Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

$Ca_2GeB_2O_7$ and $Ca_{1.78}Cd_{0.22}GeB_2O_7$: Two Acentric Borogermanates with Melilite-like Structure and Short Ultraviolet Cutoff Edge

Ru-Ling Tang,[a,b,c] Chun-Li Hu,[a] Bao-Lin Wu [a,b,c] Yan Chen,[a,b,c] and Jiang-Gao Mao*[a]

Table 1. Selected bond lengths [Å] and angles [deg.] for $Ca_2GeB_2O_7$ and $Ca_{1.78}Cd_{0.22}GeB_2O_7$.

Ca(1)-O(1)	2.349(7)	Ca(1)-O(1)	2.333(2)
Ca(1)-O(2)#7	2.361(5)	Ca(1)-O(3)#1	2.3453(16)
Ca(1)-O(2)#8	2.361(5)	Ca(1)-O(3)#2	2.3453(16)
Ca(1)-O(3)	2.376(7)	Ca(1)-O(2)	2.382(2)
Ca(1)-O(3)#5	2.526(5)	Ca(1)-O(2)#1	2.5061(17)
Ca(1)-O(3)#9	2.526(5)	Ca(1)-O(2)#3	2.5061(17)
Ca(1)-O(2)	2.543(5)	Ca(1)-O(3)#4	2.5405(16)
Ca(1)-O(2)#10	2.543(5)	Ca(1)-O(3)#5	2.5405(16)
Ge(1)-O(2)#1	1.748(5)	Ge(1)-O(3)#8	1.7482(16)
Ge(1)-O(2)#2	1.748(5)	Ge(1)-O(3)#9	1.7482(16)
Ge(1)-O(2)#3	1.748(5)	Ge(1)-O(3)#5	1.7482(16)
Ge(1)-O(2)	1.748(5)	Ge(1)-O(3)	1.7482(16)
B(1)-O(3)#12	1.391(13)	B(1)-O(2)#9	1.380(4)
B(1)-O(1)#13	1.450(12)	B(1)-O(1)#13	1.462(3)
B(1)-O(2)#8	1.586(8)	B(1)-O(3)#14	1.576(3)
B(1)-O(2)#7	1.586(8)	B(1)-O(3)	1.576(3)
O(2)#1-Ge(1)-O(2)#2	107.98(16)	O(3)#8-Ge(1)-O(3)#9	112.42(10)
O(2)#1-Ge(1)-O(2)#3	112.5(3)	O(3)#8-Ge(1)-O(3)#5	108.02(5)
O(2)#2-Ge(1)-O(2)#3	107.98(16)	O(3)#9-Ge(1)-O(3)#5	108.02(5)
O(2)#1-Ge(1)-O(2)	107.98(16)	O(3)#8-Ge(1)-O(3)	108.02(5)
O(2)#2-Ge(1)-O(2)	112.5(3)	O(3)#9-Ge(1)-O(3)	108.02(5)
O(2)#3-Ge(1)-O(2)	107.98(16)	O(3)#5-Ge(1)-O(3)	112.42(10)
O(3)#12-B(1)-O(1)#13	119.0(9)	O(2)#9-B(1)-O(1)#13	118.5(3)
O(3)#12-B(1)-O(2)#8	115.2(6)	O(2)#9-B(1)-O(3)#14	115.92(17)
O(1)#13-B(1)-O(2)#8	102.3(6)	O(1)#13-B(1)-O(3)#14	101.95(17)
O(3)#12-B(1)-O(2)#7	115.2(6)	O(2)#9-B(1)-O(3)	115.92(17)
O(1)#13-B(1)-O(2)#7	102.3(6)	O(1)#13-B(1)-O(3)	101.95(17)
O(2)#8-B(1)-O(2)#7	100.2(7)	O(3)#14-B(1)-O(3)	99.8(2)

Symmetry transformations used to generate equivalent atoms:

#1 -y, x, -z #2 -x, -y, z #3 y, -x, -z #4 x, y, z-1 #5 y, -x, -z+1 #6 -x, -y, z-1 #7 -y, x, -z+1 #8 -x-1/2, y- 1/2, -z+1 #9 -y-1, x, -z+1 #10 -y-1/2, -x-1/2, z #11 -x-1, -y, z #12 x, y, z+1 #13 y, -x-1, -z+1

Table S3. Atomic coordinates (x 10^4), equivalent isotropic displacement parameters ($Å^2$ x 10^3) and bond valence sums (BVS) for $Ca_2GeB_2O_7$ and $Ca_{1.78}Cd_{0.22}GeB_2O_7$.

Atom	x	y	z	Wyckoff	Occupancy	U(eq)	BVS
Ca(1)	3394(2)	1606(2)	5085(4)	4e	1	9(1)	2.241
Ge(1)	0	0	0	2a	1	9(1)	4.000
B(1)	1303(11)	3697(11)	9550(20)	4e	1	11(2)	2.874
O(1)	5000	0	1620(20)	2c	1	10(2)	2.328
O(2)	1844(7)	784(7)	2014(11)	4e	1	11(1)	1.721
O(3)	1448(7)	3552(7)	2415(14)	8f	1	13(2)	1.981
Ca(1)	3406(1)	1594(1)	-101(1)	4e	0.889	2(1)	
Cd(1)	3406(1)	1594(1)	-101(1)	4e	0.111	2(1)	
Ge(1)	0	0	5000	2a	1	1(1)	
B(1)	3682(3)	1318(3)	4555(7)	4e	1	1(1)	
O(1)	5000	0	3373(6)	2c	1	3(1)	
O(2)	1844(2)	798(2)	2977(3)	4e	1	4(1)	
O(3)	1449(2)	3551(2)	2588(5)	8f	1	3(1)	