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Mixed phosphine and group-13 metal ligator complexes $[(PR_3)_aM(ECp^*)_b]$ (M = Mo, Ni; E = Ga, Al; R = C_6H_5, cyclo-C_6H_{11})

Mariusz Molon, Timo Bollermann, Christian Gemel, Julian Schaumann and Roland A. Fischer*

Anorganische Chemie II, Organometallics and Materials Chemistry, Ruhr University Bochum,

Universitätsstraße 150, 44780 Bochum, Germany

Supporting Information

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Table 3 Important crystallographic data of compounds **1** to **4**

	1	**2a**	**2b**	**3a**	**3b**	**4**
empirical formula	$MoGa_2P_4C_{32}H_{66}$	$NiGa_2P_2C_{56}H_{60}$	$NiAl_2P_2C_{56}H_{60}$	$NiGa_2P_2C_{56}H_{96}$	$NiGa_2P_2C_{26}H_{48}$	$NiGa_3PC_{48}H_{75}$
molecular weight	810.11	993.13	907.65	1029.42	620.73	950.92
temperature (K)	111(2)	113(2)	113(2)	113(2)	105(2)	105(2)
wavelength Mo-K_α (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
crystal size (mm)	0.30 x 0.28 x 0.20	0.2 x 0.2 x 0.02	0.30 x 0.20 x 0.20	0.20 x 0.20 x 0.10	0.38 x 0.14 x 0.11	0.20 x 0.20 x 0.20
crystal system, space group	Orthorhombic, $P2_12_12_1$	Monoclinic, *P2 1/c*	Triclinic, *P-1*	Triclinic, *P-1*	Monoclinic, *C2/c*	Cubic, *I-43d*
a (Å)	11.6503(2)	16.5596(10)	11.5183(5)	11.9834(7)	20.8362(13)	26.9627(3)
b (Å)	14.6989(4)	15.2068(8)	21.7943(9)	16.4634(11)	10.2222(3)	26.9627(3)
c (Å)	23.1578(5)	23.3095(15)	22.2311(8)	17.9050(12)	16.8438(18)	26.9627(3)
α (°)	90.00	90.00	117.737(4)	87.267(6)	90.00	90.00
β (°)	90.00	101.783(6)	92.013(3)	73.270(6)	121.849(10)	90.00
γ (°)	90.00	90.00	94.562(3)	85.217(5)	90.00	90.00
cell volume ($Å^{-3}$)	3965.69(15)	5746.1(6)	4907.3(3)	3370.1(4)	3047.4(4)	19601.5(4)
Z	4	4	4	2	4	16
density $\rho_{calc.}$ (mg m^{-3})	1.357	1.148	1.229	1.014	1.353	1.289
absorption coefficient μ(mm^{-1})	1.841	1.342	0.532	1.145	2.483	2.072
F (000)	1688	2064	1920	1104	1296	7984
2θ range for data collection□(°)	3.17 – 25.00	2.85 – 25.00	2.77 – 25.00	2.90 – 25.00	3.01 – 24.99	3.38 – 25.00
index ranges	-13≤h≤13, -13≤k≤17, -27≤l≤27	-19 ≤h≤15, -12≤k≤18, -27≤l≤24	-13≤h≤13, -25≤k≤25, -26≤l≤26	-14≤h≤14, -19≤k≤19, -21≤l≤21	-24≤h≤24, -11≤k≤11, -19≤l≤20	-29≤h≤32, -32≤k≤31, -32≤l≤31
reflexions collected	29247	21121	46113	37627	7746	63101
unique reflexions	6978	10110	17267	11846	2666	2878
R_{int}	0.0308	0.1143	0.0719	0.0933	0.0398	0.0735
data/restraints/parameters	6978/81/400	10110/66/550	17267/6/1119	11846/0/550	2666/0/141	2878/4/258
absorption correction	Semi-empirical	empirical (sadabs)	empirical (sadabs)	empirical (sadabs)	empirical (sadabs)	empirical (sadabs)
goodness-of-fit on F^2 (GOF)	0.990	0.919	0.970	0. 982	1.066	1.147
final R indices [I > 2σ(I)]	R_1 = 0.0271 wR_2 = 0.0600	R_1 = 0.0844 wR_2 = 0.1697	R_1 = 0.0540 wR_2 = 0.0938	R_1 = 0.0621 wR_2 = 0.1377	R_1 = 0.0314 wR_2 = 0.0725	R_1 = 0.0390 wR_2 = 0.0744
R indices (all data)	R_1 = 0.0410 wR_2 = 0.0635	R_1 = 0.1575 wR_2 = 0.1975	R_1 = 0.0987 wR_2 = 0.1065	R_1 = 0.1057 wR_2 = 0.1531	R_1 = 0.0390 wR_2 = 0.0764	R_1 = 0.0505 wR_2 = 0.0784
Largest diff. peak and hole (e A^{-3})	0.783 and -0.324	0.723 and -0.811	0.414 and -0.296	0.639 and -0.414	0.473 and -0.385	0.267 and -0.210

Diffraction data of **5** is of poor quality therefore only the unit cell parameters will be provided:
a = 14.689(2) Å, b = 10.005(2) Å, c = 17.673(5) Å, α = β = γ = 90.00°, V = 2597.3(10) $Å^3$