Prediction of New Displacive Ferroelectrics through Systematic Pseudosymmetry Search. Results for Materials with $Pba2$ and $Pmc2_1$ Symmetry.

Supplementary material

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This Supplementary material contains the tables with the coordinates of the initial (polar) and the calculated high-symmetry (non-polar) structures of the compounds considered as possible ferroelectrics among those listed in the Inorganic Crystal Structure Database (ICSD) with symmetry space group $Pmc2_1$. Each table gives the supergroup for which the structure has been obtained to be pseudosymmetric as well as the transformation matrix P relating the bases of this supergroup and $Pmc2_1$, the origin shift p of the origin in $Pmc2_1$ with respect to that of the supergroup. Also, the asymmetric unit of the polar and the high-symmetry structure are given with respect to the basis of the group $Pmc2_1$. The origin in the polar group is fixed at position $z = u$, where u corresponds to the optimized position of the origin in the polar structure for which the maximal displacement among all atoms in the structure has minimal value.

The coordinates given under "High-symmetry structure" are obtained from the ICSD structure data as follows:

$$(x, y, z)^{\mathcal{G}}_{Pmc2_1} = (x, y, z,)^{Pmc2_1} + \text{displacement} - (0, 0, u)$$

Under"Initial structure" we have listed the atomic positions of the polar structures with respect to the new origin. These 'new-origin' coordinates are simply related to

the original Pmc2$_1$ coordinates found in the ICSD database:

$$(x, y, z,)^{Pmc2_1}_{\text{new origin}} = (x, y, z,)^{Pmc2_1} - (0, 0, u)$$

The transformation of the new-origin positions into the basis of the corresponding supergroup is accomplished by the following relation:

$$\mathbf{r}^{\mathcal{G}} = P\mathbf{r}^{\mathcal{G}}_{Pmc2_1} + \mathbf{p}$$

where $\mathbf{r}^{\mathcal{G}}$ is a column that contains the coordinates of the point with respect to the basis of the supergroup $\mathcal{G}$, and $\mathbf{r}^{\mathcal{G}}_{Pmc2_1}$ is a column with the coordinates of the same point with respect to the basis of $Pmc2_1$.

The Wyckoff positions of the occupied atomic orbits of initial and high-symmetry structure are specified by their Wyckoff letters and multiplicities. The splitting relations between the orbits of the non-polar and polar structures are indicated by curly brackets.

Table 1. *Initial and calculated high-symmetry structures for $BaHgS_2$.* $\mathbf{a} = 4.215$, $\mathbf{b} = 14.388$, $\mathbf{c} = 7.338$*;* $\mathcal{G} = Pbam$, $P = (\mathbf{c}, \mathbf{a}, \mathbf{b})$, $p = (\frac{1}{4}\, 0, 0)$*;* $u = 0.142$. *WP=Wyckoff positions.*

Atom	Initial structure				High-symmetry structure			
	WP	x	y	z	WP	x	y	z
Ba(1)	2a	0	0.391	0.678	4g {	0	0.395	0.661
Ba(2)	2a	0	0.102	0.356		0	0.105	0.339
Hg(1)	2b	1/2	0.351	0.193	4h {	1/2	0.355	0.167
Hg(2)	2b	1/2	0.140	-0.142		1/2	0.145	-0.167
S(1)	2b	1/2	0.986	0.128	4h {	1/2	1.008	0.079
S(4)	2b	1/2	0.469	-0.030		1/2	0.492	-0.079
S(2)	2b	1/2	0.736	-0.043	2b	1/2	3/4	0
S(3)	2a	0	0.779	0.468	2c	0	3/4	1/2

Table 2. *Initial and calculated high-symmetry structures for Nd_4GeO_8.* $\mathbf{a} = 5.737$, $\mathbf{b} = 7.396$, $\mathbf{c} = 19.874$*;* $\mathcal{G} = Cmcm$, $P = (\mathbf{c}, \mathbf{a}, \mathbf{b})$, $p = (\frac{1}{4}\,0\,\frac{1}{4})$*;* $u = 0.481$. *WP=Wyckoff positions.*

Atom	Initial structure				High-symmetry structure			
	WP	x	y	z	WP	x	y	z
Ge(1)	2b	1/2	0.258	0.700	4c	1/2	1/4	0.691
Ge(2)	2a	0	0.756	0.817		0	3/4	0.809
Nd(1)	2a	0	0.265	0.519	4c	0	1/4	0.513
Nd(2)	2b	1/2	0.231	0.492		1/2	1/4	0.487
Nd(3)	2a	0	0.292	0.724	4c	0	1/4	0.718
Nd(4)	2b	1/2	0.787	0.789		1/2	3/4	0.782
Nd(5)	4c	0.242	0.769	0.609	8f	0.240	3/4	0.603
Nd(6)	4c	0.261	0.274	0.902		0.260	1/4	0.897
O(1)	2a	0	0.531	0.623	8g	0	0.496	0.621
O(3)	2a	0	0.041	0.633		0	0.004	0.621
O(9)	2b	1/2	0.004	0.890		1/2	0.996	0.879
O(10)	2b	1/2	0.512	0.881		1/2	0.504	0.879
O(2)	2b	1/2	0.063	0.619	8g	1/2	0.001	0.640
O(4)	2b	1/2	0.545	0.662		1/2	0.499	0.640
O(7)	2a	0	0.056	0.838		0	1.000	0.860
O(8)	2a	0	0.540	0.885		0	0.500	0.860
O(5)	4c	0.186	0.668	0.767	8f	0.187	3/4	0.756
O(6)	4c	0.312	0.192	0.755		0.313	1/4	0.744
O(11)	4c	0.215	0.010	0.005	8e	1/4	0.009	1
O(12)	4c	0.258	0.492	0.016		1/4	0.491	1

Table 3. *Initial and calculated high-symmetry structure for $Sr(OH)_2(H_2O)$.* $\mathbf{a} = 3.6478$, $\mathbf{b} = 6.1981$, $\mathbf{c} = 6.7131$*;* $\mathcal{G} = Pmma$, $P = (\mathbf{b}, \mathbf{c}, \mathbf{a})$*;* $u = 0.059$. *WP=Wyckoff positions.*

Atom	Initial structure				High-symmetry structure			
	WP	x	y	z	WP	x	y	z
H(1)	4c	0.290	0.884	0.271	4k	0.290	0.884	1/4
O(1)	2a	0	0.781	0.317	2e	0	0.781	1/4
O(2)	2b	1/2	0.065	0.183	2f	1/2	0.065	1/4
O(3)	2b	1/2	0.563	-0.024	2d	1/2	1/2	0
Sr(1)	2a	0	0.372	0.191	2e	0	0.372	1/4

Table 4. *Initial and calculated high-symmetry structure for β-Ba(OH)$_2$(H$_2$O).* $\mathbf{a} = 3.8947$, $\mathbf{b} = 6.6357$, $\mathbf{c} = 6.9523$; $\mathcal{G} = Pmma$, $P = (\mathbf{b}, \mathbf{c}, \mathbf{a})$; $u = 0.044$. *WP=Wyckoff positions.*

Atom	Initial structure				High-symmetry structure			
	WP	x	y	z	WP	x	y	z
H(1)	4c	0.22	0.865	0.249	4k	0.22	0.865	1/4
O(1)	2a	0	0.792	0.317	2e	0	0.792	1/4
O(2)	2b	1/2	0.039	0.183	2f	1/2	0.039	1/4
O(3)	2b	1/2	0.564	-0.011	2d	1/2	1/2	0
Ba(1)	2a	0	0.355	0.206	2e	0	0.355	1/4

Table 5. *Initial and calculated high-symmetry structures for Na(AlSi$_2$O$_6$)$_3$(H$_2$O)$_{1.1}$.* $\mathbf{a} = 7.521$, $\mathbf{b} = 8.221$, $\mathbf{c} = 5.225$; $\mathcal{G} = Pmma$, $P = (\mathbf{b}, \mathbf{c}, \mathbf{a})$; $u = 0.233$. *WP=Wyckoff positions.*

Atom	Initial structure				High-symmetry structure			
	WP	x	y	z	WP	x	y	z
Al/Si(1)	2a	0	0.894	-0.233	2e	0	0.894	-1/4
Al/Si(2)	4c	0.717	0.606	0.753	4k	0.717	0.606	3/4
H(1)	2b	1/2	0.081	-0.023	2b	1/2	0	0
H(2)	2b	1/2	0.067	-0.213	2f	1/2	0.067	-1/4
Na(1)	2a	0	0.323	-0.210	2e	0	0.323	-1/4
O(1)	2b	1/2	0.642	0.736	2f	1/2	0.642	3/4
O(2)	4c	0.216	0.467	0.537	4h	0.216	1/2	1/2
O(3)	4c	0.179	0.783	0.687	4k	0.179	0.783	3/4
O(4)	2a	0	0.064	0.582	2a	0	0	1/2
O(5)	2b	1/2	0.082	0.145	2f	1/2	0.082	1/4
O(6)	2b	1/2	0.844	0.244	2f	1/2	0.844	1/4
O(7)	2b	1/2	0.984	0.193	2f	1/2	0.984	1/4

Table 6. *Initial and calculated high-symmetry structures for* $La_2Fe_{1.76}S_5$. $\mathbf{a} = 4.001$, $\mathbf{b} = 32.936$, $\mathbf{c} = 11.291$; $\mathcal{G} = Pmma$, $P = (\mathbf{b}, \mathbf{c}, \mathbf{a})$; $u = 0.004$. *WP=Wyckoff positions.*

Atom	Initial structure				High-symmetry structure			
	WP	x	y	z	WP	x	y	z
Fe(1)	2a	0	0.352	0.238	2e	0	0.352	1/4
Fe(2)	2a	0	0.150	0.769	2e	0	0.150	3/4
Fe(3)	2b	1/2	0.101	0.273	2f	1/2	0.101	1/4
Fe(4)	2b	1/2	2/5	0.734	2f	1/2	2/5	3/4
Fe(5)	2a	0	0.036	0.212	2e	0	0.036	1/4
Fe(6)	2a	0	0.460	0.769	2e	0	0.460	3/4
Fe(7)	2b	1/2	0.295	0.227	2f	1/2	0.295	1/4
Fe(8)	2b	1/2	0.221	0.716	2f	1/2	0.221	3/4
La(1)	2a	0	0.189	0.062	4i	0	0.189	0.056
La(5)	2a	0	0.188	4/9		0	0.189	4/9
La(2)	2a	0	0.313	0.538	4i	0	0.311	0.558
La(6)	2a	0	0.310	0.922		0	0.311	0.942
La(3)	2b	1/2	0.439	0.049	4j	1/2	0.439	0.054
La(7)	2b	1/2	0.438	4/9		1/2	0.439	0.446
La(4)	2b	1/2	0.063	0.563	4j	1/2	0.061	0.559
La(8)	2b	1/2	0.060	0.944		1/2	0.061	0.941
S(1)	2a	0	0.097	0.118	4i	0	0.100	0.099
S(5)	2a	0	0.102	0.421		0	0.100	0.402
S(2)	2a	0	0.402	0.598	4i	0	0.401	0.602
S(6)	2a	0	2/5	0.895		0	0.401	0.898
S(3)	2b	1/2	0.351	0.085	4j	1/2	0.350	0.100
S(7)	2b	1/2	0.349	0.386		1/2	0.350	0.401
S(4)	2b	1/2	0.151	0.615	4j	1/2	0.151	3/5
S(8)	2b	1/2	0.151	0.913		1/2	0.151	0.899
S(9)	2a	0	0.426	0.244	2e	0	0.426	1/4
S(10)	2a	0	0.077	0.765	2e	0	0.077	3/4
S(11)	2b	1/2	0.178	0.252	2f	1/2	0.178	1/4
S(12)	2b	1/2	0.326	0.735	2f	1/2	0.326	3/4
S(13)	2a	0	0.002	0.541	2a	0	0	1/2
S(14)	2a	0	0.503	0.463	2c	0	1/2	1/2
S(15)	2b	1/2	0.249	0.525	4j	1/2	0.252	0.494
S(16)	2b	1/2	0.254	0.036		1/2	0.252	0.005
S(17)	2a	0	0.269	0.293	2e	0	0.269	1/4
S(18)	2a	0	0.226	0.810	2e	0	0.226	3/4
S(19)	2b	1/2	0.019	0.305	2f	1/2	0.019	1/4
S(20)	2b	1/2	0.478	0.690	2f	1/2	0.478	3/4