

Supporting Information

for

Gallium Hydrides with a Radical-Anionic Ligand

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Table 1S. Crystal data and structure refinement details for compounds **1** and **3-6**.

	1	3	4	5	6 ×0.84C ₄ H ₁₀ O
Formula	C ₃₆ H ₄₁ ClGa ₂ N ₂	C ₇₂ H ₈₀ Ga ₂ N ₄ O ₂	C ₃₆ H ₄₂ GaN ₂	C ₄₂ H ₄₈ GaN ₂ OSi	C _{53.34} H _{60.35} GaN ₂ O _{2.84}
Formula Weight	606.88	1172.84	572.43	694.63	844.54
Crystal System	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space Group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> [Å]	10.3634(8)	15.7563(13)	10.3422(2)	10.6096(3)	12.8405(6)
<i>b</i> [Å]	19.8887(16)	12.0750(10)	20.1832(4)	23.1285(6)	26.4463(11)
<i>c</i> [Å]	15.6959(12)	16.1335(14)	15.5670(3)	15.6732(4)	15.3885(16)
<i>α</i> [°]	90	90	90	90	90
<i>α</i> [°]	104.5140(10)	97.589(2)	104.300(2)	104.8490(10)	91.394(7)
<i>γ</i> [°]	90	90	90	90	90
<i>V</i> [Å ³]	3131.9(4)	3042.6(4)	3148.75(11)	3717.52(17)	5224.1(6)
<i>Z</i>	4	2	4	4	4
<i>ρ</i> _{calc} [Mg/m ³]	1.287	1.280	1.208	1.241	1.074
<i>μ</i> [mm ⁻¹]	0.991	0.935	0.899	0.806	0.565
<i>F</i> (000)	1276	1236	1212	1468	1792
Crystal Size [mm]	0.32×0.28×0.26	0.21×0.17×0.13	0.50×0.20×0.05	0.32×0.07×0.04	0.35×0.35×0.30
<i>θ</i> _{min} / <i>θ</i> _{max} [°]	2.27 / 26.00	1.70 / 26.00	2.95 / 28.00	2.27 / 27.56	3.05 / 26.00
Index Ranges	−12 ≤ <i>h</i> ≤ 12 −24 ≤ <i>k</i> ≤ 24 −19 ≤ <i>l</i> ≤ 19	−19 ≤ <i>h</i> ≤ 19 −14 ≤ <i>k</i> ≤ 14 −19 ≤ <i>l</i> ≤ 19	−13 ≤ <i>h</i> ≤ 13 −26 ≤ <i>k</i> ≤ 26 −20 ≤ <i>l</i> ≤ 20	−13 ≤ <i>h</i> ≤ 13 −30 ≤ <i>k</i> ≤ 30 −20 ≤ <i>l</i> ≤ 20	−15 ≤ <i>h</i> ≤ 15 −32 ≤ <i>k</i> ≤ 32 −18 ≤ <i>l</i> ≤ 18
Reflections Collected (Independent Reflections)	29044 (6150)	25646 (5970)	57337 (7522)	44000 (8579)	79322 (10178)
<i>R</i> _{int}	0.0252	0.0721	0.0308	0.0635	0.1003
Data / Restraints / Parameters	6150 / 2 / 387	5970 / 0 / 369	7522 / 0 / 368	8579 / 0 / 444	10178 / 85 / 585
<i>GooF</i> on <i>F</i> ²	1.050	1.007	1.074	1.009	1.042
<i>R</i> ₁ / <i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.0382 / 0.1014	0.0508 / 0.1176	0.0340 / 0.0876	0.0495 / 0.1192	0.0746 / 0.1869
<i>R</i> ₁ / <i>wR</i> ₂ (all data)	0.0426 / 0.1037	0.0829 / 0.1325	0.0392 / 0.0897	0.0715 / 0.1303	0.1029 / 0.2004
Largest Diff. Peak and Hole [e/Å ³]	0.563 / −0.563	1.525 / −0.502	0.450 / −0.376	0.648 / −0.569	1.436 / −0.733