Supporting Information

Syntheses and Structures of New Phases in the Systems AeM_xIn_{4-x} (Ae = Sr, Ba; M = Mg, Zn): Size Effects and Site Preferences on $BaAl_4$-type Structures

Bin Li and John D. Corbett

Table S1 Crystal and Refinement Data for $SrMg_{1.24(1)}In_{2.76}$.

compound	$SrMg_{1.24(1)}In_{2.76}$
Fw	434.22
space group, Z	*I*-4*m*2, 2
a (Å)	4.6831(3)
c (Å)	12.658(2)
Vol (Å^3)	277.61(4)
ρ_{calc} (g/cm^3)	5.20
μ (Mo Kα, mm^{-1})	20.8
R1/wR2, I>2σ(I)	0.027/0.062
R1/wR2,all data	0.027/ 0.062
largest diff. peak and hole (e. Å^{-3})	0.60 and -1.28

Table S2. Atomic Coordinates with $x = 0$, Isotropic-Equivalent Displacement Parameters (Å^2 x 10^3), and Site Occupancies for $SrMg_{1.24(1)}In_{2.76}$.

atom	site	y	z	U(eq)	Occupancy
Sr	2*a*	0	0	17(1)	1.00
In1	4*e*	0	0.6107(1)	16(1)	1.00
In2/Mg2	2*c*	½	¼	17(1)	0.76/0.24(1)
Mg	2*d*	½	¼	9(1)	1.00

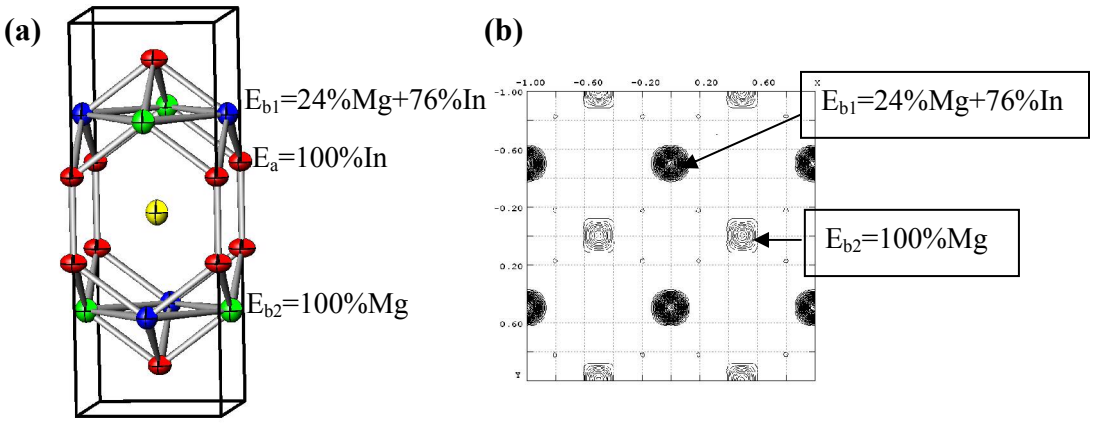
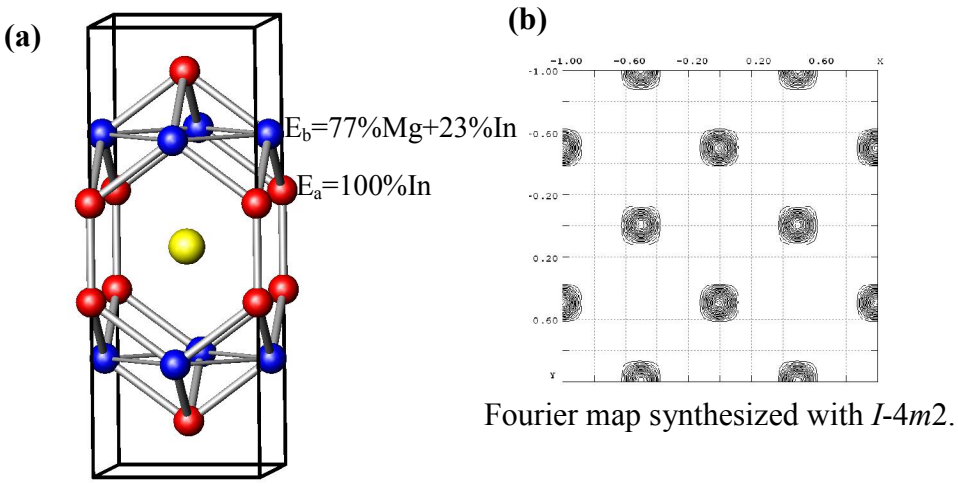


Figure S1 (a) Structure of $SrMg_{1.24(1)}In_{2.76}$ (*I*-4*m*2) with indications of atomic occupancies. (b) Fourier synthesis map with contouring level of 4eÅ^{-3} on the *xy* plane (z = ¼), corresponding to the square net in (a). The totally different electron densities at the four basal atom sites indicate disappearance of the proper 4-fold axis in the $BaAl_4$-type structure.



Fourier map synthesized with *I*-4*m*2.

Figure S2 (a) Structure of $SrMg_{1.532(4)}In_{2.468}$ **I** (*I*4/*mmm*) with indications of atomic occupancies. (b) Similar peak heights are also shown at the four basal atom sites (the *xy* plane with z = ¼) in the Fourier maps synthesized with *the low symmetry space group* (*I*-4*m*2). The contouring level is 5 eÅ^{-3}.

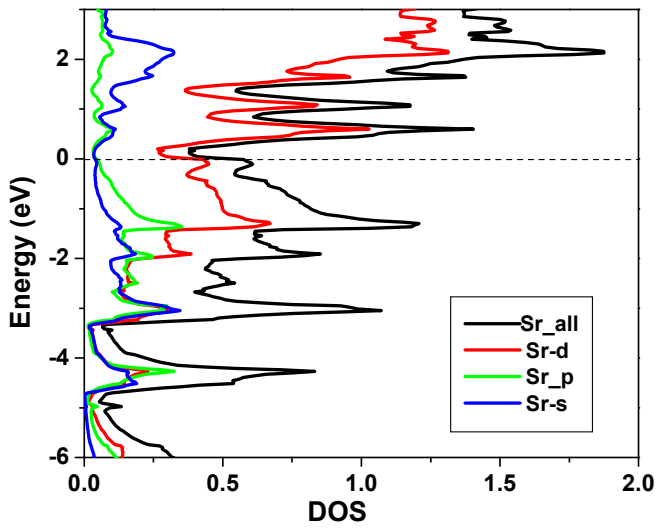


Figure 3S Partial DOS curves for Sr in $SrMgIn_3$ calculated by TB–LMTO–ASA method: all orbitals (black); Sr-d orbitals (red); Sr-p orbitals (green) and Sr-s orbitals (blue). The dotted line denotes the Fermi level.