Supporting Information

A New Tetragonal Structure Type $A_2Ca_{10}Sb_9$ (A = Li, Mg).

Electronic Variability Around a Zintl Phase.

Ashok K. Ganguli,^{*,#} Shalabh Gupta,[#] and John D. Corbett^{†*}

Table S1. Crystallographic and Refinement Details.

Empir. formula	Li Mg Ca ₁₀ Sb ₉	Mg ₂ Ca ₁₀ Sb ₉	Li _{1.38} Ca _{10.62} Sb ₉
F. w.	1527.78	1545.14	1531
T, K	273(2)	293(2)	298(2)
Crystal system, Z	Tetragonal, 4	Tetragonal, 4	Tetragonal, 4
Space group	P4(2)/mm	P4(2)/mm	P4(2)/mm
Unit cell dimen., Å			
<i>a</i>	11.8658(5)	11.8438(6)	11.9053(7)
<i>c</i>	17.181(2)	17.2967(16)	17.152(2)
<i>V</i> , Å ³	2419.0(3)	2426.3(3)	2431.1(3)
Dens.(calc.)(g/cm ³)	4.195	4.230	4.236
Absorp.coeff., mm ⁻¹	12.013	12.003	12.138
F(000)	2696	2732	2740
Crystal size, mm	0.08 x 0.07 x 0.07	0.07 x 0.06 x 0.06	0.08 x 0.06 x 0.06
Θ range, deg.	2.09-28.27	2.08 to 28.27.	2.08 to 28.28.
Index ranges	-15<= <i>h</i> <=15, -15<= <i>k</i> <=10, -22<= <i>l</i> <=20	-15<= <i>h</i> <=15, -15<= <i>k</i> <=15, -23<= <i>l</i> <=23	-15<= <i>h</i> <=9, -15<= <i>k</i> <=15, -22<= <i>l</i> <=21
Refl. collected	14545	19667	13912
Indep. Refl.[R(int)]	1617 [0.0489]	1607 [0.0542]	1625 [0.0591]
Completeness	97.9 %	97.1 %	97.7 %
Data / restraints / param.	1617 / 0 / 65	1607 / 0 / 64	1625 / 0 / 69
Goodness-of-fit on F ²	1.026	1.103	1.033
R1, wR2 [I>2σ(I)]	0.0260, 0.0538	0.0288, 0.0606	0.0421, 0.0918
(all data)	0.0346, 0.0559	0.0369, 0.0630	0.0581, 0.0985
Largest diff. peaks, e.Å ⁻³	2.684, -0.899	1.967, -1.793	8.920, -3.928

Table S2. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{A}_2\text{Ca}_{10}\text{Sb}_9$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

1	U11	U22	U33	U23	U13	U12
Ca(1)	11(1)	21(1)	16(1)	2(1)	1(1)	1(1)
Ca(2)	15(1)	16(1)	15(1)	-1(1)	0(1)	-1(1)
Ca(3)	14(1)	14(1)	24(1)	0	0	-3(1)
Ca(4)	18(1)	18(1)	27(1)	0	0	-2(1)
Mg	23(1)	23(1)	20(2)	0	0	10(2)
Li	24(7)	24(7)	0(7)	0	0	45(8)
Sb(1)	13(1)	13(1)	19(1)	2(1)	2(1)	3(1)
Sb(2)	15(1)	15(1)	16(1)	-2(1)	-2(1)	3(1)
Sb(3)	11(1)	14(1)	13(1)	0	0	-2(1)
Sb(4)	19(1)	19(1)	14(1)	0	0	5(1)
Sb(5)	11(1)	11(1)	16(1)	0	0	-1(1)
Sb(6)	9(1)	9(1)	11(1)	0	0	0
2						
Ca(1)	21(1)	12(1)	18(1)	2(1)	1(1)	1(1)
Ca(2)	18(1)	17(1)	16(1)	-1(1)	2(1)	-3(1)
Ca(3)	14(1)	14(1)	26(1)	0	0	-3(1)
Ca(4)	20(1)	20(1)	26(1)	0	0	4(1)
Mg(1)	35(2)	35(2)	23(2)	0	0	-10(2)
Mg(2)	31(2)	31(2)	20(2)	0	0	20(2)
Sb(1)	10(1)	10(1)	12(1)	0	0	0
Sb(2)	12(1)	12(1)	17(1)	0	0	-1(1)
Sb(3)	13(1)	13(1)	18(1)	1(1)	-1(1)	-3(1)
Sb(4)	17(1)	17(1)	18(1)	-5(1)	5(1)	-5(1)
Sb(5)	22(1)	12(1)	14(1)	0	0	-5(1)
Sb(6)	36(1)	36(1)	15(1)	0	0	23(1)

3

Sb(1)	12(3)	12(3)	20(5)	0(0)	0(0)	4(3)
Sb(2)	15(1)	15(1)	26(1)	5(0)	5(0)	3(3)
Sb(3)	22(1)	18(1)	14(1)	0	0	10(4)
Sb(4)	30(1)	30(1)	20(1)	0	0	2(6)
Sb(5)	12(4)	12(7)	19(7)	0	0	1(1)
Sb(6)	9(3)	9(3)	11(6)	0	0	0
Ca(1)	23(1)	12(1)	17(1)	0(1)	2(1)	1(1)
Ca(2)	16(9)	15(9)	40(3)	0(1)	0(1)	1(1)
Ca(3)	21(1)	21(1)	25(2)	0	0	9(2)
Ca(4)	20(1)	20(1)	40(3)	0	0	4(2)
Ca(5)	27(3)	27(3)	13(3)	0	0	16(3)
Li[12(6)]

Figure S1: Magnetic susceptibilities of $\text{LiMgCa}_{10}\text{Sb}_9$ at 10 (circles) and 30 (triangles) kOe as a function of temperature (K).