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Key indicators

 Single-crystal X-ray study
 $T = 120$ K
 Mean $\sigma(\text{C}-\text{C}) = 0.005$ 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>.

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

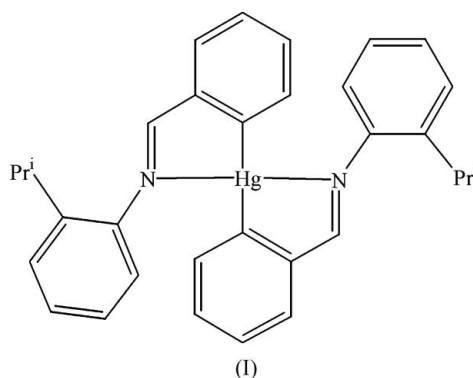
 The structure of the centrosymmetric cyclomercurated 2-phenyliminophenyl title compound, $[\text{Hg}(\text{C}_{16}\text{H}_{16}\text{N}_2)_2]$, has been determined at 120 (2) K. The coordination geometry at the Hg atom is essentially square planar.

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Comment

The structure 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).



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 $\text{C}_{32}\text{H}_{32}\text{N}_2\text{Hg}$ requires: C 59.58, H 4.99, N 4.4%; found: C 59.54, H 5.01, N 4.41%.

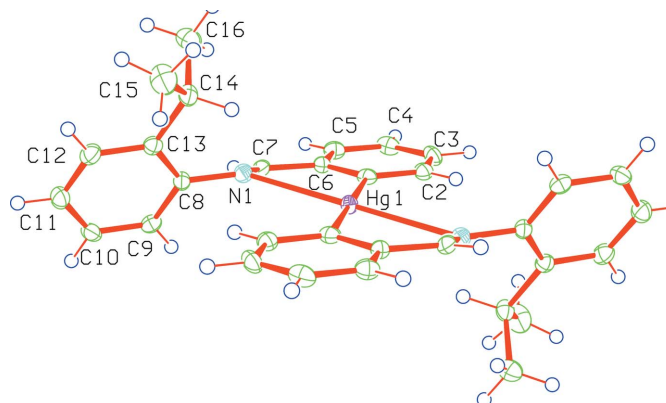


Figure 1

 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(C₁₆H₁₆N)₂]
M_r = 645.19
 Monoclinic, *P*2₁/*c*
a = 12.585 (3) Å
b = 8.2963 (17) Å
c = 13.244 (3) Å
 β = 101.58 (3)°
V = 1354.7 (5) Å³

Z = 2
D_x = 1.582 Mg m⁻³
 Mo *K*α radiation
 μ = 5.70 mm⁻¹
T = 120 (2) K
 Prism, yellow
 0.16 × 0.12 × 0.04 mm

Data collection

Enraf–Nonius KappaCCD area-
 detector diffractometer
 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* > 2σ(*I*)
R_{int} = 0.039
 θ_{\max} = 27.5°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.023
wR (*F*²) = 0.058
S = 1.06
 3078 reflections
 162 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0195P)^2 + 0.6915P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.65 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -1.50 \text{ e } \text{Å}^{-3}$

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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References

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