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

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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.

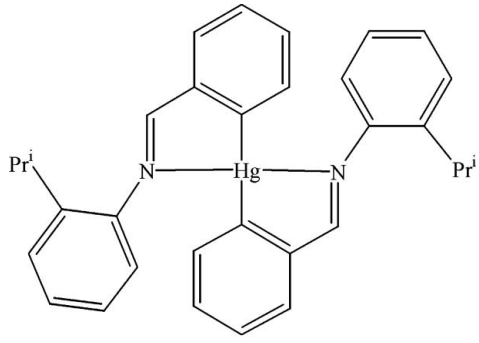
Key indicators

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%.

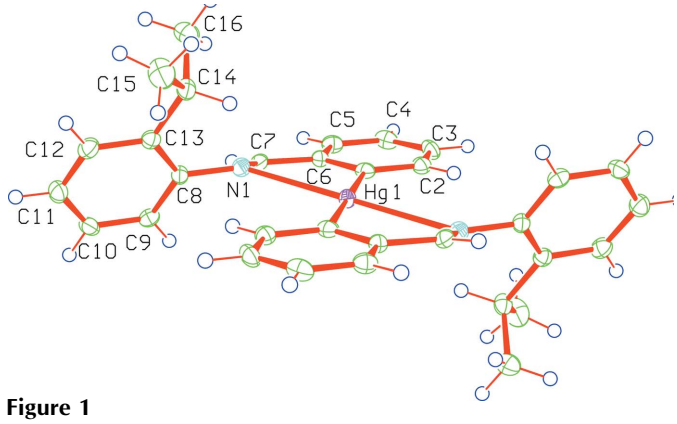


Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Unlabelled atoms are related to labelled atoms by $2-x$, $-y$, $2-z$. Displacement ellipsoids are shown at the 30% probability level.

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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