963$ (17) Å	$T = 120$ (2) K
$c = 13.244$ (3) Å	Prism, yellow
$\beta = 101.58$ (3)°	0.16 × 0.12 × 0.04 mm
$V = 1354.7$ (5) Å^3	

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer	9987 measured reflections
φ and ω scans	3078 independent reflections
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)	2244 reflections with $I > 2\sigma(I)$
$T_{min} = 0.462$, $T_{max} = 0.804$	$R_{int} = 0.039$
	$\theta_{max} = 27.5°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0195P)^2 + 0.6915P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.023$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.058$	$\Delta\rho_{max} = 0.65$ e Å^{-3}
$S = 1.06$	$\Delta\rho_{min} = -1.50$ e Å^{-3}
3078 reflections	
162 parameters	
H-atom parameters constrained	

H atoms were positioned geometrically and treated as riding, with C—H = 0.95–1.00 Å and U_{iso}(H) values of 1.2 or 1.5 times U_{eq}(C). The deepest hole is located 0.87 Å from Hg1.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; 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). E**62**, m1469–m1470 [https://doi.org/10.1107/S1600536806020150]

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Crystal data

$[Hg(C_{16}H_{16}N)_2]$
$M_r = 645.19$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.585$ (3) Å
$b = 8.2963$ (17) Å
$c = 13.244$ (3) Å
$\beta = 101.58$ (3)°
$V = 1354.7$ (5) Å^3
$Z = 2$
$F(000) = 636$
$D_x = 1.582$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6064 reflections
$\theta = 2.9$–27.5°
$\mu = 5.70$ mm^{-1}
$T = 120$ K
Prism, yellow
0.16 × 0.12 × 0.04 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SORTAV; Blessing, 1995)
$T_{min} = 0.462$, $T_{max} = 0.804$
9987 measured reflections
3078 independent reflections
2244 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.9°$
$h = -16\rightarrow16$
$k = -9\rightarrow10$
$l = -17\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.058$
$S = 1.06$
3078 reflections
162 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
$w = 1/[\sigma^2(F_o^2) + (0.0195P)^2 + 0.6915P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.65$ e Å^{-3}
$\Delta\rho_{min} = -1.50$ e Å^{-3}

Special details

Experimental. ^{1}H NMR ($CDCl_3$, 200 MHz): δ 8.51 (s, 1H, CH, $J_{HHg} = 9.81$ Hz), 7.63–7.10 (m, 14H, aryl-H), 6.68 (m, 2H, aryl-H), 3.47 (sept, 1H, CH, $J_{HH} = 7.20$ Hz), 0.85 (d, 6H, CH_3, $J_{HH} = 7.20$ Hz). $^{13}C\{^1H\}$ ($CDCl_3$, 100 MHz): δ 167.3, 164.6, 149.9, 143.6, 142.4, 139.1, 133.4, 131.3, 127.3, 126.3, 125.7, 125.1, 118.1, 27.7, 23.2.

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Hg1	1	0	1	0.01587 (6)
N1	1.11390 (19)	−0.2604 (3)	1.10205 (17)	0.0194 (5)
C1	0.9102 (2)	−0.0930 (4)	1.1028 (2)	0.0191 (6)
C2	0.8151 (3)	−0.0174 (3)	1.1180 (3)	0.0204 (7)
H2	0.792	0.0798	1.0824	0.024*
C3	0.7540 (3)	−0.0832 (4)	1.1847 (2)	0.0233 (7)
H3	0.69	−0.0301	1.1947	0.028*
C4	0.7861 (3)	−0.2257 (4)	1.2364 (2)	0.0240 (7)
H4	0.7439	−0.2707	1.2814	0.029*
C5	0.8799 (2)	−0.3026 (4)	1.2226 (2)	0.0222 (7)
H5	0.9014	−0.4009	1.2576	0.027*
C6	0.9432 (2)	−0.2362 (3)	1.1573 (2)	0.0177 (6)
C7	1.0429 (2)	−0.3225 (4)	1.1468 (2)	0.0193 (7)
H7	1.0546	−0.4282	1.1744	0.023*
C8	1.2043 (2)	−0.3549 (4)	1.0883 (2)	0.0180 (6)
C9	1.1894 (3)	−0.5072 (3)	1.0444 (3)	0.0191 (7)
H9	1.1182	−0.5501	1.0247	0.023*
C10	1.2776 (3)	−0.5972 (4)	1.0290 (2)	0.0225 (7)
H10	1.2671	−0.7017	0.9994	0.027*
C11	1.3808 (3)	−0.5339 (4)	1.0572 (3)	0.0257 (8)
H11	1.4417	−0.5954	1.0477	0.031*
C12	1.3954 (3)	−0.3805 (4)	1.0992 (2)	0.0236 (7)
H12	1.4668	−0.3382	1.1183	0.028*
C13	1.3082 (2)	−0.2867 (4)	1.1142 (2)	0.0184 (6)
C14	1.3232 (2)	−0.1206 (4)	1.1643 (2)	0.0214 (7)
H14	1.2567	−0.0562	1.1362	0.026*
C15	1.4204 (3)	−0.0284 (4)	1.1401 (4)	0.0373 (10)
H15A	1.4878	−0.0807	1.1748	0.056*
H15B	1.419	0.0829	1.1646	0.056*
H15C	1.4168	−0.0284	1.0655	0.056*
C16	1.3312 (3)	−0.1361 (4)	1.2808 (2)	0.0320 (8)
H16A	1.2651	−0.1867	1.2943	0.048*
H16B	1.3395	−0.0288	1.3124	0.048*
H16C	1.3941	−0.2027	1.3103	0.048*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.01480 (10)	0.01619 (10)	0.01730 (10)	0.00034 (6)	0.00482 (6)	0.00045 (6)
N1	0.0160 (14)	0.0202 (13)	0.0216 (13)	−0.0013 (11)	0.0028 (10)	−0.0021 (11)
C1	0.0187 (16)	0.0215 (17)	0.0166 (14)	−0.0037 (13)	0.0024 (11)	−0.0041 (12)
C2	0.0170 (17)	0.0226 (17)	0.0209 (17)	−0.0017 (13)	0.0021 (13)	−0.0049 (12)
C3	0.0182 (17)	0.0252 (18)	0.0282 (17)	−0.0002 (14)	0.0087 (13)	−0.0094 (14)
C4	0.0244 (18)	0.0276 (18)	0.0224 (16)	−0.0083 (15)	0.0103 (13)	−0.0046 (13)
C5	0.0256 (18)	0.0213 (17)	0.0193 (15)	−0.0039 (14)	0.0039 (12)	−0.0003 (12)
C6	0.0166 (16)	0.0185 (16)	0.0175 (14)	0.0004 (12)	0.0020 (11)	−0.0028 (12)
C7	0.0173 (16)	0.0192 (16)	0.0193 (15)	0.0007 (13)	−0.0017 (12)	−0.0016 (12)
C8	0.0176 (16)	0.0191 (15)	0.0173 (14)	0.0033 (13)	0.0036 (11)	0.0005 (12)
C9	0.0174 (17)	0.0212 (17)	0.0180 (16)	−0.0037 (13)	0.0019 (13)	0.0020 (11)
C10	0.0281 (18)	0.0220 (17)	0.0178 (15)	0.0023 (15)	0.0056 (12)	−0.0037 (13)
C11	0.0247 (19)	0.032 (2)	0.0222 (18)	0.0076 (15)	0.0079 (14)	0.0004 (14)
C12	0.0176 (17)	0.0276 (18)	0.0245 (16)	−0.0009 (14)	0.0013 (12)	−0.0001 (14)
C13	0.0191 (16)	0.0205 (16)	0.0157 (14)	0.0006 (13)	0.0037 (11)	0.0017 (12)
C14	0.0178 (16)	0.0165 (16)	0.0292 (16)	−0.0006 (13)	0.0030 (13)	−0.0020 (13)
C15	0.027 (2)	0.032 (2)	0.054 (3)	−0.0079 (16)	0.0132 (19)	−0.0061 (17)
C16	0.037 (2)	0.0272 (19)	0.0297 (18)	−0.0003 (16)	0.0029 (15)	−0.0074 (15)

Geometric parameters (Å, º)

Hg1—C1^{i}	2.084 (3)	C9—C10	1.387 (4)
Hg1—C1	2.084 (3)	C9—H9	0.95
N1—C7	1.276 (4)	C10—C11	1.381 (5)
N1—C8	1.423 (4)	C10—H10	0.95
C1—C2	1.401 (5)	C11—C12	1.387 (4)
C1—C6	1.409 (4)	C11—H11	0.95
C2—C3	1.393 (5)	C12—C13	1.391 (4)
C2—H2	0.95	C12—H12	0.95
C3—C4	1.386 (4)	C13—C14	1.525 (4)
C3—H3	0.95	C14—C15	1.531 (5)
C4—C5	1.386 (4)	C14—C16	1.532 (4)
C4—H4	0.95	C14—H14	1
C5—C6	1.401 (4)	C15—H15A	0.98
C5—H5	0.95	C15—H15B	0.98
C6—C7	1.475 (4)	C15—H15C	0.98
C7—H7	0.95	C16—H16A	0.98
C8—C9	1.388 (4)	C16—H16B	0.98
C8—C13	1.402 (4)	C16—H16C	0.98
C1^{i}—Hg1—C1	180.0000 (10)	C11—C10—H10	120.2
C7—N1—C8	119.3 (3)	C9—C10—H10	120.2
C2—C1—C6	118.4 (3)	C10—C11—C12	119.9 (3)
C2—C1—Hg1	121.3 (2)	C10—C11—H11	120
C6—C1—Hg1	120.3 (2)	C12—C11—H11	120

C3—C2—C1	120.8 (3)	C11—C12—C13	121.7 (3)
C3—C2—H2	119.6	C11—C12—H12	119.1
C1—C2—H2	119.6	C13—C12—H12	119.1
C4—C3—C2	120.3 (3)	C12—C13—C8	117.6 (3)
C4—C3—H3	119.9	C12—C13—C14	122.3 (3)
C2—C3—H3	119.9	C8—C13—C14	119.9 (3)
C3—C4—C5	119.9 (3)	C13—C14—C15	113.3 (3)
C3—C4—H4	120	C13—C14—C16	109.9 (2)
C5—C4—H4	120	C15—C14—C16	111.0 (3)
C4—C5—C6	120.4 (3)	C13—C14—H14	107.5
C4—C5—H5	119.8	C15—C14—H14	107.5
C6—C5—H5	119.8	C16—C14—H14	107.5
C5—C6—C1	120.2 (3)	C14—C15—H15A	109.5
C5—C6—C7	117.8 (3)	C14—C15—H15B	109.5
C1—C6—C7	122.0 (3)	H15A—C15—H15B	109.5
N1—C7—C6	122.4 (3)	C14—C15—H15C	109.5
N1—C7—H7	118.8	H15A—C15—H15C	109.5
C6—C7—H7	118.8	H15B—C15—H15C	109.5
C9—C8—C13	120.7 (3)	C14—C16—H16A	109.5
C9—C8—N1	120.7 (3)	C14—C16—H16B	109.5
C13—C8—N1	118.5 (3)	H16A—C16—H16B	109.5
C10—C9—C8	120.4 (3)	C14—C16—H16C	109.5
C10—C9—H9	119.8	H16A—C16—H16C	109.5
C8—C9—H9	119.8	H16B—C16—H16C	109.5
C11—C10—C9	119.6 (3)		

C6—C1—C2—C3	−0.6 (4)	C13—C8—C9—C10	2.5 (4)
Hg1—C1—C2—C3	178.1 (2)	N1—C8—C9—C10	178.5 (3)
C1—C2—C3—C4	−0.6 (5)	C8—C9—C10—C11	−0.4 (5)
C2—C3—C4—C5	0.5 (4)	C9—C10—C11—C12	−0.8 (5)
C3—C4—C5—C6	0.7 (4)	C10—C11—C12—C13	0.0 (5)
C4—C5—C6—C1	−1.8 (4)	C11—C12—C13—C8	2.0 (4)
C4—C5—C6—C7	179.2 (3)	C11—C12—C13—C14	177.5 (3)
C2—C1—C6—C5	1.8 (4)	C9—C8—C13—C12	−3.3 (4)
Hg1—C1—C6—C5	−176.9 (2)	N1—C8—C13—C12	−179.4 (3)
C2—C1—C6—C7	−179.3 (3)	C9—C8—C13—C14	−178.8 (3)
Hg1—C1—C6—C7	2.0 (4)	N1—C8—C13—C14	5.1 (4)
C8—N1—C7—C6	−175.5 (2)	C12—C13—C14—C15	33.3 (4)
C5—C6—C7—N1	−169.2 (3)	C8—C13—C14—C15	−151.4 (3)
C1—C6—C7—N1	11.8 (4)	C12—C13—C14—C16	−91.5 (3)
C7—N1—C8—C9	51.0 (4)	C8—C13—C14—C16	83.8 (3)
C7—N1—C8—C13	−132.9 (3)		

Symmetry code: (i) −*x*+2, −*y*, −*z*+2.