

CHEMISTRY 
A EUROPEAN JOURNAL

Supporting Information

© Copyright Wiley-VCH Verlag GmbH & Co. KGaA, 69451 Weinheim, 2008

Organometallic Chemistry of Ga⁺: Switching On and Off the Electron Pair of Monovalent Gallium in the Coordination Sphere of Ruthenium.*

Thomas Cadenbach,¹ Christian Gemel,¹ Timo Bollermann,¹ Israel Fernandez,² Gernot Frenking,³ and Roland A. Fischer*¹

¹*Anorganische Chemie II - Organometallics & Materials, Ruhr-Universität Bochum, D-44780 Bochum (Germany), fax (+49)234 321 4174;* ²*Dpto. Química Orgánica, Facultad de Química, Universidad Complutense de Madrid, 28040 Madrid (Spain).* ³*Fachbereich Chemie, Philipps-Universität Marburg, Hans-Meerwein-Strasse, D-35032 Marburg (Germany), fax (+49)6421-282-5566.*

Table S1. Details of the structure determinations of products 1-6

Crystal parameters.	1	2	3	4	5	6
Empirical formula	C ₃₄ H ₃₀ Ga ₃ Ru	C ₁₁₇ H ₂₀₈ P ₄ Ga ₄ Ru ₂	C ₇₆ H ₇₉ BF ₂₄ Ga ₄ Ru	C ₁₄₄ H ₁₃₆ B ₂ F ₅₀ Ga ₈ Ru ₂	C ₁₄₇ H ₁₃₇ B ₂ F _{50.50} Ga ₈ Ru ₂	C ₁₀₀ H ₁₁₈ BF ₂₆ Ga ₃ P ₂ Ru
Molecular weight	748.81	2219.73	1839.15	3598.05	3644.59	2196.92
Temperature (K)	113(2)	113(2)	113(2)	100(2)	103(2)	113(2)
Wavelength Mo-K _α (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal size (mm)	0.25 × 0.2 × 0.15	0.25 x 0.15 x 0.10	0.25 × 0.2 × 0.15	0.30 × 0.20 × 0.15	0.20 × 0.10 × 0.10	0.40 × 0.20 × 0.10
Crystal system, space group	Tetragonal, I4/m	Monoclinic, P2(1)/c	Orthorhombic, Pbca	Monoclinic, P2(1)/c	Triclinic, P-1	Monoclinic, P2(1)/c
<i>a</i> (Å)	19.8445(6)	20.9566(18)	25.546(3)	15.3517(4)	14.1090(6)	22.929(5)
<i>b</i> (Å)	19.8445(6)	24.925(3)	21.2722(8)	18.2016(6)	14.7960(7)	17.448(3)
<i>c</i> (Å)	18.8042(7)	23.0088(19)	29.176(2)	27.2028(10)	36.0416(18)	25.47(3)
α (°)	90	90	90	90	86.712(4)	90
β (°)	90	92.018(7)	90	102.118(3)	80.878(4)	101.84(4)
γ (°)	90	90	90	90	88.267(4)	90
Cell volume (Å ³)	7405.2(4)	12011.1(19)	15855(2)	7431.8(4)	7414.8(6)	9972(10)
<i>Z</i>	8	4	8	2	2	4
Density ρ_{calc} . (g cm ⁻³)	1.343	1.228	1.541	1.608	1.632	1.463
Absorption coefficient μ (mm ⁻¹)	2.577	1.225	1.625	1.733	1.739	1.076
<i>F</i> (000)	2968	4728	7392	3592	3639	4496
θ range for data collection (°)	2.54 - 27.58	2.68 - 27.70	2.67 - 27.59	2.81 - 27.66	2.74 - 25.05	2.69 - 27.62
Index ranges	-25 ≤ <i>h</i> ≤ 25, -22 ≤ <i>k</i> ≤ 25, -24 ≤ <i>l</i> ≤ 24	-27 ≤ <i>h</i> ≤ 23, -32 ≤ <i>k</i> ≤ 32, -29 ≤ <i>l</i> ≤ 29	-33 ≤ <i>h</i> ≤ 32, -27 ≤ <i>k</i> ≤ 27, -38 ≤ <i>l</i> ≤ 37	-20 ≤ <i>h</i> ≤ 20, -23 ≤ <i>k</i> ≤ 23, -35 ≤ <i>l</i> ≤ 35	-16 ≤ <i>h</i> ≤ 11, -17 ≤ <i>k</i> ≤ 16, -42 ≤ <i>l</i> ≤ 42	-18 ≤ <i>h</i> ≤ 29, -22 ≤ <i>k</i> ≤ 22, -33 ≤ <i>l</i> ≤ 33
Reflexions collected	37838	95267	290868	74060	30540	90864
Reflexions unique	4402	27422	18306	17247	24536	22956
Refinement method	[R(int) = 0.0438] Full-matrix least-squares on <i>F</i> ²	[R(int) = 0.1130] Full-matrix least-squares on <i>F</i> ²	[R(int) = 0.1514] Full-matrix least-squares on <i>F</i> ²	[R(int) = 0.0435] Full-matrix least-squares on <i>F</i> ²	[R(int) = 0.1137] Full-matrix least-squares on <i>F</i> ²	[R(int) = 0.0823] Full-matrix least-squares on <i>F</i> ²
Data/Restraints/Parameters	4402/0/200	27422/0/1160	18306/0/955	17247/0/988	24536/0/1896	22956/0/1198
Absorption correction	Empirical	Empirical	Empirical	Empirical	Empirical	Empirical
Goodness-of-fit on <i>F</i> ² (<i>GOF</i>)	0.983	0.659	0.824	1.309	0.861	0.806
Final <i>R</i> indices [<i>I</i> > 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0334, <i>wR</i> ₂ = 0.0936	<i>R</i> ₁ = 0.0446, <i>wR</i> ₂ = 0.0729	<i>R</i> ₁ = 0.0483, <i>wR</i> ₂ = 0.0927	<i>R</i> ₁ = 0.0449, <i>wR</i> ₂ = 0.1069	<i>R</i> ₁ = 0.0701, <i>wR</i> ₂ = 0.1403	<i>R</i> ₁ = 0.0410, <i>wR</i> ₂ = 0.0838
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0505, <i>wR</i> ₂ = 0.0980	<i>R</i> ₁ = 0.1516, <i>wR</i> ₂ = 0.0828	<i>R</i> ₁ = 0.1247, <i>wR</i> ₂ = 0.1050	<i>R</i> ₁ = 0.0849, <i>wR</i> ₂ = 0.1197	<i>R</i> ₁ = 0.1494, <i>wR</i> ₂ = 0.1548	<i>R</i> ₁ = 0.1074, <i>wR</i> ₂ = 0.0927
Largest difference peak and hole (e Å ⁻³)	1.710 and -0.459	0.933 and -0.734	0.959 and -0.541	1.345 and -0.667	0.968 and -0.975	1.434 and -1.157

$$R_1 = \frac{\sum (|F_{\text{obs}}| - |F_{\text{calc}}|)}{\sum |F_{\text{obs}}|} \quad wR_2 = \frac{[\sum_w (F_{\text{obs}}^2 - F_{\text{calc}}^2)^2 / \sum_w (F_{\text{obs}}^2)^2]^{1/2}}{\quad} \quad GOF = \frac{[\sum_w (F_{\text{obs}}^2 - F_{\text{calc}}^2)^2 / (N_{\text{obs}} - N_{\text{par}})]^{1/2}}{\quad}$$