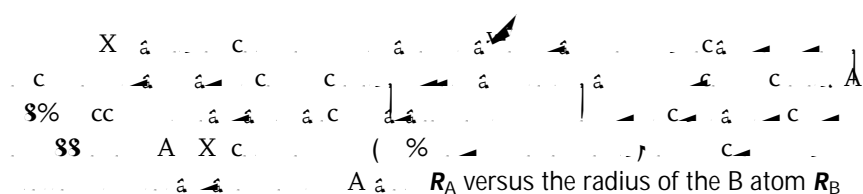
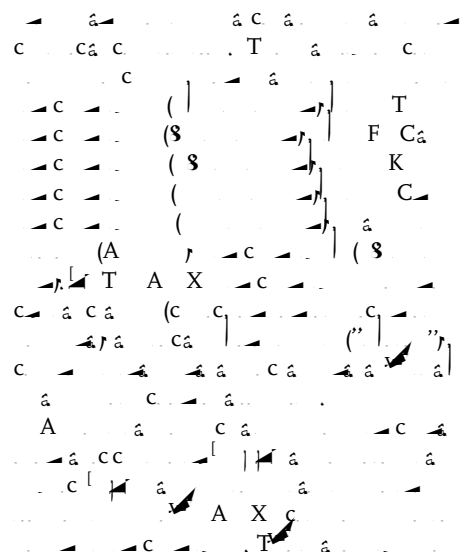


Diagrammatic Separation of Different Crystal Structures of A_2BX_4 Compounds Without Energy Minimization: A Pseudopotential Orbital Radii Approach

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for many A_2BX_4 compounds of known structure types and seeking heuristically simple, straight boundaries in the R_A versus R_B plane that best separate the domains of different structure types. The radii are sums $R_A = R_s(A) + R_p(A)$ of the quantum-mechanically calculated "orbital radii" $R_s(R_p)$, rather than empirical radii or phenomenological electronegativity scales. These success rates using first-principles orbital radii uniformly exceed the success rates using classic radii. Such maps afford a quick guess of the crystal structure of a yet unmade A_2BX_4 compound by placing its atomic orbital radii on such maps and reading off its structure type.



1. Introduction

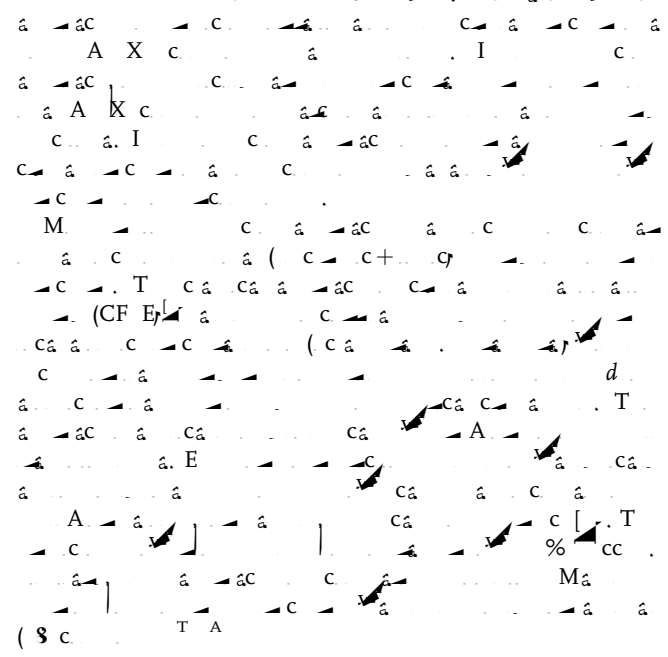
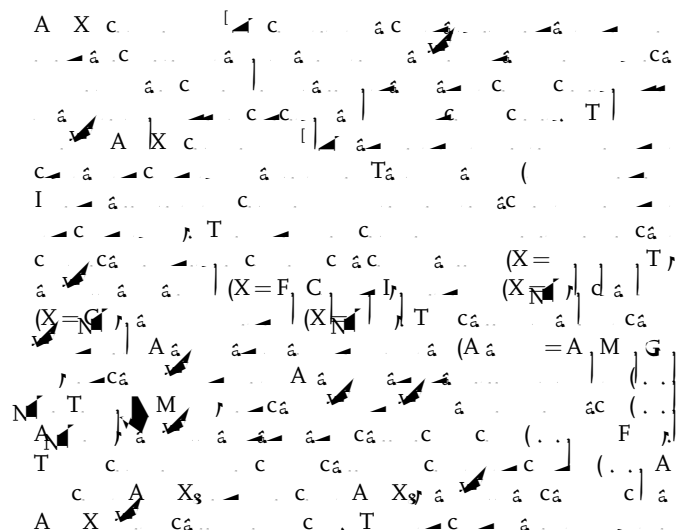


Table 1. Crystal structure types of A_2BX_4 compounds. The labels b1–b38 and d1, d3, and d9 of structures in the first column are taken from Wyckoff,^[5] whereas labels S1–S3 indicate Y_2CrS_4 -type, Yb_3S_4 -type, and Sr_2PbO_4 -type structures, respectively. The notation “none” refers to cases where no known Pearson symbol nor mineral name exists.

Label	Prototype Compd.	Space Group	Pearson's Symbol/Mineral Name	No. of Compd.
b5	Al_2MgO_4	$Fd\bar{3}m (O_h^7)$	cF56;Spinel	255
d9	Th_3P_4	$I\bar{4}3d (T_h^6)$	none	87
b9	Fe_2CaO_4	$Pnma (D_{2h}^{16})$	none	78
b11	K_2SO_4	$Pnma (D_{2h}^{16})$	none	69
d3	Cr_3S_4	$C2/m (C_{2h}^3)$	mC14	57
b10	Al_2BeO_4	$Pnma (D_{2h}^{16})$	Olivine	48
b1	K_2MgF_4	$I4/mmm (D_{4h}^{17})$	none	41
b6	Mn_3O_4	$I4_1/amd (D_{4h}^{19})$	tl28;Hausmanite; distorted Spinel	27
b4	Ag_2HgI_4	$P\bar{4}2m (D_{2d}^1)$	tl14;Thiogallate	24
b33	Li_2WO_4	$R\bar{3} (C_{3i}^2)$	Phenakite	14
S1	Y_2CrS_4	$Pca2_1 (C_{2v}^5)$	none	14
S2	Yb_3S_4	$Pnma (D_{2h}^{16})$	none	13
d1	Pb_3O_4	$P4_2/mbc (D_{4h}^{13})$	none	9
b21	Al_3BaO_4	$P6_322 (D_6^6)$	none	7
S3	Sr_2PbO_4	$Pbam (D_{2h}^9)$	none	6
b18	Na_2SO_4	$Fddd (D_{2h}^{24})$	Thenardite	4
b2	K_2PtCl_4	$P4/mmm (D_{4h}^1)$	none	3
b3	$K_2Pd(NO_2)_4$	$P2_1/c (C_{2h}^5)$	none	2
b7	Cr_2CuO_4	$I\bar{4}2d (D_{2d}^{12})$	distorted Spinel	2
b13	$KHSO_4$	$Pbca (D_{2h}^{15})$	none	2
b20	$LiKSO_4$	$P6_3 (C_6^6)$	none	2
b22	$KNaSO_4$	$P\bar{3}m1 (D_{3d}^3)$	Aphthitalite	2

Table 2. Crystal structure types of A

Label	Prototype Compd.	Space Group	Pearson's Symbol/Mineral Name	No. of Compd.
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c... a... c... T... a... ac... c... c... a...
 c... + c... a... c... c...
 a... a... a... c... a... T... a... ac...
 a... a... a... c... c... c... c... (8 %
 cc)
 I... a... c... c... a...
 a... c... a... a... a... c...
 Ha... Fc... T... c... a... ca... a...
 a... Ma... a... I... M...
 a... a... T... a... a... A... M... a...
 §... c... T... Ha... Fc... ca... a...
 a... Ca... a... M... C... (M=M, M, Z)
 a... M... c... a... M... Z... (M=A, F... a...)
 c... a... c... c... c... a...
 ca... ca... a... c... a... c...
 c... T... cc... c... a... ac...
 a... a... ca... a... a... a... a... ca... ca...
 a... a... a... a... a... a... a... c...

The image shows a musical score with lyrics and musical notation. The lyrics are in a non-Latin script, likely Georgian, and are written in a stylized font. The musical notation includes notes, stems, and bar lines. The score is arranged in several lines, with the lyrics and notation aligned horizontally. The lyrics are:
c c c T ca a C C
C Ga T C c M a T a
c a a c (I a)
A a c ac a
M ac T a
c (F a I a) a
c a a / ca ca c
a a a c (cc a c)
T c a a c
a a (F a) a c
c a a c F a
Ca G M a Z G a
a C C C H C M a C a
T c
a c c c a a
a c a
T a a c a a a c c

Aa ... | c ... c ... a ca ... c ...
T ... a ... d ... a a ... c ... a a ... a ...
ca ... c ... a ... a ... (...
I ... a ... T ... c ... c ... a ... U ... c ...
... a ... a ... a ... c ... a ... a ... a ... T ...
cc ... a ... c ... a ... a ... ca ...
... a ... a ... c ... a ... (F ... a ...
... I ... a ... a ... % a ... % c ... a ...
cc ... a ... a ... a ... a ... % a ... % ... c ...
a ... a ...



