Suplementary Materials.
Comparative Interrelationship of the Structural, Nonlinear- optical and Other Acentric Properties for Oxide, Borate and Carbonate Crystals

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Table S1. Real binary acentric binary oxide (polar piezoelectric).

	Chemical	Sym-	L, pm	L, pm	P_s	d	r	$\chi^{(2)}$	Ref
№	formula	metry	M-O	E-O	μC/cm^2	pC/N	pm/V	pm/V	
	1	2	3	6	7	8	9	10	11
1	ZnO	C_{6v}	197.3	197.3		13.9	2.6	7	453
2	$ErMnO_3$	C_{6v}	224.4	185.4	5.6			~1.25	255
3	$YbMnO_3$	C_{6v}	223.1	186.7	5.6			~1.25	254
4	$YMnO_3$ 293K	C_{6v}	227.5	186.3	5.5			~1.24	297
5	BeO	C_{6v}	166	166				~0.23	721
5	$YMnO_3$ 180K	C_{6v}	226.8	186.3					297
6	$LuMnO_3$	C_{6v}	223.4	185.9					253
7	$ScMnO_3$	C_{6v}	205	179					341
8	$AlPO_4$	C_{6v}	166.2	145.9					232
9	$Rb_{0.33}(Ga_{0.1}W_{0.9})O_3$	C_{6v}	312	165					192
10	Cu_2WO_4	C_{6v}	175.3	169.7					23
11	$Zn_2Mo_3O_8$	C_{6v}	208	191					39-40
12	$Fe_2Mo_3O_8$	C_{6v}	196.2	195.6					71
13	PbV_6O_{11}	C_{6v}	248.5	182.6					46
14	$Fe_{2.5}V_{1.5}^{3+}V_6^{4+}O_{16}$	C_{6v}	198	189					335
15	Li_2GeO_6	C_{6v}	193	175					143
16	Li_2SiO_6	C_{6v}	192	163					143
17	$CaAl_{12}O_{19}$	C_{6v}	270	174					58
18	$Ba_5(ReO_5)_3O_2$	C_{6v}	264	175					325
19	$Sr_4Ru_{3.05}O_{12}$	C_{6v}	256	184					59
20	$La_8Ru_4O_{21}$	C_{6v}	238.2	192					182
21	$YGaO_3$	C_{6v}	227.7	184					326
22	$K_4Sb_2O_3$	C_{6v}	248	173.9					286
23	K_6MgO_4	C_{6v}	267	199					207
24	$YMn_{0.75}(Cu_{0.75}Mo_{0.25})_{0.75}O_3$	C_{6v}	225	176					679
1	$PbTiO_3$	C_{4v}	253	178	70	580	13.8	42.8	299
2	$BaTiO_3$	C_{4v}	280	186	25	587	1640	19.3	300
3	$Ba_6Ti_2Nb_8O_{30}$	C_{4v}	274	188	7.1			~8.94	603
4	$Ba_6Zr_2Nb_8O_{30}$	C_{4v}	275	186	5.5			~6.93	603
5	$Ba_{62}Nb_8O_{30}$	C_{4v}	265	191	12.1			~6.32	603
6	$Li_2B_4O_7$	C_{4v}	196.7	135.5				3	368
7	$NaNbO_3$	C_{4v}	277.7	196.4	12			~1.78	452
8	$Ba_6Ti_2Ta_8O_{30}$	C_{4v}	264	189	0.8			~1.27	603
9	$Ba_6\ Zr_2Ta_8O_{30}$	C_{4v}	263	187	1.6			~1.27	603
10	$Ba_6\ Hf_2Ta_8O_{30}$	C_{4v}	264	188	1.1			~1.27	603
	$PbTiO_3$ 25C	C_{4v}	252	176					518
	$PbTiO_3$ -183C	C_{4v}	251	175					518
	$PbTiO_3$ -115C	C_{4v}	251	176					518
11	$Sr_6Nb_{34}O_{91}$	C_{4v}	252.3	166.6					456
12	$Sr(FeNb)_{0.5}O_3$	C_{4v}	279.4	197.6					454
13	$(Nb_{7.6}U_{2.4})(Ba_{5.2}K_{0.8})O_{30}$	C_{4v}	279	277					220
14	$Nd_{0.33}TaO_3$	C_{4v}	246	188					364
15	$Ba_4Nd_2Ti_4Ta_6O_{30}$	C_{4v}	262.8	181.6					547

16	$Ba_5Nd_2Ti_3Ta_7O_{30}$	C_{4v}	267.2	183.4					547
17	$LiMo_8O_{10}$	C_{4v}	201	170					34
18	$ZnMo_8O_{10}$	C_{4v}	201	188.1					34
19	$K_2V_3O_8$	C_{4v}	276.9	158.2					185
20	$Rb_2V_3O_8$	C_{4v}	284.4	156.4					185
21	$Cs_2V_5O_{13}$	C_{4v}	324	160.7					206
22	$Bi_2V_{0.6}Ge_{0.4}O_{5.3}$	C_{4v}	222	164					279
23	VSe_2O_6	C_{4v}	165.7	160.5					208
24	$Ba_{0.67}Sr_{0.33}TiO_3$	C_{4v}	279	199.3					607
25	$Ba_{0.92}Ca_{0.08}TiO_3$	C_{4v}	271	198.52					430
26	Bi_2PdO_4	C_{4v}	214.3	200.2					405
27	α-$Sr_3Fe_2O_{7-x}$	C_{4v}	242	170					523
28	$Sr_4Tl_2O_7$	C_{4v}	252	208					525
29	$CuReO_4$	C_{4v}	190.3	171.5					698
30	$BiCoO_3$	C_{4v}	225.9	171.7					667
1	$BiFeO_3$	C_{3v}	254	190	100			3401	718
2	$LiNbO_3$	C_{3v}	205.0	187.62	50	78	32.2	40.68	186
3	KIO_3	C_{3v}	303.2	177.5	30	39	~5	24.7	251
4	$LiTaO_3$	C_{3v}	204.1	190.8	50	26	44	19.4	84
5	$TlIO_3$	C_{3v}	301.6	182				~9.7	604
6	$Pb(Fe_{1/2}Ta_{1/2})O_3$ 300K	C_{3v}	276.4	196.8	28			~5	460
7	$KBrO_3$	C_{3v}	278	168				2.5	721
8	$BaTiO_3$	C_{3v}	282	190	17.8			~2	301
9	β-BaB_2O_4	C_{3v}	261.3	132.9			2.5	1.78-2.5	187
10	$Pb(Fe_{0.5}Nb_{0.5})O_3$	C_{3v}	273	206	6.7			~1.3	362
11	γ-KNO_3	C_{3v}	287	128	6.3			~1.27	333
12	$Pb(Sc_{0.5}Nb_{0.5})O_3$	C_{3v}	262.5	202.5	3.6			~ 1	458
13	$Ca_3V_2O_8$	C_{3v}	232	169	5.3	1.5	1.1	0.66	195
14	$Li_{0.8735}Nb_{1.0253}O_3$	C_{3v}	203.9	190.0					406
15	$Li_{0.941}Nb_{1.0118}O_3$	C_{3v}	205.3	187.87					186
16	$Li_{0.92}Cu_{0.08}NbO_3$	C_{3v}	210	203					302
17	$Li_{0.86}Cu_{0.14}NbO_3$	C_{3v}	209	204					302
18	$Li_{0.76}Cu_{0.24}NbO_3$	C_{3v}	212	203					302
19	$Li_{0.74}Nb_{0.94}Co_{0.28}O_3$	C_{3v}	210.2	179.5					406
20	$Li_{0.8}Nb_{0.96}Ni_{0.2}O_3$	C_{3v}	209.5	188.2					406
21	$BaNb_3O_6$	C_{3v}	277.5	192.4					490
22	$PbNb_2O_6$	C_{3v}	260	173					94
23	$PbNb_2O_7$	C_{3v}	217	173					94
24	$Pb_{2.44}Nb_2O_{7.44}$	C_{3v}	221	178					95
25	$Pb_{2.31}Nb_2O_{7.31}$	C_{3v}	217	182					95
26	R-$Mn_4Nb_2O_9$ 9GPa 1700C	C_{3v}	214.3	197.3					505
27	$Li_{1.2}Cu_{0.8}Ta_2O_6$	C_{3v}	215	196					511
28	$AgTaO_3$	C_{3v}	246.1	194.1					363
29	$Pb(Fe_{1/2}Ta_{1/2})O_3$ 10K	C_{3v}	276.8	200.1					460
30	P_4O_{10}	C_{3v}	143.1	143.1					372
31	$(Hg_3)_3(PO_4)_4$	C_{3v}	213.1	150.2					183
32	β-$Ca_3(PO_4)_2$	C_{3v}	231.6	149.8					67
33	β-$Ca_3(PO_4)_2$	C_{3v}	221.1	151					549
34	$Ca_{2.89}Mg_{0.11}(PO_4)_2$	C_{3v}	216.3	147.7					502
35	Ga_3PO_7	C_{3v}	186.3	150.8					231
36	Fe_3PO_7	C_{3v}	189.2	150.2					99
37	$BaVO_{2.5}$	C_{3v}	267	186					202
38	Ca_3SiO_5	C_{3v}	228	158					144
39	$Ca_{2.98}Si_{0.98}Al_{0.04}$ 1200C	C_{3v}	209	162					393
40	$HgTiO_3$	C_{3v}	220	196					109
41	$MnTiO_3$	C_{3v}	211	186.5					152
42	$PbHf_{0.8}Ti_{0.2}O_3$ 10K	C_{3v}	249	201					247

43	$PbHf_{0.8}Ti_{0.2}O_3$ 150K	C_{3v}	251	201					247
44	$PbHf_{0.8}Ti_{0.2}O_3$ 290K	C_{3v}	254	202					247
45	$PbHf_{0.8}Ti_{0.2}O_3$ 440K	C_{3v}	261	202					247
46	$LiReO_3$	C_{3v}	200	192.7					112
47	Li_2ReO_3	C_{3v}	201	195					112
48	β-Ag_2CO_3 483K	C_{3v}	209.0	124.67					449
49	$Ca_3Co_2O_6$	C_{3v}	239	191.6					166
5-	β-$Cs_2Cr_3O_{10}$	C_{3v}	311	153					213
51	$Bi_{2.4}La_{3.6}O_9$	C_{3v}	234.5	?234.5					131
52	$PbZn_{1/3}Nb_{2/3}O_3$ 4.2K	C_{3v}	256.5	196.4					681
53	$PbZn_{1/3}Nb_{2/3}O_3$ 295K	C_{3v}	261.4	197.7					681
54	$KAlSiO_4$	C_{3v}	296.2	158.1					696
55	$BiAlO_3$	C_{3v}	225.4	185.3					663
56	9R-Ca_3GeO_5	C_{3v}	203	177					400
1	$KNbO_3$	C_{2v}	265	195	30	107	450	20.1	417
2	$Ca_2Nb_2O_7$	C_{2v}	228	182		40	25.5	15	91
3	γ-$LiIO_3$	C_{2v}	187.2	180.3				13	64
4	$SbNbO_4$	C_{2v}	200	182	18	*	84	~5.8	90
5	Bi_2WO_6	C_{2v}	221	169	40			4	18
6	PbB_4O_7	C_{2v}	248.3	144			2.8	2.5-3.2	221
7	γ-Bi_2MoO_6	C_{2v}	215	175	25			3.1	32
8	β-$Gd_2(MoO_4)_3$	C_{2v}	227.2	173.1	20	4	4.1	2.98	37
9	$Tb_2(MoO_4)_3$	C_{2v}	225.6	174	19			2.9	73
10	$Sr_6Ti_2Nb_8O_{10}$	C_{2v}	257	186	9.8			1.79	603
11	$PbNb_2O_6$	C_{2v}	246	174	12			~1.78	4
12	Li_2GeO_3	C_{2v}	192.4	171.1		11.4-17		1.53	384
13	$Sr_2Nb_2O_7$	C_{2v}	243	184	6-9	*		~1.41	410,412
14	$Sr_6Ti_2Ta_8O_{10}$	C_{2v}	248	179	1.6			1.27	603
15	LiB_3O_5	C_{2v}	198.3	134.6			0.84	1.24	188
16	$NaNbO_3$ N	C_{2v}	241	187	10			~1	93
17	$NaNO_2$	C_{2v}	244.34	125.54	8			0.84	256
18	SrB_4O_7	C_{2v}	252.3	136.5			0.78	0.78	227
19	$LiGaO_2$	C_{2v}	194.9	183.5		8.6		0.686	55
20	$Rb_{0.33}(Nb_{0.33}W_{0.7})O_3$	C_{2v}	306	160.5	2			~0.5	192
21	$Cs_2Nb_4O_{11}$	C_{2v}	289	174				0.42	413
22	$AgIO_3$	C_{2v}	237	178				0.05	115
23	$Na_{13}Nb_{35}O_{94}$	C_{2v}	247.4	182.5					66
24	$KNbO_3$	C_{2v}	274.6	187.4					724
25	$K_4Nb_6O_{17}$	C_{2v}	250	170					88
26	$Cs(Ti_2Nb)O_7$	C_{2v}	297	174					170
27	$Ca_5TiNb_4O_{12}$	C_{2v}	230	181					611
28	$SrNb_6O_{16}$	C_{2v}	260.9	174.8					492
29	$Sr_5Nb_5O_{16}$	C_{2v}	242	165					505
30	$Tl_8Nb_{27.2}O_{72}$	C_{2v}	265	187					87
31	$Pb_{2.8}Nb_2O_{7.8}$	C_{2v}	216	180					5
32	$PbNb_2O_6$	C_{2v}	242	174					95
33	$Nb_2Zr_6O_{17}$	C_{2v}	203.2	191.9					722
34	$Nb(PO_4)O$	C_{2v}	187.1	143					89
35	$Bi_3Nb_{17}O_{47}$	C_{2v}	212	148					455
36	$(Bi_{0.99}Sb_{0.01})(Nb_{0.79}Ta_{0.21})O_4$	C_{2v}	218	182					408
37	$Ni_4Nb_2O_9$	C_{2v}	193.7	174.1					414
38	$Ni_4Nb_2O_9$	C_{2v}	193.7	174.1					92
39	T-Ta_2O_5	C_{2v}	184	184					158
40	$LaTaO_4$	C_{2v}	239	188					10
41	$(Mo_{0.93}Ta_{0.07})O_{14}$	C_{2v}	177	164					223
42	$Ta_{38}WO_{98}$	C_{2v}	192	164					510
43	$Ta_{30}W_2O_{81}$	C_{2v}	191	189					509

44	$Ta_{22}W_4O_{67}$	C_{2v}	192	164					83
45	$[Fe_{0.3}Mn_{0.7}]Ta(O_2)O_2$	C_{2v}	210	210					147
46	$Ce_{1-x}TaO_{4-\delta}$ 900° C	C_{2v}	243.3	193.6					592
47	B_2O_3	C_{2v}	137.3	137.3					349
48	LiB_3O_5	C_{2v}	198.6	134.81					575
49	CaB_2O_4 III	C_{2v}	227.5	132.8					366
50	Al_5BO_9	C_{2v}	184.6	135.9					228
51	γ-$Ce(BO_3)_4$ 7.5 GPa	C_{2v}	239.3	142.7					606
52	EuB_4O_7	C_{2v}	253.1	142.7					229
53	o-P_2O_5	C_{2v}	144.5	144.5					68
54	Li_3PO_4	C_{2v}	190.7	154.2					503
55	MgP_4O_{11}	C_{2v}	200.9	141.2					350
56	CaP_4O_{11}	C_{2v}	227.5	143.2					464
57	α-$Sr_2P_2O_7$	C_{2v}	249	147					476
58	$AlPO_4$	C_{2v}	154	131					474
59	$Zr(PO_3)_4$-II	C_{2v}	207.4	140.5					482
60	$(VO)_2P_2O_7$	C_{2v}	153.1	147.5					16
61	WPO_5	C_{2v}	183.7	146.2					19
62	β-UP_2O_7	C_{2v}	221.6	142.4					514
63	$Na_2W_2O_7$ (II)	C_{2v}	238.5	172					22
64	$Ag_8W_4O_{16}$	C_{2v}	220	173					80
65	$Bi_2W_2O_9$	C_{2v}	213	173					418
66	$Bi_{1.75}Sb_{0.25}WO_6$	C_{2v}	192	190					273
67	$Bi_{1.5}Sb_{0.5}WO_6$	C_{2v}	199	188					273
68	$Bi_{1.25}Sb_{0.75}WO_6$	C_{2v}	195	189					273
69	$BiSbWO_6$	C_{2v}	193	186					273
70	$Bi_{0.75}Sb_{1.25}WO_6$	C_{2v}	186	183					273
71	$W_{0.4}Mo_{0.6}O_3$	C_{2v}	152.2	152.2					173
72	γ-Mo_4O_{11}	C_{2v}	175.6	174					102
73	$Cu_3Mo_2O_9$	C_{2v}	179	169					72
74	$In_{11}Mo_{40}O_{62}$	C_{2v}	214.7	189.1					35
75	LT-$ZrMo_2O_8$	C_{2v}	205.45	164.25					535
76	$Sb_2Mo_{10}O_{31}$	C_{2v}	185	166					125
77	$MoO_2(SO_4)$ II	C_{2v}	165.0	143.7					419
78	$LaMo_{7.7}O_{14}$	C_{2v}	249.1	198.7					33
79	$PrMo_{7.6}O_{14}$	C_{2v}	240.5	193.3					421
80	$NdMo_8O_{14}$	C_{2v}	236.2	195.1					36
81	$NdMo_{7.7}O_{14}$	C_{2v}	239.1	193.1					236
82	$SmMo_8O_{14}$	C_{2v}	231.6	194.9					36
83	LiV_2O_5	C_{2v}	190	163					43
84	Li_3VO_4	C_{2v}	196.1	171.4					238
85	α'-NaV_2O_5	C_{2v}	243	153					240
86	α $Cu_2V_2O_7$	C_{2v}	188.0	173.6					275
87	$MgVO_3$	C_{2v}	194.7	165					78
88	$Mg_{0.01}V_2O_5$	C_{2v}	250	157.8					79
89	Sr_2VO_4	C_{2v}	231	171					48
90	α-ZnV_3O_8	C_{2v}	191	159					276
91	β-Tl_3VO_4	C_{2v}	250.2	167.9					313
92	$Bi_2VO_{5.5}$	C_{2v}	189	176					184
93	$Bi_2V_{0.8}Ge_{0.2}O_{5.4}$	C_{2v}	222	142					279
94	$Bi_2V_{0.4}Ge_{0.6}O_{5.2}$	C_{2v}	226	180					279
95	$Te_2V_2O_9$	C_{2v}	184.3	163.6					291
96	ThV_2O_7	C_{2v}	226	156					47
97	$Li_2(Si_{0.25}Ge_{0.75})_2O_5$	C_{2v}	189.8	161.1					424
98	Na_2GeO_3	C_{2v}	229.2	171.2					384
99	$Li_2Si_2O_5$	C_{2v}	192.7	156.5					282
100	Li_2SiO_3	C_{2v}	193.2	159.1					384
101	Na_2SiO_3	C_{2v}	228.2	159.2					384

102	ε-$Na_2Si_2O_5$	C_{2v}	233.3	157.1					53
103	$Cs[AlSi_5O_{12}]$	C_{2v}	331.0	159.8					487
104	$MgSiO_3$ 1100C	C_{2v}	206	150					386
105	$Gd_2Si_2O_7$	C_{2v}	227	158.1					53
106	$K_{0.8}(Mg_{x/2}Ti_{2-x/2})O_4$	C_{2v}	269	175					169
107	$K_{0.8}(Zn_{x/2}Ti_{2-x/2})O_4$	C_{2v}	269	175					169
108	α'-Ba_2TiO_4	C_{2v}	254	179		>0			355
109	$Fe_{0.13}Ti_{1.81}O_{1.92}$	C_{2v}	188	188					111
110	$La_2Ti_2O_7$ 1173K	C_{2v}	243	176					391
111	$NaAlO_2$	C_{2v}	231.2	174.1					56
112	β-$AgAlO_2$	C_{2v}	235	175					582
113	MgP_4O_{11}	C_{2v}	200.9	141.2					350
114	$Ca_5Al_6O_{14}$	C_{2v}	228.3	172.7					317
115	$Ca_2Fe_{1.43}Al_{0.57}O_5$	C_{2v}	244.8	179.4					324
116	$Ca_2Fe_{1.28}Al_{0.72}O_5$	C_{2v}	244.8	178.8					324
117	α-$NaGaO_2$	C_{2v}	216	175					215
118	$CaGa_2O_4$	C_{2v}	218	179					519
119	$Ca_3Ga_4O_9$	C_{2v}	225.8	179.5					199
120	$Ca_5Ga_6O_{14}$	C_{2v}	226	178					356
121	$GaFeO_3$	C_{2v}	186.6	181.3					329
122	$NdGaO_3$	C_{2v}	213	174					434
123	Gd_3GaO_6	C_{2v}	208	183					249
124	Ca_3GeO_5	C_{2v}	203	177					200
125	α-Sb_2O_4	C_{2v}	185.7	185.7					520
126	$K_3Sb_5O_{14}$	C_{2v}	247	187					396
127	$Pb_2Sb_2O_7$	C_{2v}	241.1	191.0					357
128	$Sb_6O_7(SO_4)_2$	C_{2v}	199.4	146.0					541
129	SO_2	C_{2v}	143	143					721
130	S_3O_9	C_{2v}	136.5	136.5					721
131	S_3O_9	C_{2v}	132.4	132.4					721
132	$CdSeO_4$	C_{2v}	222.9	161.7					397
133	β-Hg_2SeO_3	C_{2v}	224	163					543
134	$Pb_3O_2(SeO_3)$	C_{2v}	217	166					584
135	Bi_2SeO_5	C_{2v}	206.4	167.9					398
136	α'-$Na_2S_2O_3$	C_{2v}	224.7	146.6					289
137	$CdSO_4$	C_{2v}	211.5	144					210
138	$HgSO_4$	C_{2v}	211.8	148.6					210
139	$Te_2O_3(SO_4)$	C_{2v}	190.7	145.5					521
140	$Te_2V_2O_9$	C_{2v}	184.3	163.6					331
141	$UTeO_5$	C_{2v}	188	179				593	606
142	α-KNO_3	C_{2v}	281.4	123.5					565
143	$Bi_2O_2CO_3$	C_{2v}	221	128					450
144	U_3O_8	C_{2v}	207	207					585
145	CsCuO	C_{2v}	297.7	186.3					293
146	$In_2Cu_2O_5$	C_{2v}	207.4	188.4					264
147	$Sc_2Cu_2O_5$	C_{2v}	207.7	191.1					266
148	$Y_2Cu_2O_5$	C_{2v}	218	191.9					263
149	$Ho_2Cu_2O_5$	C_{2v}	210	187					448
150	$Lu_2Cu_2O_5$	C_{2v}	214.4	188.8					266
151	$Sr_2In_2O_5$	C_{2v}	250	197					213
152	β-$NaFeO_2$ 298K	C_{2v}	231.2	184					415
	β-$NaFeO_2$ 773K	C_{2v}	228.8	183.0					415
	β-$NaFeO_2$ 1023K	C_{2v}	235	185.2					415
	β-$NaFeO_2$ 1173K	C_{2v}	238	183.5					415
	β-$NaFeO_2$ 1223K	C_{2v}	239	182.9					415
153	$Sr_2Fe_2O_5$	C_{2v}	193.5	182					161-2
154	$Sr_4Fe_6O_{13}$	C_{2v}	240	179					334
155	$Na_2[NiO_2]$	C_{2v}	229.8	189.1					217

156	$Ca_3Mn_2O_7$	C_{2v}	229.3	185.7					298
157	$Pb_3Mn_7O_{15}$	C_{2v}	227	183					403
158	$Co_2Mn_3O_8$	C_{2v}	205	181					337
159	CrO_3	C_{2v}	157.8	157.8					213
160	$Bi_6Cr_2O_{15}$	C_{2v}	208.9	162.9					132
161	Rb_2TbO_3	C_{2v}	280.8	205.8					261
162	Cs_2PrO_3	C_{2v}	298.6	206.3					261
163	$Be_4Pr_9O_{20}$	C_{2v}	230.5	157.6					262
164	$LaYbO_3$	C_{2v}	218	211					216
165	Rb_2PbO_3	C_{2v}	260.7	212.5					345
166	Cs_2PbO_3	C_{2v}	303	207.9					344
167	$PbZrO_3$ 220kV/cm	C_{2v}	283	204					361
168	Ba $Ir_{1.45}Ti_{1.55}O_{10}$	C_{2v}	267	194					719
169	$SbSb_{0.5}Ta_{0.5}O_4$	C_{2v}	195	186					723
170	$Na_2[NiO_2]$	C_{2v}	229.8	189.1					217
171	Sm_3OsO_7,	C_{2v}	238.1	195.7					690
172	Eu_3OsO_7	C_{2v}	237.5	195					690
173	Gd_3OsO_7	C_{2v}	236	195.2					690
174	Sm_3RuO_7	C_{2v}	237.3	194.7					689
175	Eu_3RuO_7	C_{2v}	237.2	194.6					689

1	$TeSeO_4$	C_s	190.2	167.8				~8	65
2	$Bi_4Ti_3O_{12}$	C_s	219	173	30			~5.6	106
3	$Na_{0.2}K_{0.8}NbO_3$	C_s	251.4	186.1					493.506
4	$Na_{0.35}K_{0.65}NbO_3$	C_s	233.1	185.3					493
5	$Na_{0.90}K_{0.10}NbO_3$	C_s	237.3	184.4					528
6	$Na_{0.98}K_{0.02}NbO_3$	C_s	234	185.4					528
7	$Na_{0.2}K_{0.8}NbO_3$	C_s	251.4	186.1					493,541
8	$Se_4Nb_2O_{13}$	C_s	175	156					407
9	$NdTaO_4$	C_s	235	187					365
10	$Zn_3(BO_3)_2$	C_s	186	136					595
11	YBO_3	C_s	232.7	149.4					591
12	$Y_{17.33}(BO_3)(B_2O_5)O_{16}$	C_s	205	136					130
13	$LiPO_3$	C_s	187.9	144.6					501
14	$AlPO_4$	C_s	172.8	151.6					284
15	C-$Ga(PO_3)_3$	C_s	192.4	148.6					310
16	γ-$Ca(PO_3)_2$	C_s	231.70	146.66					659
17	$In(PO_3)_3$	C_s	211.7	144.4					351
18	$In(PO_3)_3$ – C’	C_s	204	135					500
19	$Sc(PO_3)_3$	C_s	205.5	147.4					309
20	$Ti(PO_3)_3$	C_s	199.3	147.2					283
21	$Zr(PO_3)_4$-I	C_s	201	139					479
22	$V(PO_3)_3$	C_s	194.9	146.1					466
23	$Cr(PO_3)_3$	C_s	186	142					308
24	$Mo(PO_3)_3$	C_s	205.2	147.7					133
25	$Ni_{1.184}Mn_{0.816}P_2O_7$	C_s	210	144					272
26	RhP_3O_9	C_s	197.8	147.1					463
27	Nd_3PO_7	C_s	222	141					472
28	ErP_3O_9	C_s	216	140					70
29	$(UO_2)_2P_6O_{17}$	C_s	170	136					467
30	ε-WO_3	C_s	170	170					21
31	$Cs_6W_{11}O_{36}$	C_s	294	157					118
32	V_6O_{13} 95K	C_s	165.01	165.01					556

33	$Cu_{1.82}V_4O_{11}$	C_s	178	160					175
34	CuV_2O_5 β	C_s	179	147					241
35	CuV_2O_5 ε	C_s	194	162					241
36	$Cu_{2.33}V_4O_{11}$	C_s	175.2	161.4					312
37	β-$AgVO_3$	C_s	222	161					50
38	$Ag_{2.95}V_4O_{12}$	C_s	217	143					378
39	$Ag_{1.43}V_4O_{10}$	C_s	245	164					50
40	$K_2Si_2O_5$	C_s	257.6	154.0					282
41	$Na_{17}Al_5O_{16}$	C_s	222	170					318
42	$Cs_8Sb_{22}O_{37}$	C_s	300	184					61
43	$K_2S_4O_6$	C_s	261	143.4					126
44	$As_2O(SO_4)_2$	C_s	172	137					537
45	$Te(S_2O_7)_2$	C_s	196	137					330
46	Li_5BiO_5	C_s	193	184					340
47	$Os_3Sn_{15}O_{14}$	C_s	253.11	202.6					443
48	$Na_4[FeO_3]$	C_s	220	186					489
49	$Sr_3La_4O_9$	C_s	237.1	237.1					265
50	$Sr_3(La, Sm)_4O_9$	C_s	230	230					142
51	$Sr_3Pr_4O_9$	C_s	230	230					142
52	$Sr_3Nd_4O_9$	C_s	230.8	230.5					294
53	Li_2ZrO_3	C_s	203	190					259
54	$Li_2Ge_2O_5$	C_s	192.5	167.4					720

1	α-$LiIO_3$	C_6	208.1	180.8	0	45.3	9.8	13.7	63
	$Al(IO_3)_3$	C_6	189.4	178.3				13	176
2	Tl_3PO_4	C_6	252.9	153.6				0.4	369
3	$BaGa_2O_4$	C_6	258.7	177.3	0.1			0.12	60, 248
4	$BaAl_2O_4$	C_6	269	170	0.1			0.106	57
5	SiP_2O_7	C_6	170	148					15
6	$K_{0.26}WO_3$	C_6	293	181.6					120
7	$K_{0.13}V_{0.13}Mo_{0.87}O_3$	C_6	289	168					235
8	$TlAsO_4$	C_6	253	169					485
9	$Ba(ZnGe)O_4$	C_6	255	168					171
10	$(Na_{0.9}Ca_{3.2}REE_{5.3})(Si_{4.3}P_{1.7})O$	C_6	232.6	160.3					353
11	$(Na_{1.0}Ca_{1.4}REE_{7.0})(Si_{5.7}P_{0.3})O$	C_6	238.4	161.6					353
12	$(Ca_{3.5}REE_{5.9})(Si_{5.8}P_{0.2})O$	C_6	238.4	162.0					353
13	$BaAl_{1.88}Mn_{0.12}O_4$	C_6	266.0	162.7					432
14	$BaFe_{1.5}Al_{0.5}O_4$	C_6	261.1	170.1					322
15	$BaSrGa_4O_8$	C_6	247.5	173					562
16	FeI_3O_9	C_6	198	179					250
1	$TlBO_2$	C_4	248	136				>0	599
2	β-$Ca_2P_2O_7$	C_4	231.8	148.0					96
3	β-$Ca_2P_2O_7$	C_4	230.1	148.7					416
4	$Rb_2W_{32}O_{107}$	C_4	294	166					121
5	$Bi_{14}W_4O_{27}$	C_4	187	175.8					101
6	β-$Sr_2V_2O_7$	C_4	247	163					44
7	$Sm_2Si_2O_7$	C_4	227.1	157.6					388
8	$(Ba_{1.14}K_{0.05})\Sigma_{1.19}(Ti_{5.81}V_{1.34}Cr_{0.36}Fe_{0.20}Mn_{0.16}Al_{0.09})\Sigma_{7.98}O_{16}$	C_4	267.1	189.8					246
9	$Ba_{1.12}Ti_8O_{16}$	C_4	267.1	189.2					137
10	$CuBi_2O_4$	C_4	218	192					339
1	$Co(IO_3)_2$	C_3	209	179	21.7			0.05	113

2	$LaNb_7O_{19}$	C_3	245.8	184.2					168
3	Li_7TaO_6	C_3	199.9	190.8					529
4	$(Ca_{1.89}Sm_{0.16})(Ta_{1.86}Ti_{0.10})O_7$	C_3	213	190					546
5	B_2O_3	C_3	133	133					594
6	$GaAsO_4$ 6GPa 1273K	C_3	174	153					702
7	$BaSi_4O_9$ 4GPa, 1000C	C_3	273.5	160.1					694
8	$Na_4Ti_5O_{12}$	C_3	214	178					431
9	$Ca_3Nb_2O_8$	C_3	228.1	181.9					527
10	$Sr_7Al_{12}O_{25}$	C_3	253	166					321
11	$RbNO_3$ IV 298K	C_3	295	121					488
12	$RbNO_3$ IV 403K	C_3	303	115					488
13	$Be_4O(NO_3)_6$	C_3	159	117					400
14	$HgCr_2O_7$	C_3	198	157.4					685
15	$Ba_3Y_2Yb_2O_9$	C_3	242.2	216.9					296
16	$Ba_3Dy_4O_9$	C_3	259.6	219.0					296
17	$Ba_3Ho_4O_9$	C_3	245.5	212.3					347
18	$Ba_3Er_4O_9$	C_3	263.1	216					296
19	$Ba_3Tm_4O_9$	C_3	259.04	215.86					347
20	$Ba_3Yb_4O_9$	C_3	260	214					346
21	β-$MnSb_2O_6$	C_3	211.5	196.4					337
1	$Ca_2Nb_2O_7$	C_2	230.5	179.4				15	494,507
2	$Hg(IO_3)_2$	C_2	223	180				13.7	571
3	β-$Hg(IO_3)$	C_2	221.5	181					570
4	$Mg(IO_3)_2$	C_2	204	175				13.7	699
5	$Zn(IO_3)_2$	C_2	201	171				13.7	699
6	Tl_2MoO_4	C_2	256	170				~5.5	148
7	γ-$PbGe_4O_9$	C_2	243	163				~3.6	244
8	BiB_3O_6	C_2	208.7	134				3.2	230
9	$La_2Ti_2O_7$	C_2	238	177	5-9	*		1.1	2, 107
10	$Nd_2Ti_2O_7$	C_2	240	182	5			~0.5-1	108
11	Pb_3GeO_5	C_2	215.9	172.7	0.2			0.13	385
	Pb_3GeO_5	C_2	208	172					628
	Pb_3GeO_5 500C	C_2	243	173					630
12	$SrAl_2O_4$	C_2	251	172.9	1			0.1	320
13	α-$Cu(IO_3)$	C_2	195.8	180.4				0.04	114
14	$Mn(IO_3)_2$	C_2	200	178				>0	699
15	$Co(IO_3)_2$	C_2	200	176				>0	699
16	Nb_2O_5	C_2	173	168					413
17	$Cu_{0.5}Nb_{1.5}O_{3.7}$	C_2	187.7	187.7					268
19	$GaNbO_4$	C_2	189.1	179.7					86
20	$TiNb_{24}O_{62}$	C_2	172	165					411
21	$WNb_{12}O_{33}$	C_2	191	170					6
22	$W_4Nb_{26}O_{77}$	C_2	185	182					410
23	$W_5Nb_{16}O_{55}$	C_2	191	176					6
24	UNb_6O_{16}	C_2	227.7	179.5					267
25	H-Ta_2O_5	C_2	185.3	170.9					508
26	Z-Ta_2O_5	C_2	171	171					226
19	Li_3TaO_4	C_2	180	175					532
27	$Ca_2Ta_2O_7$	C_2	216	190					11
28	$Al_{0.33}Ta_{15}W_{0.66}O_{40}$	C_2	193	166					222
29	$Ce_6Ta_6O_{25}$	C_2	218.1	189					530
30	$Bi_2B_8O_{15}$	C_2	208.4	124					270
31	$Bi_2B_8O_{15}$ α	C_2	205.73	134.18					270
32	$CuCdP_2O_7$	C_2	203	143					270
33	$Ca_4(PO_4)_2O$	C_2	213.6	151.1					534
34	$Sr_2P_6O_{17}$	C_2	243.3	140.4					478
35	$(CdCu)P_2O_7$	C_2	203	143					191/522

36	$P_4W_{10}O_{38}$	C_2	179	148					82
37	α-$Pb_3P_{0.3}V_{1.7}O_8$ 85K	C_2	241.1	146.1					484
38	VP_2O_7	C_2	186.2	146.3					311
39	$W_2O_3(PO_4)_2$	C_2	161	137					481
40	$Al_2(WO_4)_3$	C_2	171.8	171.2					17
41	V_2MoO_8	C_2	164.4	164.4					178
42	$(Mo_{0.3}V_{0.7})O_5$	C_2	165.9	165.9					237
43	$La_6Mo_8O_{33}$	C_2	229	169					
44	$Fe_2(MoO_4)_3$	C_2	190	163					42
45	α- $Nd_2(MoO_4)_3$	C_2	249.2	180					136
46	$Na_{0.9}Mo_6O_{17}$	C_2	246.8	170.8					38
47	BaV_3O_8	C_2	267.5	161.9					49
48	$Pb_3V_2O_8$ 85K	C_2	239.1	158.4					484
49	α-$Bi_4V_2O_{10}$	C_2	207	160??					557
50	CoV_2O_6	C_2	198	168					104
51	γ-$PbGe_4O_9$	C_2	243	163					244
52	Pb_2SiO_4	C_2	215	164					389
53	$Cs_{0.35}Al_{0.35}Si_{2.65}O_6$	C_2	324.6	159.4					392
54	α-$SrSiO_3$	C_2	239	153					316
55	$BaTi_2O_5$	C_2	267.3	171					559
56	$Pr_2Ti_2O_7$	C_2	228	178					608
57	$Cd_3Se_3O_{10}$	C_2	213.2	162					358
58	$Hg_3Se_3O_{10}$	C_2	219.7	161.3					288
59	$Hg_2(NO_3)_2$	C_2	218.1	119.4					568
60	β-UO_3	C_2	169	169					123
61	$K_2U_2O_7$	C_2	249	185					526
62	$Ca_4Fe_9O_{17}$	C_2	232.2	183.7					295
63	$CaFe_4O_7$	C_2	210.4	169.1					336
64	La_2NiO_4	C_2	238	177					163
65	$BiMnO_3$	C_2	211	178					257
66	Bi_2UO_6	C_2	219	191					687
67	Te_2O_5	C_2	189.2	184.8					675
1	KIO_3	C_1	272	172.1				15	3
2	$(NbO)_2P_4O_{13}$	C_1	163.5	138.1					415
3	$Bi_7Ta_3O_{18}$	C_1	201.9	187.3					531
4	$Cd_{1.25}Ca_{0.75}P_2O_7$	C_1	235.7	149.3					164
5	$Cd_2B_2O_5$	C_1	214	130					573
6	β-$Tl_2B_4O_7$	C_1	245	135					139
7	L-$SmBO_3$	C_1	225	130					576
8	$AlPO_4$	C_1	172.6	151.5					284
9	CeP_5O_{14}	C_1	238.3	145.4					98
10	UP_4O_{12}	C_1	214	132					480
11	Sb_2WO_6	C_1	193.1	173.9					20
12	$V_{0.95}Mo_{0.97}O_5$	C_1	179	151					376
13	$CuVO_3$ (I)	C_1	198.4	177.6					177
14	$As_2V_4O_{13}$	C_1	166.1	163.8					239
15	$La_2Ge_2O_7$	C_1	233.7	171.0					179
16	$Gd_2Ge_2O_7$	C_1	217	168					383
17	$PbAl_2O_4$	C_1	226	174					319
18	$PbGa_2O_4$	C_1	228	181					319
19	$Ga_2Te_4O_{11}$	C_1	184.4	183.5					328
20	$Sb_2(S_2O_7)_3$	C_1	202.9	140.3					542
21	$Sr_3Te_4O_{11}$	C_1	237	178					290

Table S1.Continued. Real binary acentric binary oxide (non - polarl piezoelectric).

	Chemical	Sym-	L, pm	L, pm	P_s	d	r	$\chi^{(2)}$	Ref
№	formula	metry	M-O	E-O	μC/cm^2	pC/N	pm/V	pm/V	
1	1	2	3	6	7	8	9	10	12
1	$Bi_{12}Si_{0.87}O_{20}$	T	206.4	164.7	0	37.8	4.2	2.05	138
2	$Bi_{12}GeO_{12}$	T	206.9	175.8	0	37.6	3.4	1.8	193
3	$Bi_{12}TiO_{20}$	T	199	172	0			~1.8	146
4	$NaClO_3$	T	241.9	148.5	0	2.7		0.4	119
5	$NaBrO_3$	T	241	164.8	0			0.28	119
6	$Bi_{12}GeO_{12}$	T	207.2	176.4					486
7	$LiCuNb_3O_9$	T	201.8	191.7					496
8	β-$SnWO_4$	T	221.4	174.6					122
9	ZrW_2O_8	T	204.5	170.7					234
10	ZrW_2O_8	T	205.1	171.3					555
11	β-$La_2W_{1.7}Mo_{0.3}O_9$	T	253.3	178.5					515
12	β-$La_2Mo_2O_9$	T	249.6	173					516
13	$Bi_{12}Ti_{0.90}O_{19.80}$	T	207.07	182.9					486
14	$Nd_4Re_{5.5}O_{19}$	T	244.52	188.0					285
15	$K_3[SbO_3]$	T	265.9	192.3					287
16	$Cs_3[SbO_3]$	T	288.8	192.8					287
17	α- Bi_2O_3	T	222	222					138
18	γ-Bi_2O_3	T	204.5	198.0					486
19	$Bi_{12}(Bi^{III}_{0.5}Tl^{III}_{0.5})O_{19.50}$	T	252.7	206.45					442
20	Bi_3ReO_8	T	212.4	172.8					580
21	$K_9Ni_2O_7$	T	262.2	180.4					218
22	$K_2Pb_2O_3$	T	280	218					447
23	k-$CeZrO_4$	T	204	173					292
1	$(Ca_{0.94}Na_{0.06})(Ta_{3.86}Nb_{0.13})O_{10.97}$	D_6	249.2	195.9					172
2	$CaTa_4O_{11}$	D_6	246	196					9
3	$Ca(Ta_{2.82}Nb_{1.18})O_{11}$	D_6	246.5	195.7					624
4	$SrTa_4O_{11}$	D_6	251.8	198					225
5	$AlPO_4$ 25C	D_6	172.8	151.8					499
	$AlPO_4$ 500C	D_6	166	155					499
	$AlPO_4$ 530C	D_6	168	149					499
	$AlPO_4$ 550C	D_6	161	148					499
	$AlPO_4$ 580C	D_6	162	143					499
	β-$AlPO_4$ 585-631C	D_6	171.0	149.0					513
6	$CePO_4$	D_6	234	156					470
7	$Ge_{0.24}WO_3$	D_6	225.3	190.5					24
8	$LiAlSi_2O_6$ III	D_6	206.8	164.1					429
9	$LiAlSi_2O_6$ III	D_6	193.3	163.3					387
10	$K_{0.92}Ba_{0.25}Fe_{1.25}Ge_{0.75}O_4$	D_6	286	177.7					597
11	β- $BaGa_2O_4$	D_6	287.6	182					327
12	γ-$CaSO_4$	D_6	238.5	147.7					563
1	β-TeO_2	D_4	188	188	0			0.59	116
2	CsB_9O_{14}	D_4	314	123					271
3	BaB_8O_{13}	D_4	269.4	112.2					589
4	$K_5V_3O_{10}$	D_4	265.9	161.5					277
5	$Eu_2Ge_2O_7$	D_4	222	176					613
6	$Tb_2Ge_2O_7$	D_4	227.4	173.2					612
7	$Er_2Ge_2O_7$	D_4	219.5	173.3					382
8	$LuGe_2O_7$	D_4	214	169					427
9	SiO_2	D_4	160.1	160.1					426
10	$LiAlSi_2O_6$ II	D_4	226.9	163.7					428
11	Mg_2TiO_4 774K	D_4	198.1	191.2					600
12	Mn_2TiO_4	D_4	203	193					605

13	γ-$LiAlO_2$	D_4	194.8	175.5					323
14	$Sb_2O(SO_4)_2$	D_4	192.1	144.0					540
15	$Bi_8O_{11}(SO_4)$	D_4	194	144					596
16	Li_2TeO_4	D_4	202	183.3					252
17	$K_3[CuO_2]$	D_4	258.7	178.0					444
18	γ-Fe_2O_3	D_4	190	186					258
19	γ-$NaFeO_2$ 1273K	D_4	236.2	180.7					402
	γ-$NaFeO_2$ 1323K	D_4	237.4	182.0					402
20	Na_2HgO_2	D_4	235	197					219
1	$BAsO_4$	D_3	157	144	0			1.54	721
2	$AlAsO_4$	D_3	174.1	166.6	0			1.53	52
3	$FePO_4$ 294K	D_3	179.3	146.9	0			1.52	373
4	$GaAsO_4$	D_3	182.6	166.5	0			1.4	51
5	$GaPO_4$	D_3	180.7	152.3	0			0.5	97
6	$GaPO_4$ 20C	D_3	180.7	152.9	0			0.5	437
7	$AlPO_4$	D_3	173.2	152.0	0			0.41	52
8	SiO_2 10^{-4}Gpa	D_3	161.0	161.0	0	2.3	5.86*	0.4	390
9	$SrGe_4O_9$	D_3	260.1	172.6	0			0.18	245
10	$BaGe_4O_9$	D_3	271.3	171.2	0			0.13	145
11	GeO_2	D_3	173.41	173.41	0	~30			243
12	Ag_3BO_3	D_3	212.5	136.3					306
13	$GdBO_3$	D_3	230	136					587
14	α-$AlPO_4$ 25C	D_3	173.02	152.1					587
	α-$AlPO_4$ 92C	D_3	172.9	151.8					587
	α-$AlPO_4$ 183C	D_3	172.7	151.8					587
	α-$AlPO_4$ 275C	D_3	172.6	151.6					587
	α-$AlPO_4$ 366C	D_3	172.4	151.1					587
	α-$AlPO_4$ 458C	D_3	172.0	150.7					587
	α-$AlPO_4$ 486C	D_3	171.9	150.5					587
	α-$AlPO_4$ 523C	D_3	172.2	150.7					587
	$AlPO_4$ 568C	D_3	171.8	150.4					587
	$GaPO_4$ 500C	D_3	181.2	152.9					437
15	$GaPO_4$ 750C	D_3	181.0	152.3					437
16	$FePO_4$ 20K	D_3	182.1	151.7					373
17	$CaAs_2O_6$	D_3	230	186					379
	$AlAsO_4$ 20C	D_3	174.3	166.6					380
	$AlAsO_4$ 500C	D_3	173.4	165.9					380
	$AlAsO_4$ 750C	D_3	172.6	164.9					380
	$AlAsO_4$ 2.99GPa	D_3	173.4	166.5					381
	$AlAsO_4$ 4.87GPa	D_3	173.5	166.8					381
18	SiO_2 10.2Gpa	D_3	160.66	160.66					390
19	$La_3Ga_5SiO_{14}$	D_3	235.4	172.0					435
20	$Na_{2.54}Ca_{1.73}Ge_3O_9$	D_3	224	164.6					280
21	$La_3Ga_5GeO_{14}$	D_3	238.0	179.4					278
22	$MnSb_2O_6$	D_3	209	191					62
23	$Mn_2Sb_2O_7$	D_3	204	167					62
24	$Hg_3(SO_4)O_2$	D_3	207.0	145.1					615
25	$Hg_3(CrO_4)O_2$	D_3	207.5	162.9					566
26	Tl_2TeO_6	D_3	207	195					359
27	Yb_2TeO_6	D_3	223	189					151
28	$BaZnO_2$	D_3	264	196					154
29	α-$Ca_3Fe_{14.82}O_{25}$	D_3	193	179					127
30	γ- $Ca_3Fe_{14.82}O_{25}$	D_3	217.4	188.7					128
31	$BaNi_{5/6}O_{5/2}$	D_3	251	187					572
32	$SrHgO_2$	D_3	242.2	194.9					514
1	Y_3TaO_7	D_2	214	203				2.2	140

2	β-RbB_3O_5	D_2	284	134				1.5	305
3	CsB_3O_5	D_2	303	135	0			1.15	13
4	TlB_3O_5	D_2	266.2	135				1.15	13
5	$Rb_2Nb_4O_{11}$	D_2	280.4?	199.2?				0.54	453
6	$Cd(IO_3)_2$	D_2	226.2	181.1				0.05	117
7	$AlPO_4$	D_2	178.0	151.1					14
8	$BaNb_2O_6$	D_2	266	188					
9	$Cs_{0.7}(Nb_{2.7}W_{2.3})O_{14}$	D_2	304.4	169.0					457
11	$Sr_{0.97}NbO_3$	D_2	269.0	196					491
12	$TlNb_{3.09}O_{8.22}$	D_2	274	192					
13	$Te_3Nb_2O_{11}$	D_2	184	180					116
14	$Nb_8W_9O_{47}$	D_2	188	148					8
15	$Nb_7W_{10}O_{47}$	D_2	173.9	171.1					1
16	$Nb_{16}W_{18}O_{94}$	D_2	175	175					409
17	$Th_2Ta_2O_9$	D_2	218.4	184.4					512
18	B_2O_3	D_2	135.6	135.6					578
19	α-RbB_3O_5	D_2	257	131					602
20	α-CsB_9O_{14}	D_2	310.8	130.2					579
21	$Na_4P_2O_7$	D_2	227.2	151.2					504
22	BeP_2O_6 III (h)	D_2	155	145					371
23	$Ba(PO_3)_2$	D_2	273	143					475
24	β-$Cd(PO_3)_2$	D_2	218.8	146.9					468
25	$AlPO_4$	D_2	168	156					469
26	$GaPO_4$	D_2	173	156					469
27	$Ti_5O_4(PO_4)_4$	D_2	172.1	150.5					283
28	$AsPO_5$	D_2	172	149					465
29	Sb_5PO_{10}	D_2	192	149					189
30	$P_4W_8O_{32}$	D_2	181	149					477
31	$P_4W_{12}O_{44}$	D_2	180	152					29
32	$P_4W_{16}O_{56}$	D_2	181	152					29
33	LaP_3O_9	D_2	241.5	147.4					69
34	NdP_3O_9	D_2	233	149					100
35	PrP_3O_9	D_2	238	148.2					548
36	$Cs_{0.06}WO_3$	D_2	324.5	168.8					81
37	V-Y_2WO_6	D_2	223	184					25
38	V-Gd_2WO_6	D_2	226	186					26
39	δ-Nd_2WO_6	D_2	229	187					27
40	ε-Y_2WO_6	D_2	212	176					124
41	V-Er_2WO_6	D_2	222	184					129
42	$Cu_{3.85}Mo_3O_{12}$	D_2	192.8	166					75
43	$Zn_{3.77}V_{1.54}Mo_{1.46}O_{12}$	D_2	200	170					274
44	La_3MoO_7	D_2	232.5	186.1					30
45	Pr_3MoO_7	D_2	228.0	185.4					420
46	U_2MoO_8	D_2	206	166					41
47	$Cu_4V_{2.15}O_{9.38}$	D_2	201	163					156
48	$Zn_{3.77}V_{1.54}Mo_{1.46}O_{12}$	D_2	200	170					314
49	PbV_2O_6 III	D_2	253	149					377
50	γ-$Bi_4V_2O_{10}$	D_2	224	156					45
51	$V_{0.95}Cr_{0.05}O_2$	D_2	168	168					141
52	Y_2GdSbO_7	D_2	208	198					135
53	$SbAsO_5$	D_2	180	158					465
54	$BaSiO_3$ (h)	D_2	262.4	158.7					538
55	$Nd_2Si_2O_7$	D_2	237	159					54
56	La_3ReO_8	D_2	231.5	180.2					181
57	β-Li_5GaO_4	D_2	185	184					436
58	$Bi_{12}GaO_{20}$	D_2	204.9	172					146
59	γ-$CaSO_4$	D_2	258.8	148.2					160
60	Tl_2SeO_4	D_2	264.1	164.2					583

61	La_2TeO_6	D_2	240.1	189					151
62	Gd_2TeO_6	D_2	226	188.9					564
63	$AgNO_3$	D_2	238.4	118					332
64	$Ba(NO_2)_2$	D_2	277.5	123.6					399
65	UO_3	D_2	180	180					446
66	Rb_2SnO_2	D_2	277	206					155
67	$NaOH{\cdot}4H_2O$	D_2	233.6	177					150
68	Rb_3AgO_2	D_2	265	200					343,360
69	BeP_2O_6 III (h)	D_2	155	145					369

Table S1.Continued. Real binary acentric binary oxide (non-polarl piezoelectric).

	Chemical	Sym-	L, pm	L, pm	P_s	d	r	$\chi^{(2)}$	Ref
№	formula	metry	M-O	E-O	$\mu C/cm^2$	pC/N	pm/V	pm/V	
1	1	2	3	6	7	8	9	10	12
1	γ - $LiBO_2$	D_{2d}	195.7	148.3				6.3	12
2	$Gd_2(MoO_4)_3$	D_{2d}	229.3	173.2	0				37
3	$(Nd_{0.023}Gd_{0.977})_2(MoO_4)_3$	D_{2d}	225.8	171.5					536
4	Rb_3NbO_8	D_{2d}	280.4	199.2					453
5	$FeNb_2O_6$	D_{2d}	199.0	196.4					76
6	$Rb_3[Ta(O_2)_4]$	D_{2d}	281.2	198.9					599
7	CuB_2O_4	D_{2d}	191.3	146.2					367
8	PdB_2O_4	D_{2d}	198	144.6					304
9	Na_3PO_4	D_{2d}	222	148					550
10	$Tl_4P_4O_{12}$	D_{2d}	270	144					498
11	β-$VO(PO_3)_2$	D_{2d}	192	152					483
12	W_5O_{14}	D_{2d}	195	195					174
13	$Na_{0.33}WO_3$	D_{2d}	221	179					28
14	La_2MoO_6	D_{2d}	225	177					74
15	β-$Cs_2V_4O_9$	D_{2d}	313.3	161.9					165
16	$Mg_3As_2O_8$	D_{2d}	200.7	167.5					77
17	$Co_3(AsO_4)_2$	D_{2d}	201.9	168.6					105
18	$Cd_2Ge_7O_{16}$	D_{2d}	226	172					197
19	$Al_4Ge_3O_{12}$	D_{2d}	188	175					394
20	Zr_3GeO_8	D_{2d}	203.9	180.3					315
21	Zn_2SiO_4 – II	D_{2d}	198	162					517
22	$CaYAl_3O_7$	D_{2d}	238.3	172.4					433
	$CaYAl_3O_7$:Cr	D_{2d}	238.6	172.8					433
	$CaYAl_3O_7$:Cr,B	D_{2d}	237.9	172.8					433
	$CaYAl_3O_7$:Mg,Cr	D_{2d}	238.6	171.2					433
	$CaYAl_3O_7$:Ca,Cr	D_{2d}	238.4	172.6					433
23	$(Sr_{0.5}Pr_{0.5})_2Ga_3O_7$	D_{2d}	245	184					395
24	β-Bi_2O_3	D_{2d}	209.6	209.6					567
25	$Li_4[Cu_4O_4]$	D_{2d}	180.7	184.6					157
26	$Na_4[Cu_4O_4]$	D_{2d}	230.1	183					157
27	$Rb_4[Cu_4O_4]$	D_{2d}	278.6	181.9					157
28	SeO_3	D_{2d}	154	154					438
29	Sn_2OSO_4	D_{2d}	213.7	144.8					439
30	$Na_4[Ag_4O_4]$	D_{2d}	232.2	205.4					157
31	$K_4[Ag_4O_4]$	D_{2d}	264.6	205.8					157
32	$Rb_4[Ag_4O_4]$	D_{2d}	283	202.3					157
33	$Cs_4[Ag_4O_4]$	D_{2d}	297.6	205.8					157
1	BPO_4	S_4	152.7	146.3				> 0	461
2	PNb_9O_{25}	S_4	176	165					402
3	VNb_9O_{25}	S_4	178.3	167.3					269
4	$W_3Nb_{14}O_{44}$	S_4	178	178					7
5	$W_8Nb_{18}O_{69}$	S_4	191	191					7
6	VTa_9O_{25}	S_4	182.0	175.3					269

7	$(La_{0.272}Sr_{0.728})(Al_{0.648}\ Ta_{0.352})O_3$	S_4	271	191.4					561
8	$Cs_2W_3O_{10}$	S_4	309	170					352
9	KMo_4O_6	S_4	277	201.3					31
10	$(Ag_3Hg)(V_{0.7}\ As_{0.3})O_4$	S_4	239.5	167.8					581
11	$K_4[Cu_4O_4]$	D_{2d}/S_4	261.6	184.2					157

	Chemical	Sym-	L, pm	L, pm	P_s	d	r	$\chi^{(2)}$	Ref]
№	formula	metry	M-O	E-O	$\mu C/cm^2$	pC/N	pm/V	pm/V	
1	1	2	3	6	7	8	9	10	12
1	$Bi_4Ge_3O_{12}$.	T_d	215.5	175	0	0.87	1.03	1.46	194
2	$Bi_4Si_3O_{12}$	T_d	212.5	161.9	0	1.6	0.52	0.9	354
3	$Gd_3Sb_5O_{12}$.	T_d	228.1	195				0.18	135
4	$Yb_3Sb_5O_{12}$.	T_d	221.4	195				0.15	134
5	$Zn_4O(BO_2)_6$	T_d	184	152		*		0.22	211
6	$Zn_4O(BO_2)_6$	T_d	195.7	147.4					497
7	Li_3NbO_4	T_d	205.7	185.8					303
8	$K_{0.88}Cs_{0.12}B_{1.09}Si_{1.91}O_6$	T_d	286.7	152.5					425
9	$K_{0.50}Cs_{0.50}B_{1.08}Si_{1.92}O_6$	T_d	298.3	153.9					425
10	$K(BSi_2O_6)$	T_d	280.0	155.4					462
11	$Co_4(BO_2)_6O$	T_d	197.26	147.25					533
12	Ag_3PO_4	T_d	237.9	155.1					370
13	$Ca_3Bi(PO_4)_3$	T_d	228.0	149.5					471
14	$Ba_3La(PO_4)_3$	T_d	270.5	148.8					471
15	$In_3(PO_4)_3$	T_d	208.4	152.4					551
16	$Sc(PO_3)_3$	T_d	207.1	147.1					374
17	$Sc_4(P_4O_{12})_3$	T_d	207.1	147.6					307
18	$Pb_{11}Nb(PO_4)_9$	T_d	233	155					417
19	$Pb_4(PO_4)_2CrO_4$	T_d	241.5	156.7					473
20	$Pb_4(PO_4)_2SO_4$	T_d	244.4	150.3					553
21	$Li_{11}Fe(WO_4)_7$	T_d	198	186					375
22	$Bi_4Ge_3O_{12}$	T_d	214.9	173.6					629
23	$Tb_{55}(GeO_4)_{12}O_{59}$	T_d	219	175					631
24	β-$Rb_2ZnGe_5O_{12}$	T_d	318	163					281
25	$CsAlGe_2O_6$	T_d	309.4	173.5					422
26	$Tb_{55}Ge_{12}O_{107}$	T_d	220	175					159
27	$Bi_4Si_3O_{12}$	T_d	215	163					427
28	Dy_2TiO_5	T_d	217.6	202.9					110
29	$Cu_2Al_4O_7$	T_d	196.6	174.7					196
30	$MgAl_2O$	T_d	191.3	191.6					203
31	$Ca_{12}Al_{14}O_{21}$	T_d	236	172.5					153
32	$Ca_4Al_6O_9$	T_d	246	175					205
33	$Pb_2Ru_2O_{7-y}$	T_d	259	195					190
34	Na_3SbO_3	T_d	235.5	189.6					212
35	α-$BaSO_4$	T_d	310	148					614
36	Na_3BiO_3	T_d	244.2	205.4					212
37	$Pb_2Ir_2O_{6.5}$	T_d	226.7	196.8					78
38	$Pb_2Ir_2O_{6.5}$	T_d	226.7	196.8					167
21	Na_6PbO_4	T_d	224.2	223.6					209
22	$Ca_{12}Be_{17}O_{29}$	T_d	231.4	155					445
1	$DyTa_7O_{19}$	D_{3h}	234	187	0			2.1	224
2	$NdTa_7O_{19}$	D_{3h}	203.9?	189.6	0			1.2	545
3	$LaTa_7O_{19}$	D_{3h}	252	189.6	0			1	149
4	$CeTa_7O_{19}$	D_{3h}	224	188.6	0			~0.9	204
5	$Cu_5Ta_{11}O_{30}$	D_{3h}	191.5	189.8					85
6	$Pr_2Nb_{11}O_{30}$	D_{3h}	243.6	189.4					451
7	$BiTaW_2O_{10}$	D_{3h}	196	194					506
8	YBO_3	D_{3h}	226	135					577

9	σ-$Ba_2P_2O_7$	D_{3h}	277.6	148.5					233
10	NaV_6O_{11}	D_{3h}	273.9	178.5					103
11	α-Ag_2CO_3 423K	D_{3h}	217.9	125.3					449
12	Ca_2InO_4	D_{3h}	239	198					201
13	$Ca_{4.74}Ir_3O_{12}$	D_{3h}	235	203.7					342
14	$Ba_3Pt_2O_7$	D_{3h}	250	157					260
15	$SrBe_3O_4$	D_{3h}	265.36	160.1					441
1	$ThMo_2O_8$	C_{3h}	234	168				>0	76

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Table II. Real ternary borates.

	Chemical	Sym	L, pm		d	P_s	$\chi^{(2)}$	Ref.

№	formula	- metry	M-O	M-O	B-O	pC/N	μC/cm^2	pm/V	
1	$PB_2(BO_3)(NO_3)$	C_{6v}	231.3	122.2	139.2			2.4	215
2	$PB_7O(OH)_5(BO_3)CO_3$	C_{6v}	219.4	128.3	139.2			1.7	216
3	$Ba_3Y(BO_3)_3$	C_{6v}	266	222	129			~1.2	14
	β-$Ba_3Y(BO_3)_3$	C_{6v}	265.0	212.2	130			~1.2	85
4	$Ba_3Yb(BO_3)_3$	C_{6v}	268	214	130			~1.2	60
5	$Ba_3Dy(BO_3)_3$	C_{6v}	266	212	130			~1.2	60
6	$Ba_3Ho(BO_3)_3$	C_{6v}	264	218	130			~1.2	60
7	$Ba_3Er(BO_3)_3$	C_{6v}	263	219	130			~1.2	60
8	$Ba_3Tm(BO_3)_3$	C_{6v}	262	220	130			~1.2	60
9	$Ba_3Lu(BO_3)_3$	C_{6v}	268	217	130			~1.2	60
10	$Ba_3Sc(BO_3)_3$	C_{6v}	265	206	132			~1.2.	37
11	$Ba_7(BO_3)_3F_3$	C_{6v}	261	261	136.2			~0.9	219
12	$Ca_3La_3(BO_3)_5$	C_{6v}	247	232	135			>0	32
13	$Ca_3La_3(BO_3)_5$	C_{6v}	250.1	231.39	135.8			>0	172
14	$Ba_3(BO_3)(PO_4)$	C_{6v}	267.0	153.4	133			>0	140
15	$BaEu_6(Si_3B_6O_{24})(OH)_2$	C_{6v}	296.7	161.0	142.2			>0	197
1	$Li_2B_4O_7$	C_{4v}	196.7	196.7	*135.5*			3	61
2	$LaBaCuBO_5$	C_{4v}	281	196	132			>0.	206
3	$LaBaCuO_2BO_3$	C_{4v}	281.51	197.3	132			>0.	210
4	$PrBaCuO_2BO_3$	C_{4v}	278.95	195.5	132			>0.	210
5	$NdBaCuO_2BO_3$	C_{4v}	279.1	194.4	132			>0.	210
6	$NdBaCuO_2BO_3$	C_{4v}	279.60	195.8	132			>0.	207
1	$Pb_3(B_6O_{16})B(OH)_4$	C_{3v}	274	274	136			>2.3	217
2	β-BaB_2O_4	C_{3v}	261.3	261.3	*135.1*			2.3	17
3	$K_3Nb_3B_2O_{12}$	C_{3v}	277	184	*135*			1.2	81
4	$Cd_3Zn_3(BO_3)_4$	C_{3v}	201.4	201.4	137.4			.1	*104*
5	$NaMg_3(Al_6Si_6B_3)(O,OH)_{30}$, dravite	C_{3v}	~242	~160	~136			0.57	201
6	$NaFe^{2+}{}_3(Al_6Si_6B_3)(O,OH)_{30}$, shirl	C_{3v}	~237	~160	~136			~0.5	201
7	$Ca(MgAl_5Si_6B_3)(O,OH)_{30}$, uvite	C_{3v}	240	~160	~136			~0.5	201
8	$Na(LiAl_2Al_6(BO_3)_3Si_6O_{18}(OH)_3O$ Darrellhenryite,	C_{3v}	~230	~160	~136			~0.5	201
9	$NaMg_3Al_6Si_6O_{18}(BO_3)_3(OH)_3F$ fluor-dravite	C_{3v}	~240	~160	~136			~0.5	202
10	$K(MgAl_2)(Al_5Mg)Si_6O_{18}(BO_3)_3(OH)_3$° Maruyamaite	C_{3v}	~270	~160	~136			~0.5	203
11	$Na(GaFeAl)_3(Al_3Ga_2Fe)Si_6O_{18}(BO_3)_3(OH)(3)O$ tourmaline	C_{3v}	253.7	161.8	136.9			~0.5	204
12	$NaFe^{3+}{}_3(Al_4Mg_2)Si_6O_{18}(BO_3)_3$, bosiite	C_{3v}	250.6	160.4	160.4			~0.5	205
13	$SrLiB_9O_{15}$	C_{3v}	271	199	*131.1*			>0	49
14	$BaLiB_9O_{15}$	C_{3v}	291	191	*134.1*			>0	49
15	$BaNaB_9O_{15}$	C_{3v}	283	229	134			>0	49
16	$BaHf(BO_3)_2$	C_{3v}	279.1	205	137.5			>0	*128*
17	$BaZr(BO_3)_2$	C_{3v}	279.8	206.5	137.7			>0	*128*
1	$KNbOB_2O_5$	C_{2v}	275.6	175.5	132.9			6.1	152
2	$Pb_{0.7}Ba_{0.3}B_4O_7$	C_{2v}	265	248.3	144.2			5.1	
3	$CsNbOB_2O_5$	C_{2v}	310.1	177.4	133			~4	3
4	$CsNbOB_2O_5$	C_{2v}	310.1	177.5	135.3			~4	98/*22*
5	$CsTaOB_2O_5$	C_{2v}	311	190.6	131			~4	3/*24*
6	$TlNbB_2O_6$	C_{2v}	276	176	~130			~4	25/ *23*
7	$Al_{4.5}Ga_{0.5}BO_9$	C_{2v}	~190	~190	~136			1.26-4	185-186

8	PbB_4O_7	C_{2v}	248.3	248.3	144.2			3.2	20/26
9	SrB_4O_7	C_{2v}	252.3	252.3	137			3	19
	SrB_4O_7	C_{2v}	247	247	136.5			3	26/78
10	$RbNbB_2O_6$	C_{2v}	289	167	124			2.4	8/28
11	$BaBiBO_4$	C_{2v}	271	199	137.4			1.8	149
12	$KTaB_2O_6$	C_{2v}	286.9	184.13	134.7			1.79	173/*66*
13	$Bi_2ZnB_2O_7$	C_{2v}	213.6	193.2	132.6			1.6	150/35
14	$Pb_4B_2O_7$.	C_{2v}	220.5	220.5	133.5			1.39	*151*
15	LiB_3O_5	C_{2v}	198.3	198.3	*134.6*			*1.24*	18
16	LiB_3O_5	C_{2v}	198.6	198.6	134.2			*1.24*	89
17	$CaBi_2B_2O_7$	C_{2v}	232	205	135.5			1.13	162/*61*
18	$SrBi_2B_2O_7$	C_{2v}	244	2-4	134			1.1	*61*
19	$Cs_3Zn_6B_9O_{21}$	C_{2v}	314.7	190.2	128.4			1.06	139
20	CsZn2B3O7.	C_{2v}	311.9	190.7	129.4			0.98	146
21	H_2TETA)[$Al(B_5O_{10})$]	C_{2v}	171.1	~250	132.7			0.98	142
22	CsB_3GeO_7	C_{2v}	298.0	172.4	134.6			0.98	68
23	$Ba_2Zn(BO_3)_2$	C_{2v}	254	194	136			0.98	43
24	$LiBGeO_4$	C_{2v}	175.7	171.7	140			0.7-0.9	124
25	$Mg[B_6O_9(OH)_2]\cdot 4H_2O$	C_{2v}	202,0	202,0	134.7		147	0.84	198
26	$GdBe_2B_5O_{11}$	C_{2v}	232	158.2	134.7			0.84	187
27	$Al_5Ga_{0.5}BO_9$	C_{2v}	174.2	174.2	135.6			0.56-0.8	185-186
28	$YbBe_2B_5O_{11}$	C_{2v}	228.7	159.0	133.8			0.76	187
29	$K_3B_3O_4(OH)_4\cdot 2H_2O$	C_{2v}	274.9	274.9	133.5			0.72	196
30	$KSr_4(BO_3)_3$	C_{2v}	283.9	248.1	137			0.65	155
32	$NaCa_4(BO_3)_3$	C_{2v}	254.1	237.3	134			0.57	155
31	$KCa_4(BO_3)_3$	C_{2v}	269.4	237.3	133			0.46	155
33	$Li_5Rb_2B_7O_{14}$,	C_{2v}	291.9	187.5	129.4			0.36	194
34	$L_{i5}Cs_2B_7O_{14}$	C_{2v}	304.3	190	132.2			0.36	195
35	$RbSr_4(BO_3)_3$	C_{2v}	298	252.7	136.2			0.28	*155*
36	B_2O_3	C_{2v}	137.3	137.3	137.3			>0	214
37	α -$Li_4B_2O_5$	C_{2v}	186.8	186.8	134.0			>0	133
38	$Na_3[B_6O_9(VO_4)]$	C_{2v}	233	163.5	133				7
39	$K_3Nb_3O_6(BO_3)_2$	C_{2v}	272.8	180.3	135				81/145
40	$Rb_3Y_2(BO_3)_3$	C_{2v}	270.6	216.9	135.4				170
41	$CuTbB_5O_{10}$	C_{2v}	225.3	195					115
42	$CuTmB_5O_{10}$	C_{2v}	219.9	194.5					121
43	$CuLuB_5O_{10}$	C_{2v}	219.5	190.8					121
44	CaB_2O_4	C_{2v}	227.5	227.5	132.6				68
45	$CaAlBO_4$	C_{2v}	232.7	172.1					123
46	$CaGaBO_4$	C_{2v}	246	173					33
47	$Sr_4Mn_3(B_{0.8}Mn_{0.2})O_{10}$	C_{2v}	249	189.4					99
48	Al_5BO_9	C_{2v}	184.6	184.6	135.5				21
49	$Al_{20}B_4O_{36}$	C_{2v}	`172.4	`172.4	136.1				189
50	$Al1_{6.62}Cr_{1.38}B_4O_{36}$	C_{2v}	172.7	172.7	136				107
51	SnB_4O_7 β 7.5 GPa 1100C	C_{2v}	231.8	231.8	140.8				165
52	$La_2Sr_3(BO_3)_4$	C_{2v}	241	238					54
53	γ-$Ce(BO_2)_3$ 7.5 GPa, 1000 C	C_{2v}	239.3	239.3	144				142
54	γ- $La(BO_2)_3$	C_{2v}							142
55	γ- $Pr(BO_2)_3$	C_{2v}							142
56	γ- $Nd(BO_2)_3$	C_{2v}							142
	$Pr_2Sr_3(BO_3)_4$	C_{2v}	229	222				142	93
57	$Nd_2Sr_3(BO_3)_4$	C_{2v}	238	234					55
58	EuB_4O_7	C_{2v}	253.1	253.1					22
59	$Er_2Sr_3(BO_3)_4$	C_{2v}	230	226	145				22
60	AgB_3O_5	C_{2v}	255	255	125			>0	57
1	$Cd_4BIO(BO_3)_3$	C_s	226.3	224.2	133			2	32
2	$LuCa_4O(BO_3)_3$	C_s	232.7	222.5				184	100/58

3	$YCa_4O(BO_3)_3$	C_s	233.9	222.6				1.82	143
4	$GdCD_4O(BO_3)_3$	C_s	218.6	222.3	133.2			1.79	34
5	$Ca_4LaO(BO_3)_3$	C_s	229	222				1.4	34
6	$LaCa_4O(BO_3)_3$	C_s	231	228				1.4	79
7	$Ca_4SmO(BO_3)_3$	C_s	232.9	225.4				1.4	74
8	$Sm_2Ca_8O_2(BO_3)_6$	C_s	232.8	224.5				1.4	59
9	$Ca_4GdO(BO_3)_3$	C_s	232.0	224.5				1.4	103
10	$GdCa_4O(BO_3)_3$	C_s	233.2	224.4				1.4	58
11	$TbCa_4O(BO_3)_3$	C_s	232.8	223.8				1.4	58
12	$(Y_{0.73}Yb_{0.25}Er_{0.02})Ca_4O(BO_3)_3$	C_s	232.5	223.7				1.4	143
13	$(Y_{0.75}Yb_{0.20}Er_{0.02}Ce_{0.03})Ca_4O(BO_3)_3$	C_s	232.8	222.9				1.4	143
14	$(Y_{0.97}Yb_{0.03})Ca_4O(BO_3)_3$	C_s	233.4	222.6				1.4	143
15	$(Y_{0.85}Yb_{0.15})Ca_4O(BO_3)_3$	C_s	233.4	223.3				1.4	143
16	Ca2[B5O9]·(OH)·H2O	C_s	234.4	258	136.8			1.39	199
17	$La_2(CH_3CO_2)_2[B_5O_9(OH)]$	C_s	233.7	118.9	134.8/			1.26	190
18	$La_2(CH_3CO_2)_2[B_5O_9(OH)]·H2O$	C_s	237.8	122.8	131.,5/			1.13	190
19	γ- $LaSc_3(BO_3)_4$	C_s	242.4	202.9				1	47/72
20	$Pr_2(CH_3CO_2)_2[B_5O_9(OH)]·H_2O$	C_s	232.9	124.4	133.2/			0.95	190
21	$Ba_{11}Sr(BO_3)_8$	C_s	~261	260	~136			0.9	188
22	$Pr_2(CH_3CO_2)_2[B_5O_9(OH)]$	C_s	229.6	120.3	132.9/			~1.05	190
23	$Ce_2(CH_3CO_2)_2[B_5O_9(OH)]·$	C_s	232	/115.8	133.4			~0.9	190
24	$Ce_2(CH_3CO_2)_2[B_5O_9(OH)]·H_2O,$	C_s	234.8	124.5	133.7/			0.8	190
25	$Tl_4[B_8O_{12}(OH)_4]H_2O.$	C_s	240.8	190.6	135.1			> 0.1	193
26	$Zn_3(BO_3)_2$	C_s	186	186	136				133
27	α-$Zn_3(BO_3)(PO_4)$	C_s	198.0	152.8	136.3				117
28	$Co_3[BPO_7]$	C_s	199.2	152.2	137				15
29	YBO_3	C_s	232.7	232.7	~136				131
30	$YbBO_3$	C_s	231	231	~136				131
31	$Y_{16.86}(BO_3)_4(B_2O_5)_2O_{16}$	C_s	206	206					130
32	$TmBO_3$	C_s	231.7	231.7	~136				73
33	$Na_2Zn_2MnB_{4.67}O_{11}$	C_s	232	194					209
1	Sm_3BWO_9	C_6	227.2	182.4				2	159
2	Dy_3BWO_9	C_6	217.4	185.5				1.8	159
3	La_3BWO_9	C_6	236	195	143			1.3	159
4	Gd_3BWO_9	C_6	219.0	192.0				1	159
5	Tb_3BWO_9	C_6	219.2	190.2				1	159
6	Eu_3BWO_3	C_6	229.1	186.1				1	159
7	Nd_3BWO_9	C_6	224.8	194.5				1	159
8	Pr_3BWO_9	C_6	227.5	194.9				1	139
9	$SrBi_2B_2O_7$	C_6	244	215					162
10	$NaBSiO_4$	C_6	220	161					39
11	$CaZrB(Al_9O_{18})$	C_6	237.1	182.7					21
12	$Ca_4Mn_3O_3(BO_3)_3(CO_3)$	C_6	234	131	132				208
1	$TlBO_2$	C_4	248	248	136			> 0	109
1	$LaBGeO_5$	C_3	240.7	171.9	145.4			3.06	23
2	Eu_3BWO_9	C_3	223	184	136			1..6	159
3	B_2O_3	C_3	133	133	133			>0	134
4	β-SrB_4O_7	C_3	247.9	247.9	132.3				182
5	$BaAsBO_5$	C_3	262	162					116
6	$PbAsBO_5$	C_3	251	163					120
7	$Cr_2[BP_3O_{12}]$	C_3	187.6	149	141.1				66
8	$LaBSiO_5$	C_3	238.3	158					10
	$LaBSiO_5$	C_3	241.2	158.6					104
	$LaBSiO_5$ 293K	C_3	239.6	159					108

9	$CeBO[SiO_4]$	C_3	235	160	145			>0	95
10	$(Ce_{0.5}La_{0.5})(BO(SiO_4))$	C_3	239.7	159					135
11	$Sm_{14}(GeO_4)_2(BO_3)_6O_8$	C_3	220	171					46
12	$Nd_{14}(GeO_4)_2(BO_3)_6O_8$	C_3	223	174					46
13	$Nd_{4.3}Sm_{4.8}Eu_{4.9}(GeO_4)_2(BO_3)_6°_8$	C_3	224	173					71
14	$PrBGeO_5$	C_3	234.3	166.4					102
15	$PrBGeO_5$ 650C	C_3	236.9	170.5					102
1	BiB_3O_6	C_2	208.7	208.7				3.2	24
2	$La_2CaB_{10}O_{19}$	C_2	234.9	185.1	136			1.6	38
3	$La_2CaB_{10}O_{19}$	C_2	234.9	229.7	133.3			1.6	48
4	$Pb_3Ba_3(BO_3)_4$	C_2	~240	260	~136			1,39	188
5	$Ba_2[B_6O_9(OH)_4$	C_2	263.9	OH272.6	134.9			1.39	222
6	$Sr_2B_5O_9(OH)\cdot H_2O$	C_2	255.5	124	135.1		130	1.39	220
7	$Sr_2B_5O_9(OH)\cdot H_2O$ (2),	C_2	254.4	254.4	132.3		148	1.13	221
8	$PrSc_3(BO_3)_4$	C_2	243.4	204.7					47
9	α-LaBMoO6	C_2	243.5	173.5	132.1			1.07	131
10	$Sr_2[B6O9(OH)_4]$	C_2	263.3	287.8	134.3			0.98	148
11	$Bi_2B_8O_{15}$	C_2	208.4	208.4	134.3			0.9	31
12	$Bi_2B_8O_{15}$ α	C_2	205.73	205.73	134, 2			0.9	160
13	$BaCuB_2O_5$	C_2	270.3	188.5	134.5			0.3	1
14	$LiBSi_2O_6$	C_2	193	156.3					129
15	$Li_3Eu_2(BO_3)_3$	C_2	235	185					106
16	$Na_5B_2P_3O_{13}$	C_2	220.2	147.4					84
17	K_2LiBO_3	C_2	260.5	188					111
18	$K_2B_2Ge_3O_{10}$	C_2	271.2	171.5	144.8			>0	174
19	$CaB_2U_2O_{10}$	C_2	231.5	179.7					65
20	$UO_2B_2O_4$	C_2	176.3	176.3	132.4				180
1	$Ba_3Na(B_6O_{16})B(OH)_5$	C_1	262.7	218	135			1.5	4
2	$RBSR[C_4H_2O_6B(OH)_2]\cdot 4H_2O$	C_1	291.5	259.4	125.3			1.36	191
3	$KSR[C_4H_2O_6B(OH)_2]\cdot 4H_2O$	C_1	279.1	257.7	125.1			1.2	191
4	$Li_6CuB_4O_{10}$	C_1	188.3	175	130			0.8	161
5	$Bi_2Cu_5B_4O_{14}$	C_1	212	188	131			0.57	175
6	L-$SmBO_3$	C_1	225	225					94
7	$Cd_2B_2O_5$	C_1	214	214					101
8	$Ba_2B_{10}O_{17}$ est PDF	C_1	266.1	266.1	136		167-168	0.2	192
9	$Tl_4[B_8O_{12}(OH)_4]H_2O$.	C_s	240.8	190.6	135.1			> 0.1	193
1	RbMgBO3	T	285	211.8	136.9			0.57	143
2	$KMgBO_3$	T	278.08	209.2	135.7			0.46	179
3	$K_{0.9}Na_{0.1}MgBO_3$	T	276.9	210.84	136.5			0.46	179
4	$K_{0.8}Na_{0.2}MgBO_3$	T	276.2	209.5	137.0			0.46	179
5	$Bi_{24.5}BO_{38.25}$	T	209.4	166.0				0.46	86
1	$Li_{2.46}Al_{0.18}BO_3$	D_6	189.8	184	136			>0	147
1	BaB_8O_{13}	D_4	269.4	269.4	137			>0	
2	$Rb_5S_4BO_{16}$	D_4	269.7	145.9	131.3			>0	120-121
1	$Lu_{0.66}La_{0.95}Sc_{2.39}(BO_3)_4$	D_3	247.8	157.2	136.4			1.74	171
2	$CeSc_3(BO_3)_4$	D_3	245.1	206.1	136.8			1.7	136
3	$BiAlGa_2(BO_3)_4$	D_3	238.0	190.8	135			1.6	169
4	$BAsO_4$	D_3	157	157	144			1.54	223
5	$PrSc_3(BO_3)_4$	C_2	243.4	204.7	134			1.4	36
6	$Y_{0.57}La_{0.72}Sc_{2.71}(BO_3)_4$	D_3	244.8	205.8	135.3			1.4	137

7	$YAl_3(BO_3)_4$	D_3	232.1	183.7	138.3			1.4	42/53
8	$NdAl_3(BO_3)_4$	D_3	237.1	185.8	135			1.4	41
9	$GdAl_3(BO_3)_4$	C_2	231.8	184.3	135.3			1.4	42/52
10	$YbAl_3(BO_3)_4$	D_3	229.5	185.9	136.9			1.4	42
11	$TmAl_3(BO_3)_4$	D_3	230.5	186.0	137.4			1.4	42
12	$NdGA_3(BO_3)_4$	D_3	237.9	192.6	138.8			1.4	40
13	β-$LaSc_3(BO_3)_4$	D_3	248.3	205.7	134.2		36	1.4	72
`14	$NdBSiO_5$	D_3	236.2	161.8					38
15	$(Nd_{0.5}Bi_{0.5})Fe_3[BO_3]_4$	D_3	240.6	202.1					44
16	$NdFe_3(BO_3)_4$	D_3	240.4	195.0					127
17	$(Nd_{0.8}Gd_{0.2})Sc_3(BO_3)_4$	D_3	238.9	198					70
18	$TmAl_3(BO_3)_4$	D_3	230.5	186.0					163
19	$Y_{0.5}Lu_{0.5}Al_3(BO_3)_4$	D_3	233.6	186.1					132
20	$YAl_{1.5}Ga_{1.5}(BO_3)_4$	D_3	232	190					137
21	$BaBPO_5$	D_3	268.8	147.6	133.8			0.56	13
	$BaBPO_5$	D_3	266.6	149.7	143.9				75
22	$K_2Fe_2B_2O_7$	D_3	263.5	179.2	136.7			0/51	183
23	B_2O_3	D_3	135.6	135.6	135.6				88
24	$(K_{0.48}Na_{0.52})_2Al_2B_2O_7$	D_3	241.6	167.6					167
25	$K_2Al_2O(BO_3)_2$	D_3	270.25	169.95					118
26	$K_2Ga_2O(BO_3)_2$	D_3	264.6	176.2					109
26	$CsBaB_3O_6$	D_3	307.4	269.8	127.3			0	168
27	Ag_3BO_3	D_3	212.5	212.5					174
28	$CaBPO_5$	D_3	227	149	146				45
29	$CaBPO_5$	D_3	227	149					113
30	$BaAl_2B_2O_7$	D_3	274.60	166.5					114
31	BPO_4 7.8Gpa 1273K	D_3	151.3	151.3					144
32	BPO_4 8.0Gpa 1108K	D_3	167.3	167.3					144
33	$(Y_{0.5}Bi_{0.5})Fe_3(BO_3)_4$	D_3	237.2	197.0					137
34	$LaBSiO_5$ 443K	D_3	240	159					108
35	$LaFe_3(BO_3)_4$	D_3	241.9	194.4					127
36	$(Ce_{0.5}Nd_{0.5})Sc_3(BO_3)_4$	D_3	240.2	200.1					70
37	$(Ce_{0.41}Nd_{0.46}Gd_{0.13})Sc_3(BO_3)_4$	D_3	244.1	206.1					70
38	$(Ce_{0.80}Gd_{0.20})Sc_3(BO_3)_4$	D_3	245.7	211.3					42
39	$(Ce_{0.70}Gd_{0.30})Sc_3(BO_3)_4$	D_3	244.3	210.1					42
40	$(Ce_{0.68}Gd_{0.32})Sc_3(BO_3)_4$	D_3	238.3	202.8					70
41	$(Ce_{0.99}Lu_{0.01})(Lu_{0.20}Sc_{2.80})(BO_3)_4$	D_3	246	206					70
42	$PrBGeO_5$ 800C	D_3	237.3	171.1					102
43	$GdBO_3$	D_3	230	230					112
44	$GdFe_3(BO_3)_4$ 297K	D_3	234.74	195.8					154
45	$GdFe_3(BO_3)_4$ 90K	D_3	235.7	195.9					154
46	$Gd_{0.97}Eu_{0.03}Al_3B_4O_{12}$	D_3	234.1	185.1					50
47	$YbAl_3(BO_3)_4$	D_3	229.5	185.9					28
48	B_2O_3	D_3	*135.6*	*135.6*	*135.6*				*88*
1	β-RbB_3O_5	D_2	284	284	134			1.5	41/56
2	$Se_2B_2O_7$	D_2	169.5	169.5	140			1.18	158
3	$Cd_{1.17}Zn_{0.83}B_2O_5$	D_2	223.1	199.7	134.6			1.13	153
4	$Na_3VO_2B_6O_{11}$	D_2	234.23	163.76	135.6			0.8	177
5	β-$SrGaBO_4$	D_2	240.5	178.7	133.7			0.57	11
6	$BaZn_2(BO_3)_2$	D_2	274.0	192.6	135			0.25	9
7	$LiKB_4O_7$	D_2	264.27	187.2					26
8	$LiRbB_4O_7$	D_2	271.2	188.5					26
9	α-RbB_3O_5	D_2	257	257					141
10	CsB_3O_5	D_2	303	303					2
11	CsB_9O_{14}	D_2	310.8	310.8	145.2				30
12	$Ag_2CsB_{15}O_{24}$	D_2	320.5	231.1					119
13	$Ba_5(BO_3)_2(B_2O_5)$	D_2	250.5	250.5	140				157

14	TlB_3O_5	D_2	266.2	266.2	136				12
1	γ-$LiBO_2$	D_{2d}	195.7	195.7	148.3			6.3	5
2	$CaBiGaB_2O_7$	D_{2d}	240.2	182.6	141.6			1.01	7
3	$KBaBP_2O_8$	D_{2d}	272.1	149.8	144.9			0.46	176
4	$KSrBP_2O_8$	D_{2d}	267.6	147.8	141.7			0.36	176
5	$CsLiB_6O_{10}$	D_{2d}	314.7	196					36
6	$CsLiB_6O_{10}$	D_{2d}	314.5	196.2					138
7	CuB_2O_4	D_{2d}	188.6	188.6					168
8	CuB_2O_4	D_{2d}	191.3	191.3					69
9	$Ca_2SiB_2O_7$	D_{2d}	232.9	165.7					128
10	$SrCu_2(BO_3)_2$	D_{2d}	260.8	192.9					16
11	$Sr_{0.661}Ca_{0.339}Cu_2(BO_3)_2$	D_{2d}	256.5	191.3					29
12	$Sr_{0.735}Ba_{0.265}Cu_2(BO_3)_2$	D_{2d}	260.4	193.1					29
13	$Sr_6BP_5O_{20}$	D_{2d}	241.7	150.5	147.1				148
13	$Sr_6BP_5O_{20}$	D_{2d}	241.9	154.2	145.9				166
14	PdB_2O_4	D_{2d}	198.0	198.0					64
15	$Ho_4AlCu_2B_9O_{23}$	D_{2d}	226.0	195.1	130.5				8
16	$Lu_4AlCu_2B_9O_{23}$	D_{2d}	224.7	191.0	134.8				8
1	BPO_4	S_4	152.7	152.7	146.3			1.13	77
2	$Pb_6[PO_4][B(PO_4)_4]$	S_4	204	151	146			1.06	67
3	$LiBSiO_4$	S_4	201.6	161.7					125
4	$LiBGeO_4$	S_4	199.5	175.0					125
5	$Pb_6(AsO_4)(B(AsO_4)_4)$	S_4	219	169					120
6	BPO_4 25C	S_4	153.2	153.2					146
	BPO_4 500C	S_4	151.6	151.6					146
	BPO_4 900C	S_4	150.9	150.9					146
1	$Zn_4B_6O_{13}$	T_d	184	184				0.22	6
2	H-HBO_2	T_d	240	130					
3	$K_{0.88}Cs_{0.12}B_{1.09}Si_{1.91}O_6$	T_d	286.7	152.5					76
4	$K_{0.50}Cs_{0.50}B_{1.08}Si_{1.92}O_6$	T_d	298.3	153.9					76
5	$K(Bsi_2O_6)$	T_d	280.0	155.4					80
6	$Ca_3Er_3Ge_2BO_{13}$	T_d	232.5	174.0					105
7	$Zn_4O(BO_2)_6$	T_d	195.7	195.7					82
	$Zn_4O[B_6O_{12}]$	T_d	196.0	196.0					92
8	$Co_4(BO_2)_6O$	T_d	197.3	197.3					87
1	$Ba_3Ti_3O_6(BO_3)_2$	D_{3h}	269.3	189.6	136.0			28	97
2	$Sr_2Be_2B_2O_7$	D_{3h}	247.8	161.8				2.48	126
3	$Na_3La_9O_3(BO_3)_8$	D_{3h}	245.0	241.4	137.1			1.6	164/40
4	$K_3Nb_3O_6(BO_3)_2$	D_{3h}	278.6	194.15	136			1	62
5	$K_3Ta_3B_2O_{12}$	D_{3h}	276.2	194.2				1	83
6	$Ba_2Be_2B_2O_7$	D_{3h}							218
7	$YbBO_3$	D_{3h}	226	226					91
8	$LaAl_{2.03}(B_4O_{10})O_{0.54}$	D_{3h}	247.9	178.9					27
9	$NdAl_{2.07}[B_4O_{10}]O_{0.6}$	D_{3h}	243.3	177.9					51
10	$KGd[B_6O_{10}(OH)_2]$ P-62m	D_{3h}	*274*	234.4	144.4			>0	129
1	$LiCdBO_3$	C_{3h}	221.3	190	139			.0	96

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Table 3.

Composition, structure (S), the oxide bond length (L).and NLO-susceptibility ($\chi^{(2)}$) of carbon-contained crystals

№	Composition	S	L, пм *M-O*	L, pm *E-O*	L, pm *C-O*	$\chi^{(2)}$ pm/V	Ref
1	$PB_7O(OH)_5(BO_3)CO_3$	C_{6v}	219.4	139.2	128.3	1.7	1
2	$Pb_5O(OH)_2(CO_3)_3$	C_{6v}	215.6	215.6	126.2		2
3	$Cs_3Ba_4(CO_3)_3F_5$	C_{6v}	320	259	127.6	0.47	3
4	β-Ag_2CO_3	C_{3v}	209.0	209.0	124.7		4
5	$C_{31}H_{69}Cl_4N_9O_{25}Zn_3$	C_{3v}	194.7	167	128.4		5
6	$C_{31}H_{69}Cl_4N_9O_{25}Cu_3$	C_{3v}	193.6	166.7	127.9		5
7	$C_{31}H_{69}Cl_4N_9O25CuZn_2$	C_{3v}	195	166.6	126.8		5
8	$Sr_4Fe_2O_6CO_3$	C_{2v}	246.9	189	118.7		6
9	$Bi_2O_2CO_3$	C_{2v}	221	221	128		7
10	$KND(CO_3)_2$	C_{2v}	*270*	*230*	*127*		8
11	$Y_2(CO_3)_3 \cdot nH_2O$ (n : 2-3)	C_{2v}	234.2	234.2	124.2		9
12	$CaY_4(CO)_3 \cdot 9H_2O$	C_{2v}	*237*	*234*	*125*		10
13	$NA_3[BE(OH)(CO_3)\cdot (C_7H_6OCO_2)_2]\cdot$	C_{2v}	*237*	*159.7*	*123.2*		11
14	$NA_3EU(CO_3)_3$	C_{2v}	240.7	237.8	127.4	~1.4	12
15	$FENAC_{16}H_{24}N_4O_8\cdot 5H_2O$	C_{2v}	240	204.4	*126*		13
16	$K_2[CU(CO_3)_2]$	C_{2v}	*270*	*170*	*125*		14
17	$[L''ZN\}_2(CO_3)(C_6H_6)$	C_{2v}	229.5	190.9	124.9		15
18	$NA_3Y(CO_3)_3$	C_{2v}	*235*	*226.7*	*127.1*	1.39	16
19	$NA_3GD(CO_3)_3$	C_{2v}	*236*	*220*	*126*	1.38	16
20	$NH_4][CD(HCOO)_3]$	C_{2v}	*265*	235	129	0.6	17
21	$LICHO_2 \cdot H_2O$	C_{2v}	199	199	127	0.94	18
22	$LI_{0.9}NA_{0.1}CHO_2 \cdot H_2O$	C_{2v}	236	199	127	0.99	19
23	$NACHO_2$	C_{2v}	*237*	*237*	127	0.35	19
24	$PB(C_4H_4O_6)$	C_{2v}	240	240	126	0.64	20
25	$CE(CH_3CO_2)_2[B_5O_9(OH)]\cdot H_2O$	C_s	234.8	133.7	124.5	0.8	21
26	$LA_2(CH_3CO_2)_2[B_5O_9(OH)]$	C_s	233.7	134.8	125	1.26	21
27	$LA_2(CH_3CO_2)_2[B_5O_9(OH)]H_2O$	C_s	237.8	131.,5	125	1.13	21
28	$PR_2(CH_3CO_2)_2[B_5O_9(OH)]\cdot H_2O$	C_s	232.9	133.2	124.4	0.95	21
29	Meso- tart-$C_4H_4Li_2O_6$	C_s	191.1	191.1	126		22
30	$Na_3Lu(CO_3)_2F_2$	C_s	227.7	219.6	122.9	1.67	23*
31	$Na_8Lu_2(CO_3)_6F_2$	C_s	230	223	123.5	1.64	23*
32	$LINACO_3$	C_6	*237*	*199*	*129*		24
33	$CA_4MN_3O_3(BO_3)_3(CO_3)$	C_6	234	131	127	0.1	25
34	$NASIALO_4CA(CO_3)_{0.26}$	C_6	241.2	160.1	126.9	1.8	26
35	$Na_2Co_8(CO_3)_6(OH)_6 \cdot 6H_2O$	C_6	237.2	205.2	129.5	1.8	27
36	$HG_8\cdot(NI, MG)_6\cdot(CO_3)_{12}\cdot(OH)_{12}\cdot (H_3O)_6.(H_2O)_3$	C_6	209.9	199.4	124.8	1.79	28
37	$N\ A_6Sl_6Al_6O_{24}C\ A_{1.5} \cdot 1.6\ CO_3$	C_6	233.5	160.1	126.9	1.79	29
38	$CA_2SRC_3H_5O_2$	C_4	258	235	129	~4	30
39	$[NACA_3(CO_3)_2F_3 \cdot H_2O]$	C_3^3	246.2	246.1	123		31
40	$K_2CA_2(CO_3)_3$	C_3	267.7	236.7	126.1	1.74	32
41	L- TART -$C_4H_4Li_2O_6$	C_2	188.7	188.7	127		22
42	$K_2C_4H_4O_6\cdot 1/2H_2O$	C_2	270	240	116	4.26	19
43	$NAKC_4H_4O_6\cdot 4H_2O$	C_2	270	240	115	4.3	30
44	$NaHC_4H_4O_6 \cdot H_2O$	C_2	238.0	157.9	130		33
45	$SN\ (C_4H_4O_6)$	C_2	235	235	126	1.1	34
46	$MN\ (C_4H_4O_6)$	C_2	210	210	126	0.52	34

47	$[NdSn_2\{h(tart)_3\}12H_2O$	C_2	239.6	200.8	131.3		35
48	$[UO_2(C_2H_5CO_2)_2(CO(NH_2)_2]\cdot H_2O$	C_2	176	176	130.1		36
49	$C_{12}H_{32}Cu_2Ge_2O_{31}$,	C_2	210	190	130		37
50	$C_{12}H_{28}GdGe_2O_{28.5}$	C_2	230	190	130		37
51	C12H27Ge2O28Tm,	C_2	227	190	130		37
52	$C_{12}H_{27}Ge_2O_{28}Yb$	C_2	224	188	130		37
53	$[CD(C_4H_4O_6)(H_2O)_3]2H_2O$	C_2	236.6	230	130		34
54	$[AGGE(HCIT)_2(H_2O)_3]2\ H_2O$	C_1	226.8	181.8	130		38
55	$KSR[C_4H_2O_6B(OH)_2]\cdot 4H_2O$	C_1	279.1	257.7	125.1	1.2	39
56	$RBSR[C_4H_2O_6B(OH)_2]\cdot 4H_2O$	C_1	291.5	259.4	125.3	1.36	39
57	$[C_6H_{16}N_2O]2(HC_2O_4)_4\cdot 3H_2O$	C_1	193	192.6	125.2		40
58	$LiNACO_3$	C_1	*238*	*197*	*125*	0.45	24
59	$NA_8[aLSiO_4]_6CO_3$	T	*238*	*160*	*128*		41
60	$Mn_4Al_2(OH)_{12}CO_3\cdot 3H_2O$	D_6^6	*220*	*161*	*130*		42
61	$Mg_4Al_2(OH)_{12}CO_3\cdot 3H_2O$	D_6^6	*210*	*159*	*129*		53/42
62	$Ba_{l\,x}Sr_x)_2Cu_{l+y}O_{2+2y+z}\ O_3)_{l-y.}$	D_4	242.1	195.2	122.3		43
63	$CA_2YCO_3(OH)_2\cdot 3H_20$	D_4	237	226	128		.44
64	$K_4Eu_2(CO_3)_3F_4$	D_3^7	270	235	130	~14	45
65	$K_4Gd_2(CO_3)_3F_4$	D_3^7	269	234	129	~10	45
67	$Mn_4Al_2(OH)_{12}CO_3\cdot 3H_2O$	D_3^6	*222*	*160*	*131*		42
68	$Mg_4Al_2(OH)_{12}CO_3\cdot 3H_2O$	D_3^6	*208*	*160*	*129*		42
69	$Fe_4Mg_4Al_2(OH)_{12}CO_3\cdot 3H_2O$	D_3^6	*218*	*161*	*130*		42
70	$NA[(VO)_2(C_4H_4O_6)(C_4H_2O_6)\ (H_2O)_2]\cdot$	D_2^4	225.4	159.9	127	~0.1	46
71	$K_2[(VO)_2(C_4H_4O_6)(C_4H_2O_6)$	D_2^5	241.9	1.58.9	128	~0.1	46
72	$RB_2[(VO)_2(C_4H_4O_6)(C_4H_2O_6)$	D_2^4	286.3	160.7	129	~0.1	46
73	$CS_2[(VO)_2(C_4H_4O_6)(C_4H_2O_6)$	D_2^4	301.3	160.6	130	~0.1	46
74	$SR(CHO_2)_2$	D_2	255	255	129	0.54	19
75	$SR(CHO_2)_2\cdot 2H_2O$	D_2	254.5	254.5	129	0.35	19
76	$SR(C_4H_4O_6)\cdot\ 3H_2O$	D_2	254	254	129	0.46	34
77	$ZN\ (C_4H_4O_6)\cdot\ 2.5H_2O$	D_2	210	210	126	0.52	/34
78	$BA(C_4H_4O_6)$	D_2	265	265	127	0.35	34
79	$CA(C_4H_4O_6)\cdot 4H_2O$	D_2	240	240	127	0.23	34
80	$CUC_4H_4O_6)\cdot 3H_2O$	D_2	202	202	127	0.26	34
81	$COC_4H_4O_6)\cdot 3H_2O$	D_2	204	204	127	0.1	34
82	$FeC_4H_4O_6)\cdot 3H_2O$	D_2	212	212	127	0.1	34
83	$(NH_4)HC_2O_4$	D_2	262	262	*130*	0.06	34
84	$CA_{0.8}BA_{0.2}(C_4H_4O_6)\cdot 46/34$	D_2	*265*	*240*	*129*	0.56	47
85	$CE_2(CO_3)_3\cdot 4H_2O$	D_2	240	240	128		50
86	$CS_2C_4H_4O_2$	D_2	300	300	131	~0.1	19
87	$(NH_4)_2C_2O_4\cdot H_2O$	D_2	265	265	123	0.78	19
88	$C_{52}H_{44}O_6SB_2$	D_2	222.5	222.5	1.27		48
89	$CA(C_4H_4O_6)\cdot 6H_2O$	D_2	254.2	238.6	*130*		34
90	$BA_4LiCUO_4(CO_3)_2$	D_{2d}	264.7	184.5	126		49
91	$Na_5Lu(CO_3)_4\cdot 2H_2O$	D_{2d}	229	221	123		16
92	$[CN_3H_6]_2[CU(CO_3)_2]$	D_{2d}	195.6	195.6	124/9		51
93	$(NH_2)_2CO$	D_{2d}	260	260	126	1.2	18
94	$Sr_{2-x},Ba_xCUO_2(CO_3)$	S_4	255	196	128		52
95	$BA_3Co_2O_6(CO_3)_{0.60}$	C_{3h}	262.5	182.6	129.2		53
96	α-Ag_2CO_3	D_{3h}	217.9	217.9	125.3		4
97	$CE(CO_3)F$	D_{3h}	254.3	254.3	127.2		54

98	$K_{2.70}P\ B_{5.15}(CO_3)_5F_3$	D_{3h}	267.9	266.7	128.3	7.3	55
99	$RbSrCO_3F$	D_{3h}	300	240	127.6	1.3	3
100	$KSrCO_3F$	D_{3h}	270	239	129.4	1.3	3
101	$RbCaCO_3F$	D_{3h}	301	237	127.6	0.43	3
102	$KCaCO_3F$	D_{3h}	269	236	127.6	1.41	3
103	$CsCaCO_3F$	D_{3h}	320	238	127.6	0.43	3
104	$CsSrCO_3F$	D_{3h}	323.8	239.3	128.9	0.88	56
105	$CsPBCO_3F$	D_{3h}	313.7	270.9	128.2	6.93,	57-58
106	$RBPBCO_3F$	D_{3h}	301	268.6	129.1	6..3-17	57
107	$KCdCO_3F$	D_{3h}	282.6	224	125.2	0.91	59
108	$RbCdCO_3F$	D_{3h}	291.3	222.4	128.5	0.67	60
109	$KZnCO_3F$.	D_{3h}	276.4	199.1	128.7	0.53	60
110	$RBZnCO_3F$.	D_{3h}	287.9	194.7	127.9	0.36	60

* - Supporting information

References

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