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

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–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.

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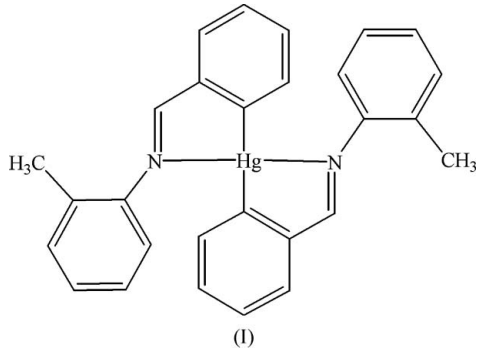
The structure of the cyclomercurated 2-phenyliminophenyl title compound, [Hg($C_{14}H_{12}N)_2$], shows that the mercury coordination is essentially square planar

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-isopropylphenylimnophenyl)-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).



(I)

Experimental

Caution: preparation of an organomercurial. Organomercurials are extremely toxic. To Hg(C_6H_4-2-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.

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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 CH_2Cl_2 (0.2 ml) in a small vial (1 × 5 cm), layering ethanol (5 ml) on top and leaving the vial to to stand for 24 h. Elemental analysis $C_{28}H_{24}HgN_2$ 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 $K\alpha$ radiation
$a = 11.9925$ (3) Å	$\mu = 6.85$ mm^{-1}
$b = 11.3864$ (3) Å	$T = 293$ (2) K
$c = 16.6542$ (5) Å	Plate, yellow
$\beta = 97.6730$ (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 $I > 2\sigma(I)$
$T_{min} = 0.254$, $T_{max} = 0.707$	$R_{int} = 0.086$
	$\theta_{max} = 27.4°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0284P)^2 + 5.7069P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.050$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.092$	$\Delta\rho_{max} = 1.54$ e Å^{-3}
$S = 1.02$	$\Delta\rho_{min} = -1.64$ e Å^{-3}
5084 reflections	Extinction correction: *SHELXL97*
283 parameters	Extinction coefficient: 0.00103 (15)
H-atom parameters constrained	

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); 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).

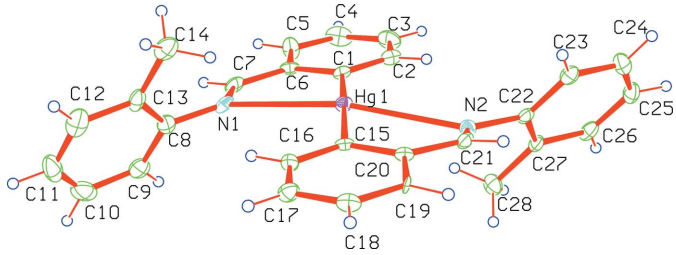

Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are shown at the 30% probability level.

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