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Key indicators

Single-crystal X-ray study

T = 293 K

Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$

R factor = 0.037

wR factor = 0.085

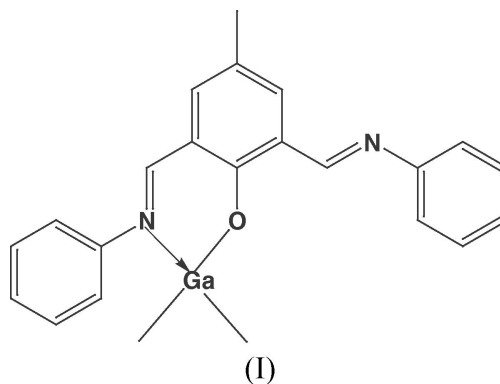
Data-to-parameter ratio = 16.2

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Dimethyl[4-methyl-2,6-bis(phenyliminomethyl)-phenolato- $\kappa^2\text{N},\text{O}$]gallium(III)

The title compound, $[\text{Ga}(\text{CH}_3)_2(\text{C}_{21}\text{H}_{17}\text{N}_2\text{O})]$, synthesized by the reaction of trimethylgallium and 4-methyl-2,6-bis(phenyliminomethyl)phenol, has the Ga atom in a tetrahedral geometry; two molecules form a dimer through a $\pi-\pi$ interaction.

Comment

Among the organometallic derivatives of group 13 elements (Atwood & Harvey, 2001; Chitsaz & Neumuller, 2001; Peters *et al.*, 1998), the trialkylgallium(III) compounds are able to react with ligands having active hydrogen to furnish compounds having N—Ga—N (Park *et al.*, 2000), N—Ga—O (Hill *et al.*, 2001) or N—Ga—S (Shen *et al.*, 2003) linkages. The title compound, (I), with the 4-methyl-2,6-bis(phenyliminomethyl)phenolate ligand displays an N—Ga—O coordination mode (Fig. 1 and Table 1).



The O1—Ga1—N2 angle is marginally larger than that of dimethyl(*N*-salicylidene-2-aminopyridine)gallium

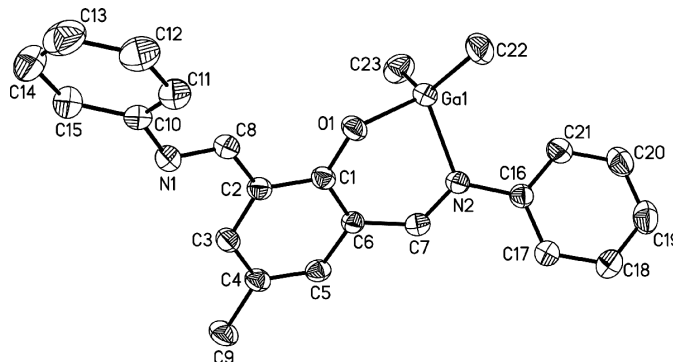


Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted.

[90.76 (7)°; Shen *et al.*, 2000], and the Ga1—O1 and Ga1—N2 bond distances are comparable with those reported for *N,N*-ethylene(salicylideneiminato)bis(dimethylgallium) [1.869 (2)/1.874(2) and 2.026 (3)/2.035(3) Å; Chong *et al.*, 1977]. There is a π - π interaction (Fig. 2) that leads to the formation of dimers [$\text{Cg1} \cdots \text{Cg1}^i = 3.50$ (2) Å, where Cg1 is the centroid of ring C1—C6; symmetry code: (i) $1 - x, 1 - y, 1 - z$].

Experimental

To a benzene solution (4 ml) of trimethylgallium (0.2 ml, 2 mmol) was added a benzene solution (4 ml) of 4-methyl-2,6-bis(phenylimino-methyl)phenol (0.629 g, 2 mmol) and the resulting mixture was stirred for 40 min at room temperature. The solvent was removed. Orange block-shaped crystals were obtained by recrystallizing the orange powder from cyclohexane–benzene (0.58 g, 70% yield). Analysis calculated for $\text{C}_{23}\text{H}_{23}\text{GaN}_2\text{O}$: C 66.86, H 5.61, N 6.78%; found: C 66.60, H 5.82, N 6.98%.

Crystal data

[$\text{Ga}(\text{CH}_3)_2(\text{C}_{21}\text{H}_{17}\text{N}_2\text{O})$]
 $M_r = 413.15$
 Monoclinic, $P2_1/c$
 $a = 9.498$ (1) Å
 $b = 13.028$ (1) Å
 $c = 16.598$ (2) Å
 $\beta = 95040$
 $V = 2045.9$ (4) Å³
 $Z = 4$

$D_x = 1.341$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 3581 reflections
 $\theta = 2.5$ – 25.4°
 $\mu = 1.36$ mm⁻¹
 $T = 293$ (2) K
 Block, orange
 $0.30 \times 0.20 \times 0.20$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
 $T_{\min} = 0.73$, $T_{\max} = 0.76$
 10679 measured reflections

4013 independent reflections
 2790 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.068$
 $\theta_{\text{max}} = 26.0^\circ$
 $h = -11 \rightarrow 11$
 $k = -14 \rightarrow 16$
 $l = -20 \rightarrow 17$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.085$
 $S = 1.05$
 4013 reflections
 247 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.025P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.42$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.26$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ga1—O1	1.8843 (18)	Ga1—C22	1.942 (3)
Ga1—N2	2.045 (2)	Ga1—C23	1.943 (3)
O1—Ga1—C22	107.56 (11)	N2—Ga1—C22	110.83 (11)
O1—Ga1—C23	108.87 (11)	N2—Ga1—C23	103.40 (11)
O1—Ga1—N2	90.81 (8)	C22—Ga1—C23	128.77 (14)

The H atoms were positioned geometrically and refined as riding, with C—H distances 0.93 or 0.96 Å (C_{methyl}), and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$. Methyl groups were rotated to fit the electron density.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve

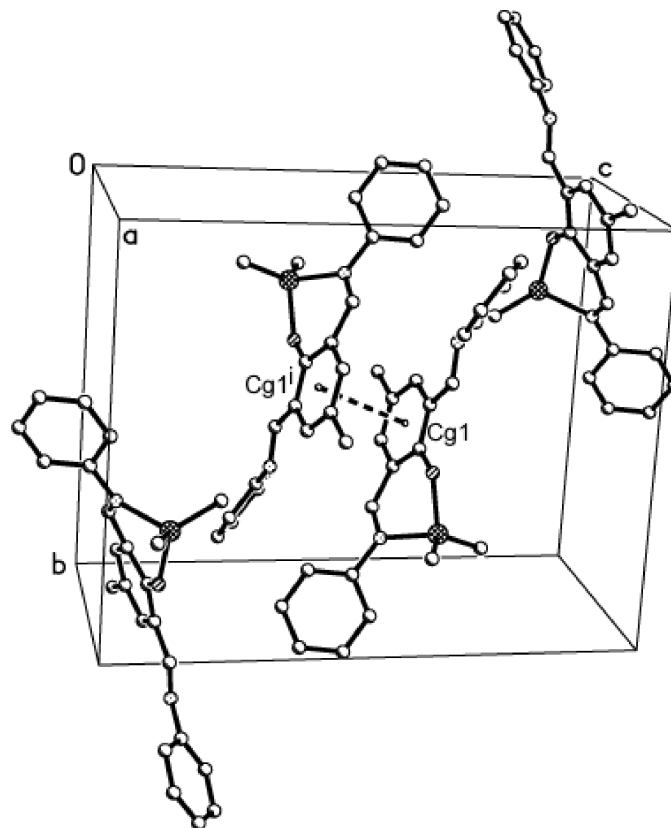


Figure 2

A view of the packing of the title compound. The dashed line shows the weak π - π interaction [symmetry code: (i) $1 - x, 1 - y, 1 - z$]. H atoms have been omitted.

structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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