Supporting Information

Synthesis, Structure and Reactivity Study of Magnesium Amidinato Complexes Derived from Carbodiimides and *N*,*N*'-Bis(2,6-diisopropylphenyl)-1,4-diaza-butadiene Ligands

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Table 1. Crystallographic details and refinement parameters of compounds **1**-**7**.

Crystal	**1**	**2**	**3**	**4**
CCDC No.	1019669	1019670	1019671	1019672
Empirical formula	$C_{54}H_{72}Mg_2N_4$	$C_{42}H_{56}Mg_2N_4$	$C_{32}H_{50}MgN_4$	$C_{73}H_{94}MgN_4$
Formula weight	825.78	665.53	515.07	1051.83
T (K)	120	120	120	120
λ (Å)	0.71069	0.71069	0.71069	0.71069
Crystal system	Monoclinic	Monoclinic	Orthorhombic	Monoclinic
Space group	*P 2$_1$/c*	*P 2$_1$/c*	*P b c a*	*C 2/c*
a (Å)	12.618(5)	12.896 (5)	20.441(5)	17.809(5)
b (Å)	11.279(5)	16.810 (5)	11.399(5)	19.577(5)
c (Å)	19.871(5)	16.810 (5)	27.842(5)	17.603(5)
α (°)	90	90	90	90
β (°)	122.834(15)	105.741(5)	90	98.479(5)
γ (°)	90	90	90	90
V (Å^3)	2376.2(15)	3883(2)	6487(3)	6070(3)
Z	2	4	8	4
D_{calc} g cm^{-3}	1.153	1.138	1.055	1.151
μ (mm^{-1})	0.090	0.095	0.079	0.075
F (000)	896	1440	2256	2288
Theta range for data collection	3.04 to 27.44 deg.	3.15 to 30.44 deg.	3.00 to 27.5 deg	3.04 to 30.45 deg.
Reflections collected / unique	37443 / 5407 [R(int) = 0.0857]	95565 / 11748 [R(int) = 0.0407]	60136 / 7404 [R(int) = 0.0646]	61348 / 9204 [R(int) = 0.0392]
Completeness to theta = 71.25	99.7 %	99.5 %	99.7 %	99.8 %
Absorption correction	Multi-scan	Multi-scan	Multi-scan	Multi-scan
Max. and min. transmission	0.9848 and 0.9777	0.978 and 0.973	0.988 and 0.980	0.986 and 0.979
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	5407 / 0 / 271	11748 / 0 / 441	7404 / 0 / 346	9204 / 0 / 363
Goodness-of-fit on F^2	1.047	1.078	1.059	0.945
Final R indices [I>2sigma(I)]	R1 = 0.0460, wR2 = 0.1064	R1 = 0.0415, wR2 = 0.1043	R1 = 0.0939, wR2 = 0.2485	R1 = 0.0462, wR2 = 0.1276
R indices (all data)	R1 = 0.0633, wR2 = 0.1166	R1 = 0.0527, wR2 = 0.1121	R1 = 0.2029, wR2 = 0.2439	R1 = 0.0557, wR2 = 0.1356
Absolute structure parameter Largest diff. peak and hole	0.428 and -0.229 e. Å $^{-3}$	0.396 and -0.272 e. Å $^{-3}$	0.421 and -0.466 e. Å $^{-3}$	0.519 and -0.255 e. Å $^{-3}$

Table 1 (contd). Crystallographic details and refinement parameters of compounds **1-7**.

Crystal	**5**	**6**	**7**
CCDC No.	1019673	1019674	1019675
Empirical formula	$C_{54}H_{72}MgN_6$	$C_{50}H_{64}MgN_4$	$C_{94}H_{116}Mg_2N_4O_2$
Formula weight	829.49	745.36	1382.53
T (K)	120	120	120
λ (Å)	0.71069	0.71069	0.71069
Crystal system	Triclinic	Monoclinic	Triclinic
Space group	*P -1*	*P* $2_1/c$	*P* -1
a (Å)	11.569(5)	15.311(5)	11.523(5)
b (Å)	12.971(5)	16.053(5)	12.684(5)
c (Å)	16.674(5)	18.041(5)	15.762(5)
α (°)	100.146(5)	90	79.062(5)
β (°)	93.771(5)	92.921(5)	73.256(5)
γ (°)	100.240(5)	90	67.014(5)
V (Å^3)	2411.6(16)	4428(2)	2023.1(13)
Z	2	4	1
D_{calc} g cm^{-3}	1.139	1.118	1.135
μ (mm^{-1})	0.079	0.078	0.080
F (000)	896	1616	748
Theta range for data collection	3.13 to 30.48 deg.	3.06 to 30.48 deg.	3.07 to 30.48 deg.
Reflections collected / unique	49598 / 14648	85075 / 134237	41678 / 12266
	[R(int) = 0.0556]	[R(int) = 0.1234]	[R(int) = 0.0815]
Completeness to theta = 71.25	99.5 %	99.5 %	99.4 %
Absorption correction	Multi-scan	Multi-scan	Multi-scan
Max. and min. transmission	0.9875 and 0.9837	0.988 and 0.982	0.986 and 0.981
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	14648 / 0 / 558	13423 / 0 / 508	12266 / 0 / 469
Goodness-of-fit on F^2	0.989	1.024	1.155
Final R indices [I>2sigma(I)]	R1 = 0.0925,	R1 = 0.0822,	R1 = 0.0688,
	wR2 = 0.1705	wR2 = 0.2295	wR2 = 0.1703
R indices (all data)	R1 = 0.0903,	R1 = 0.0897,	R1 = 0.1286,
	wR2 = 0.2408	wR2 = 0.2497	wR2 = 0.2386
Absolute structure parameter Largest diff. peak and hole	0.499 and -0.381 e. Å^{-3}	1.447 and -0.631 e. Å^{-3}	0.456 and -0.482 e. Å^{-3}