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Crystallographic report

[1,3-Di(mestityl)imidazol-2-ylidene]gallium iodide dihydride

Robert J. Baker and Cameron Jones*

Department of Chemistry, Cardiff University, PO Box 912, Park Place, Cardiff CF10 3TB, UK

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The structure of the *N*-heterocyclic gallium hydride complex, $[GaH_2I\{CN(Mes)C_2H_2N(Mes)\}]$, Mes = mesityl, shows both hydride ligands to be bonded to the distorted tetrahedral gallium centre. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; gallium; hydride; *N*-heterocyclic carbene

COMMENT

The title complex (**I**) was synthesised by the reaction of one equivalent of $[GaH_3\{CN(Mes)C_2H_2N(Mes)\}]$[1] with 'GaI'[2] and was accompanied by gallium metal deposition. In the structure (Fig. 1), all gallium–ligand bond lengths are in the normal ranges for such interactions (as determined from a survey of the Cambridge Crystallographic Database) and the gallium centre has a distorted tetrahedral coordination environment. Complex **I** is isostructural to the related indium hydride complex, $[InH_2Cl\{CN(Mes)C_2H_2N(Mes)\}]$.[1]

*Correspondence to: Cameron Jones, Chemistry Department, Cardiff University, PO Box 912, Park Place, Cardiff CF10 3TB, UK.
E-mail: jonesca6@cardiff.ac.uk
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EXPERIMENTAL AND RESULTS

A solution of $[GaH_3\{CN(Mes)C_2H_2N(Mes)\}]$ (0.79 mmol) and 'GaI' (0.79 mmol) in toluene (20 ml) was stirred at room temperature

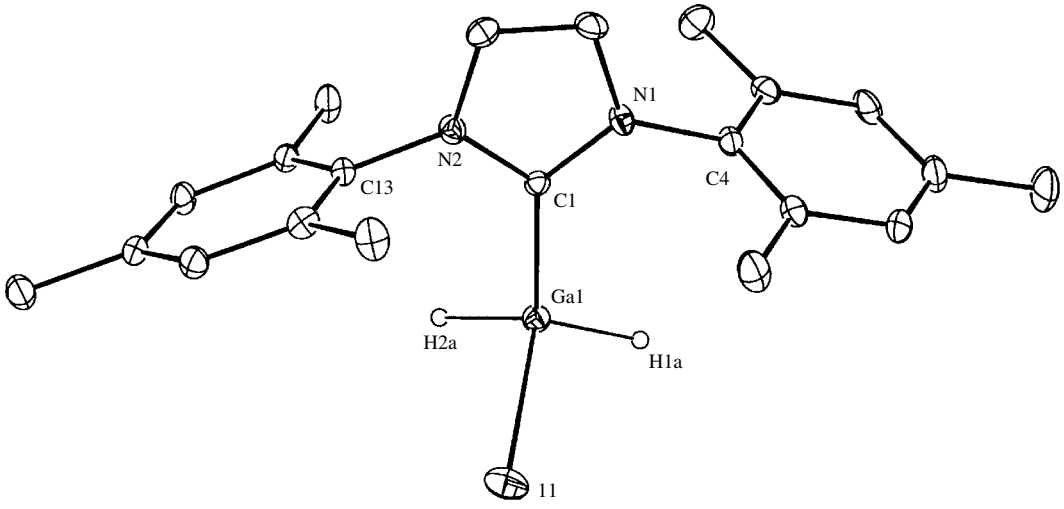

Figure 1. Molecular structure of **I**. Key geometric parameters: I(1)–Ga(1) 2.5976(7), Ga(1)–H(1a) 1.52(4), Ga(1)–H(2a) 1.59(5), Ga(1)–C(1) 2.022(4), N(1)–C(1) 1.350(6), N(2)–C(1) 1.354(6) Å; C(1)–Ga(1)–I(1) 105.23(12), N(1)–C(1)–N(2) 104.4(4), C(1)–Ga(1)–H(1a) 111.4(18), C(1)–Ga(1)–H(2a) 109.5(19), H(1a)–Ga(1)–I(1) 104.0(17), H(2a)–Ga(1)–I(1) 105.4(17), H(1a)–Ga(1)–H(2a) 120(2)°.

for 24 h. After this time, the reaction was filtered and the solution concentrated to 5 cm^3. Placement at −35 °C overnight yielded the title compound as colourless blocks (0.130 g, 32%). M.p. 177–181 °C (dec.); ^{1}H NMR (400 MHz, C_6D_6) $\delta = 2.01$ (br. s, 18 H, CH_3), 4.12 (br, 2H, Ga–H), 5.89 (s, 2H, NC_2H_2N), 6.63 (s, 4H, Ar); ^{13}C NMR (100.13 MHz, C_6D_6) $\delta = 18.5$ (*m*-CH_3), 21.4 (*p*-CH_3), 123.2 (NC_2H_2N), 130.0 (*m*-Ar), 134.2 (*p*-Ar), 135.3 (*o*-Ar), 140.4 (*ipso*-Ar); IR (Nujol, cm^{-1}) ν 1863 (br, Ga–H); APCI/MS m/z 501 [$M^+ - H_2$, 35%], 375 [$M^+ - H_2 - I$, 100%].

Intensity data for **I** were collected at 150 K on a Nonius Kappa CCD diffractometer for a colourless crystal 0.10 × 0.10 × 0.15 mm^3. $C_{21}H_{26}GaIN_2$, $M = 503.06$, orthorhombic, $P2_12_12_1$, $a = 7.8320(16)$, $b = 16.274(3)$, $c = 17.207(3)$, $V = 2193.2(8)$ Å^3, $Z = 4$, $T = 150$ K, 4253 unique data (θ_{max} 26.0°), 3709 data $I \geq 2\sigma(I)$, $R = 0.038$, $wR = 0.077$, $\rho_{max} = 0.64$ e$^-$ Å^{-3}, absolute structure parameter is −0.015(19). Programs used: SHELXS-97, SHELXL-97, X-seed and ORTEP. CCDC deposition number: 208 969.

Acknowledgements

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