Supporting Information

Non-centrosymmetric melilite-type borates $\text{Bi}_2\text{ZnB}_2\text{O}_7$ and $\text{CaBiGaB}_2\text{O}_7$

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Table 7. Powder X-ray diffraction pattern for $\text{Bi}_2\text{ZnB}_2\text{O}_7$ recorded with a Guinier-Hägg camera using $\text{Cu K}\alpha_1$ radiation and silicon as internal standard. Primitive orthorhombic unit-cell with $a = 10.830(1)$ Å, $b = 11.027(1)$ Å, $c = 4.8894(5)$ Å, $Z = 4$. The observed intensities were measured with a computer-controlled film scanner (KEJ Instruments, Sweden).

h	k	l	d_{cal} (Å)	d_{obs} (Å)	I_{obs}	h	k	l	d_{cal} (Å)	d_{obs} (Å)	I_{obs}
0	0	1	4.8894	4.8889	66	2	3	2	1.9054	1.9053	5
2	2	0	3.8634	3.8630	29	2	5	1	1.8847	1.8834	19
0	2	1	3.6582	3.6568	7	5	3	0	1.8661	1.8660	17
2	0	1	3.6290	3.6298	9	0	6	0	1.8379	1.8376	2
1	3	0	3.4808	3.4809	45	0	4	2	1.8291	1.8289	6
3	1	0	3.4309	3.4317	29	4	0	2	1.8145	1.8134	9
2	2	1	3.0313	3.0327	100	6	0	0	1.8050	1.8043	11
1	3	1	2.8356	2.8355	66	1	4	2	1.8036		
3	1	1	2.8085	2.8079	70	4	1	2	1.7904	1.7909	1
0	4	0	2.7568	2.7577	7	3	5	1	1.7564	1.7564	15
4	0	0	2.7076	2.7075	9	5	3	1	1.7435	1.7432	25
1	4	0	2.6716	2.6730	4	2	4	2	1.7329	1.7326	3
4	1	0	2.6295	2.6287	4	4	2	2	1.7236	1.7229	16
2	3	1	2.5825	2.5842	6	1	6	1	1.6991	1.6989	11
0	0	2	2.4447	2.4441	37	6	0	1	1.6933	1.6932	16
4	2	0	2.4303	2.4305	14	0	0	3	1.6298	1.6295	18
0	4	1	2.4014	2.4025	1	6	3	0	1.6202		
4	0	1	2.3686	2.3683	3	1	5	2	1.6192	1.6197	9
1	4	1	2.3445	2.3446	6	4	5	1	1.6141	1.6141	6
4	1	1	2.3158	2.3160	7	5	4	1	1.6084	1.6084	8
3	3	1	2.2788	2.2803	2	5	1	2	1.6040	1.6046	2
1	2	2	2.1888	2.1896	4	2	5	2	1.5675	1.5672	4
4	2	1	2.1763	2.1777	8	0	2	3	1.5629		
1	5	0	2.1611	2.1607	5	2	0	3	1.5606	1.5615	3
5	1	0	2.1254	2.1245	1	1	2	3	1.5469		
2	2	2	2.0658	2.0656	15	5	5	0	1.5454	1.5460	1
2	5	0	2.0426	2.0418	1	2	2	3	1.5017	1.5015	19
1	3	2	2.0006	2.0003	32	3	5	2	1.4913	1.4913	17
3	1	2	1.9910	1.9905	31	5	3	2	1.4834	1.4836	16
1	5	1	1.9766	1.9771	9	1	3	3	1.4760	1.4761	17
5	1	1	1.9492	1.9493	3	3	1	3	1.4721	1.4723	13
						1	6	2	1.4557	1.4553	3

Table 8. Powder X-ray diffraction pattern for $\text{CaBiGaB}_2\text{O}_7$ recorded with a Guinier-Hägg camera using $\text{Cu K}\alpha_1$ radiation and silicon as internal standard. Primitive tetragonal unit-cell with $a = 7.4663(4) \text{ \AA}$, $c = 4.8343(5) \text{ \AA}$, $Z = 2$. The observed intensities were measured with a computer-controlled film scanner (KEJ Instruments, Sweden).

h	k	l	$d_{\text{cal}} (\text{\AA})$	$d_{\text{obs}} (\text{\AA})$	I_{obs}
0	0	1	4.8343	4.8362	19
2	0	0	3.7331	3.7372	5
1	1	1	3.5654	3.5665	33
2	1	0	3.3390	3.3397	32
2	0	1	2.9547	2.9557	75
2	1	1	2.7474	2.7480	100
2	2	0	2.6397	2.6401	10
0	0	2	2.4172	2.4173	13
3	1	0	2.3610	2.3615	28
2	2	1	2.3168	2.3177	3
3	0	1	2.2127	2.2131	5
3	1	1	2.1215	2.1224	4
2	0	2	2.0290	2.0302	2
2	1	2	1.9580	1.9582	48
4	1	0	1.8108	1.8109	20
2	2	2	1.7827	1.7832	10
3	3	0	1.7598	1.7600	8
4	0	1	1.7413	1.7413	10
4	1	1	1.6958	1.6959	25
3	1	2	1.6890	1.6890	28
4	2	0	1.6695	1.6692	9
3	3	1	1.6537	1.6538	28
0	0	3	1.6114	1.6112	4
1	1	3	1.5412	1.5410	5
2	0	3	1.4795	1.4793	10
2	1	3	1.4513	1.4504	29
3	3	2	1.4227	1.4221	4
5	1	1	1.4014	1.4010	9
4	2	2	1.3737	1.3740	7
5	2	1	1.3327	1.3326	9
5	3	0	1.2805	1.2809	3
4	4	1	1.2733	1.2729	1
5	3	1	1.2378	1.2379	1
6	1	0	1.2274	1.2271	2
4	0	3	1.2198	1.2197	14

Table 9. Powder X-ray diffraction pattern for $\text{CdBiGaB}_2\text{O}_7$ recorded with a Guinier-Hägg camera using $\text{Cu K}\alpha_1$ radiation and silicon as internal standard. Primitive tetragonal unit-cell with $a = 7.4156(4) \text{ \AA}$, $c = 4.7933(5) \text{ \AA}$, $Z = 2$. The observed intensities were measured with a computer-controlled film scanner (KEJ Instruments, Sweden).

h	k	l	$d_{\text{cal}} (\text{\AA})$	$d_{\text{obs}} (\text{\AA})$	I_{obs}
0	0	1	4.7933	4.7901	31
2	0	0	3.7078	3.7072	6
1	1	1	3.5379	3.5370	33
2	1	0	3.3163	3.3155	49
2	0	1	2.9328	2.9328	57
2	1	1	2.7272	2.7278	100
2	2	0	2.6218	2.6224	9
0	0	2	2.3967	2.3974	12
3	1	0	2.3450	2.3451	27
2	2	1	2.3002	2.3006	1
3	0	1	2.1969	2.1975	4
3	1	1	2.1064	2.1062	8
2	1	2	1.9425	1.9429	47
4	0	0	1.8539	1.8549	2
4	1	0	1.7985	1.7987	18
2	2	2	1.7689	1.7693	6
3	3	0	1.7479	1.7477	9
4	0	1	1.7291	1.7292	12
4	1	1	1.6839	1.6839	21
3	1	2	1.6761	1.6762	24
4	2	0	1.6582	1.6585	5
3	3	1	1.6421	1.6419	38
0	0	3	1.5978	1.5980	4
1	1	3	1.5284	1.5280	4
2	0	3	1.4673	1.4673	8
2	1	3	1.4394		
4	1	2	1.4385	1.4389	27
3	3	2	1.4122	1.4120	6
5	1	1	1.3917	1.3916	5
5	2	0	1.3770	1.3773	4
2	2	3	1.3644		
4	2	2	1.3636	1.3639	5
5	2	1	1.3235	1.3235	14
4	4	0	1.3109	1.3112	2
5	3	0	1.2718	1.2715	4
6	0	0	1.2359	1.2355	6