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Supporting Information

Bis(phosphinoselenoic amides) as Versatile Chelating Ligands for Alkaline Earth Metal (Mg, Ca, Sr and Ba) Complexes: Syntheses, Structure and ε-Caprolactone Polymerisation

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Table TS1. Crystallographic data and structure refinement parameters for complexes **1-*cis*, 1-*trans*** and **2-7.**

	1 -*cis*	**1** -*trans*	**2**	**3**	**4**	**5**	**6**	**7**
CCDC No.	987282	987283	987285	987287	987284	987289	987288	987286
Empirical formula	$C_{26}H_{26}N_2P_2Se_2$	$C_{34}H_{42}N_2O_2P_2$ Se_2	$C_{38}H_{48}CaN_2O_3P_2$ Se_2	$C_{38}H_{48}N_2O_3P_2Se_2$ Sr	$C_{38}H_{48}BaN_2O_3P_2$ Se_2	$C_{38}H_{48}MgN_2O_3P_2$ Se_2	$C_{26}H_{32}B_2N_2P_2$	$C_{34}H_{46}B_2BaN_2O_2$ P_2
Formula weight	586.35	730.56	840.72	888.26	937.97	824.95	456.10	735.62
T (K)	293(2)	293(2)	150(2)	150(2)	150(2)	150(2)	293(2)	150(2)
λ (Å)	1.54184	1.54184	1.54184	1.54184	1.54184	1.54184	1.54184	1.54184
Crystal system	Monoclinic,	Orthorhombic	Triclinic	Triclinic	Triclinic,	Triclinic	Monoclinic	Triclinic
Space group	*C 2/c*	*P b c a*	*P*-1	*P*-1	*P*-1	*P-1*	*C c*	*P*-1
a (Å)	23.2423(12)	16.5026(5)	9.8642(10)	9.8678(11)	9.6600(5)	9.6053(11)	12.7050(6)	9.2659(9)
b (Å)	12.0610(7)	11.4432(3)	13.4955(12)	13.4550(14)	17.2064(10)	13.3939(14)	13.7069(7)	14.0750(13)
c (Å)	9.2715(5)	18.3315(5)	16.8868(12)	17.0933(17)	25.4384(14)	16.644(3)	14.7809(7)	14.9320(15)
α (°)	90	90	106.675(7)	106.687(9)	105.952(5)	107.905(13)	90	111.894(9)
β (°)	102.372(6)	90	101.705(8)	101.184(9)	90.358(4)	99.522(12)	91.387(4)	91.583(8)
γ (°)	90	90	106.697(9)	106.567(10)	102.056(5)	105.115(10)	90	101.013(8)
V (Å^3)	2538.7(2)	3461.77(17)	1960.4(3)	1987.4(4)	3966.6(4)	1895.5(5)	2573.3(2)	1763.2(3)
Z	4	4	2	2	4	2	4	2
D_{calc} g cm^{-3}	1.534	1.398	1.424	1.484	1.571	1.445	1.177	1.386
μ (mm^{-1})	4.957	3.790	4.567	5.028	10.938	3.701	1.640	9.855
F (000)	1176	1488	864	900	1872	848	968	752
Theta range for data collection	3.89 to 70.74 deg.	4.82 to 70.73 deg.	2.87 to 65.00 deg.	3.68 to 70.77 deg.	3.62 to 71.13 deg.	2.90 to 70.69 deg.	4.75 to 70.77 deg.	3.71 to 70.77deg.
Limiting indices	-28<=h<=27,	-15<=h<=20,	-11<=h<=11,	-10<=h<=12,	-11<=h<=11,	-10<=h<=11	-15<=h<=15,	-8<=h<=11,
-	-14<=k<=14,	-13<=k<=13,	-14<=k<=15,	-16<=k<=16,	-21<=k<=18,	-16<=k<=11	-10<=k<=16,	-17<=k<=15,
	-8<=l<=11	-17<=l<=22	-19<=l<=14	-20<=l<=15	-21<=l<=31	-20<=l<=20	-15<=l<=18	-18<=l<=15
Reflections collected / unique	4948 / 2396 [R(int) = 0.0296]	8871 / 3273 [R(int) = 0.0251]	12666 / 6651 [R(int) = 0.0738]	14710 / 7443 [R(int) = 0.0610]	31367 / 14953 [R(int) = 0.0555]	13867 / 7151 [R(int) = 0.0400]	4908 / 3221 [R(int) = 0.0330]	13627 / 6641 [R(int) = 0.0755]
Completeness to theta = 71.25	98.2 %	98.3 %	99.6 %	97.5 %	97.4 %	98.0 %	97.9 %	97.7 %
Absorption correction	Multi-scan	Multi-scan	Multi-scan	Multi-scan	Multi-scan	Multi-scan	Multi-scan	Multi-scan
Max. and min. transmission	1.000 and 0.634	1.000 and 0.659	1.000 and 0.179	1.000 and 0.586	1.000 and 0.564	1.000 and 0.849	1.000 and 0.790	1.000 and 0.527
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	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 /	2396 / 0 / 145	3273 / 0 / 193	6651 / 0 / 433	7443 / 0 / 433	14953 / 0 / 865	7151 / 0 / 433	3221 / 2 / 292	6641 / 0 / 412

parameters								
Goodness-of-fit on F^2	1.041	1.080	1.104	1.277	1.088	1.045	1.073	1.010
Final R indices [I>2sigma(I)]	R_1 = 0.0340, wR_2 = 0.0859	R_1 = 0.0329, wR_2 = 0.0888	R_1 = 0.0674, wR_2 = 0.2624	R_1 = 0.0497, wR_2 = 0.1484	R_1 = 0.0572, wR_2 = 0.1524	R_1 = 0.0415, wR_2 = 0.0979	R_1 = 0.0456, wR_2 = 0.1263	R_1 = 0.0527, wR_2 = 0.1148
R indices (all data)	R_1 = 0.0426, wR_2 = 0.0938	R_1 = 0.0346, wR_2 = 0.0903	R_1 = 0.0974, wR_2 = 0.2936	R_1 = 0.0773, wR_2 = 0.1581	R_1 = 0.0799, wR_2 = 0.1694	R_1 = 0.0555, wR_2 = 0.1080	R_1 = 0.0491, wR_2 = 0.1312	R_1 = 0.0768, wR_2 = 0.1350
Largest diff. peak and hole	0.417 and -0.48 $e.A^{-3}$	0.475 and -0.458 $e.A^{-3}$	0.164 and -1.222 $e.A^{-3}$	0.553 and -0.617 $e.A^{-3}$	1.769 and -1.288 $e.A^{-3}$	0.872 and -0.605 $e.A^{-3}$	0.195 and -0.235 $e.A^{-3}$	1.068 and -1.276 $e.A^{-3}$