TABLE I. Symmetry analysis of candidate compounds with $\mathcal{H}_{ME} \neq 0$.

Comp	Crystal symmetry (space and point group)	Site point group	Magnetic symmetry (space and point group)	Related dipoles	Related quadrupoles	Comments/$\mathcal{M}_e$
$MnTiO_3$	$R3c$ (C_{3v})	C_3	Cc' (m')	1×Mn1[+−] $\begin{pmatrix} 0 & 0 & p_z \\ 0 & 0 & p_z \end{pmatrix}$ 1×Mn2[+−] $\begin{pmatrix} \delta p_{x2} & -\delta p_{y2} & p_z \\ \delta p_{x2} & -\delta p_{y2} & p_z \end{pmatrix}$ 1×Mn3[+−] $\begin{pmatrix} -\delta p_{x3} & \delta p_{y3} & p_z \\ -\delta p_{x3} & \delta p_{y3} & p_z \end{pmatrix}$	1×Mn1[+−] $\begin{pmatrix} -\mathcal{Q}_{x1} & 0 & \delta_{xz1} \\ 0 & -\mathcal{Q}_{x1} & \delta_{yz1} \\ \delta_{xz1} & \delta_{yz1} & 2\mathcal{Q}_{x1} \end{pmatrix}\begin{pmatrix} -\mathcal{Q}'_{x1} & 0 & \delta'_{xz1} \\ 0 & -\mathcal{Q}'_{x1} & \delta'_{yz1} \\ \delta'_{xz1} & \delta'_{yz1} & 2\mathcal{Q}'_{x1} \end{pmatrix}$ 1×Mn2[+−] $\begin{pmatrix} -\mathcal{Q}_{x2} & 0 & \delta_{xz2} \\ 0 & -\mathcal{Q}_{x2} & \delta_{yz2} \\ \delta_{xz2} & \delta_{yz2} & 2\mathcal{Q}_{x2} \end{pmatrix}\begin{pmatrix} -\mathcal{Q}'_{x2} & 0 & \delta'_{xz2} \\ 0 & -\mathcal{Q}'_{x2} & \delta'_{yz2} \\ \delta'_{xz2} & \delta'_{yz2} & 2\mathcal{Q}'_{x2} \end{pmatrix}$ 1×Mn3[+−] $\begin{pmatrix} -\mathcal{Q}_{x3} & 0 & \delta_{xz3} \\ 0 & -\mathcal{Q}_{x3} & \delta_{yz3} \\ \delta_{xz3} & \delta_{yz3} & 2\mathcal{Q}_{x3} \end{pmatrix}\begin{pmatrix} -\mathcal{Q}_{x3} & 0 & \delta'_{xz3} \\ 0 & -\mathcal{Q}_{x3} & \delta'_{yz3} \\ \delta'_{xz3} & \delta'_{yz3} & 2\mathcal{Q}_{x3} \end{pmatrix}$	• **Electric behavior**: Ferroelectric • **Connection between opposite-moment sites**: $\mathcal{M}'_{[100]}$ • **Magnetoelectric term**: $\mathcal{H}_{ME} \propto \delta_x k_x^2 + \delta_y k_y^2 + \delta_z k_z^2 + \delta_{xz} k_x k_z + \delta_{yz} k_y k_z$ • **Notes**: The structure exhibits distortions with components δ on the order of 10^{-8} to 10^{-7}. These small δ values slightly modify the dipoles and quadrupoles, preventing a perfect mapping of magnetic sites by the symmetry operation, but inducing a small secondary SS.
$ScFeO_3$	$R3c$ (C_{3v})	C_3	Cc' (m')	1×Fe1[↑↓] $\begin{pmatrix} \delta x & -\delta y & -p_z \\ \delta x & -\delta y & -p_z \end{pmatrix}$ 1×Fe2[↑↓] $\begin{pmatrix} \delta x & -\delta y & -p_z \\ -2\delta x & 2\delta y & -p_z \end{pmatrix}$ 1×Fe3[↑↓] $\begin{pmatrix} -2\delta x & 2\delta y & -p_z \\ \delta x & -\delta y & -p_z \end{pmatrix}$	1×Fe1[+ −] $\begin{pmatrix} -\mathcal{Q}_{x1} & 0 & \delta_{xz1} \\ 0 & -\mathcal{Q}_{x1} & -\delta_{yz1} \\ \delta_{xz1} & -\delta_{yz1} & 2\mathcal{Q}_{x1} \end{pmatrix}\begin{pmatrix} -\mathcal{Q}_{x1} & 0 & \delta_{xz1} \\ 0 & -\mathcal{Q}_{x1} & -\delta_{yz1} \\ \delta_{xz1} & -\delta_{yz1} & 2\mathcal{Q}_{x1} \end{pmatrix}$ 1×Fe2[+ −] $\begin{pmatrix} -\mathcal{Q}_{x1} & 0 & \delta_{xz1} \\ 0 & -\mathcal{Q}_{x1} & -\delta_{yz1} \\ \delta_{xz1} & -\delta_{yz1} & 2\mathcal{Q}_{x1} \end{pmatrix}\begin{pmatrix} -\mathcal{Q}_{x1} & 0 & -2\delta_{xz1} \\ 0 & -\mathcal{Q}_{x1} & 2\delta_{yz1} \\ -2\delta_{xz1} & 2\delta_{yz1} & 2\mathcal{Q}_{x1} \end{pmatrix}$ 1×Fe3[+ −] $\begin{pmatrix} -\mathcal{Q}_{x1} & 0 & -2\delta_{xz1} \\ 0 & -\mathcal{Q}_{x1} & 2\delta_{yz1} \\ -2\delta_{xz1} & 2\delta_{yz1} & 2\mathcal{Q}_{x1} \end{pmatrix}\begin{pmatrix} -\mathcal{Q}_{x1} & 0 & \delta_{xz1} \\ 0 & -\mathcal{Q}_{x1} & -\delta_{yz1} \\ \delta_{xz1} & -\delta_{yz1} & 2\mathcal{Q}_{x1} \end{pmatrix}$	• **Electric behavior**: Ferroelectric • **Connection between opposite-moment sites**: $\mathcal{M}'_{[100]}$ • **Magnetoelectric term**: $\mathcal{H}_{ME} \propto \delta_{yz} k_y k_z - \delta_{xz} k_x k_z$ • **Notes**: The material exhibits small distortions.
$Mn_4Nb_2O_9$	Cc (C_s)	C_1	Cc ($m.1$)	2×Mn1[+ −] $\begin{pmatrix} -p_{x1} & p_{y1} & p_{z1} \\ -p_{x1} & -p_{y1} & p_{z1} \end{pmatrix}$ 2×Mn2[+ −] $\begin{pmatrix} p_{x2} & -p_{y2} & p_{z2} \\ p_{x2} & p_{y2} & p_{z2} \end{pmatrix}$ 2×Mn3[+ −] $\begin{pmatrix} -p_{x3} & -p_{y3} & p_{z3} \\ -p_{x3} & p_{y3} & p_{z3} \end{pmatrix}$ 2×Mn4[+ −] $\begin{pmatrix} -p_{x4} & p_{y4} & p_{z4} \\ -p_{x4} & -p_{y4} & p_{z4} \end{pmatrix}$	2×Mn1[+ −] $\begin{pmatrix} -\mathcal{Q}_{x1} & \mathcal{Q}_{xy1} & -\mathcal{Q}_{xz1} \\ \mathcal{Q}_{xy1} & \mathcal{Q}_{y1} & -\mathcal{Q}_{yz1} \\ -\mathcal{Q}_{xz1} & -\mathcal{Q}_{yz1} & \mathcal{Q}_{x1} - \mathcal{Q}_{y1} \end{pmatrix}\begin{pmatrix} -\mathcal{Q}_{x1} & -\mathcal{Q}_{xy1} & -\mathcal{Q}_{xz1} \\ -\mathcal{Q}_{xy1} & \mathcal{Q}_{y1} & \mathcal{Q}_{yz1} \\ -\mathcal{Q}_{xz1} & \mathcal{Q}_{yz1} & \mathcal{Q}_{x1} - \mathcal{Q}_{y1} \end{pmatrix}$ 2×Mn2[+ −] $\begin{pmatrix} \mathcal{Q}_{x2} & \mathcal{Q}_{xy2} & -\mathcal{Q}_{xz2} \\ \mathcal{Q}_{xy2} & \mathcal{Q}_{y2} & \mathcal{Q}_{yz2} \\ -\mathcal{Q}_{xz2} & \mathcal{Q}_{yz2} & -\mathcal{Q}_{x2} - \mathcal{Q}_{y2} \end{pmatrix}\begin{pmatrix} \mathcal{Q}_{x2} & -\mathcal{Q}_{xy2} & -\mathcal{Q}_{xz2} \\ -\mathcal{Q}_{xy2} & \mathcal{Q}_{y2} & -\mathcal{Q}_{yz2} \\ -\mathcal{Q}_{xz2} & -\mathcal{Q}_{yz2} & -\mathcal{Q}_{x2} - \mathcal{Q}_{y2} \end{pmatrix}$ 2×Mn3[+ −] $\begin{pmatrix} \mathcal{Q}_{x3} & \mathcal{Q}_{xy3} & \mathcal{Q}_{xz3} \\ \mathcal{Q}_{xy3} & -\mathcal{Q}_{y3} & \mathcal{Q}_{yz3} \\ \mathcal{Q}_{xz3} & \mathcal{Q}_{yz3} & -\mathcal{Q}_{x3} + \mathcal{Q}_{y3} \end{pmatrix}\begin{pmatrix} \mathcal{Q}_{x3} & -\mathcal{Q}_{xy3} & \mathcal{Q}_{xz3} \\ -\mathcal{Q}_{xy3} & -\mathcal{Q}_{y3} & -\mathcal{Q}_{yz3} \\ \mathcal{Q}_{xz3} & -\mathcal{Q}_{yz3} & -\mathcal{Q}_{x3} + \mathcal{Q}_{y3} \end{pmatrix}$ 2×Mn4[+ −] $\begin{pmatrix} \mathcal{Q}_{x4} & \mathcal{Q}_{xy4} & -\mathcal{Q}_{xz4} \\ \mathcal{Q}_{xy4} & \mathcal{Q}_{y4} & -\mathcal{Q}_{yz4} \\ -\mathcal{Q}_{xz4} & -\mathcal{Q}_{yz4} & -\mathcal{Q}_{x4} - \mathcal{Q}_{y4} \end{pmatrix}\begin{pmatrix} \mathcal{Q}_{x4} & -\mathcal{Q}_{xy4} & -\mathcal{Q}_{xz4} \\ -\mathcal{Q}_{xy4} & \mathcal{Q}_{y4} & \mathcal{Q}_{yz4} \\ -\mathcal{Q}_{xz4} & \mathcal{Q}_{yz4} & -\mathcal{Q}_{x4} - \mathcal{Q}_{y4} \end{pmatrix}$	• **Electric behavior**: Ferroelectric • **Connection between opposite-moment sites**: $\mathcal{M}_{[010]}$ • **Magnetoelectric term**: $\mathcal{H}_{ME} \propto \gamma k_y + k_y(\alpha k_x + \beta k_z)$ • **Notes**: —
$MnSiN_2$	$Pna2_1$ (C_{3v})	C_1	Pc' (m')	1×Mn1[+ −] $\begin{pmatrix} p_{x1} & -p_{y1} & p_{z1} \\ -p_{x1} & p_{y1} & p_{z1} \end{pmatrix}$ 1×Mn2[+ −] $\begin{pmatrix} p_{x2} & p_{y2} & -p_{z2} \\ p_{x2} & -p_{y2} & -p_{z2} \end{pmatrix}$	1×Mn1[+ −] $\begin{pmatrix} \mathcal{Q}_{x1} & -\mathcal{Q}_{xy1} & \mathcal{Q}_{xz1} \\ -\mathcal{Q}_{xy1} & \mathcal{Q}_{y1} & \mathcal{Q}_{yz1} \\ \mathcal{Q}_{xz1} & \mathcal{Q}_{yz1} & -\mathcal{Q}_{x1} - \mathcal{Q}_{y1} \end{pmatrix}\begin{pmatrix} \mathcal{Q}_{x1} & \mathcal{Q}_{xy1} & \mathcal{Q}_{xz1} \\ \mathcal{Q}_{xy1} & \mathcal{Q}_{y1} & -\mathcal{Q}_{yz1} \\ \mathcal{Q}_{xz1} & -\mathcal{Q}_{yz1} & -\mathcal{Q}_{x1} - \mathcal{Q}_{y1} \end{pmatrix}$ 1×Mn2[+ −] $\begin{pmatrix} \mathcal{Q}_{x2} & \mathcal{Q}_{xy2} & -\mathcal{Q}_{xz2} \\ \mathcal{Q}_{xy2} & \mathcal{Q}_{y2} & \mathcal{Q}_{yz2} \\ -\mathcal{Q}_{xz2} & \mathcal{Q}_{yz2} & -\mathcal{Q}_{x2} - \mathcal{Q}_{y2} \end{pmatrix}\begin{pmatrix} \mathcal{Q}_{x2} & -\mathcal{Q}_{xy2} & -\mathcal{Q}_{xz2} \\ -\mathcal{Q}_{xy2} & \mathcal{Q}_{y2} & -\mathcal{Q}_{yz2} \\ -\mathcal{Q}_{xz2} & -\mathcal{Q}_{yz2} & -\mathcal{Q}_{x2} - \mathcal{Q}_{y2} \end{pmatrix}$	• **Electric behavior**: Ferroelectric • **Connection between opposite-moment sites**: $\mathcal{M}'_{[010]}$ • **Magnetoelectric term**: $\mathcal{H}_{ME} \propto \gamma k_y + k_y(\alpha k_x + \beta k_z)$ • **Notes**: Atoms related by $\mathcal{M}'_{[010]}$ have moments $(4.891, \pm 0.007, 0.953)$ and $(4.896, \pm 0.002, 0.963)$. Small opposite y-components indicate the system is not strictly collinear.
Li_2CoSiO_4	$Pna2_1$ (C_{2v})	C_1	C_ac ($m.1'$)	4×Co1[+ −] $\begin{pmatrix} -p_x & -p_y & -p_z \\ -p_x & p_y & -p_z \end{pmatrix}$ 4×Co2[+ −] $\begin{pmatrix} p_x & p_y & -p_z \\ p_x & -p_y & -p_z \end{pmatrix}$	4×Co1[+ −] $\begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}\begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$ 4×Co2[+ −] $\begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}\begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$	• **Electric behavior**: Ferroelectric • **Connection between opposite-moment sites**: $\mathcal{M}_{[010]}$ • **Magnetoelectric term**: $\mathcal{H}_{ME} \propto \gamma k_x k_y$ • **Notes**: —

TABLE II. Symmetry analysis of candidate compounds with $\mathcal{H}_{ME} = 0$.

Comp	Crystal symmetry (space and point group)	Site point group	Magnetic symmetry (space and point group)	Related dipoles	Related quadrupoles	Comments/$\mathcal{M}_{\mathcal{A}}$
$BaFe_2Se_3$	*Pnma* (D_{2h})	C_1	C_ac ($m.1'$)	4×Fe1[+ −] $\begin{pmatrix} -p_x & -p_y & -p_z \\ p_x & -p_y & -p_z \end{pmatrix}$ 4×Fe2[+ −] $\begin{pmatrix} p_x & -p_y & -p_z \\ -p_x & -p_y & -p_z \end{pmatrix}$ 4×Fe3[+ −] $\begin{pmatrix} p_x & p_y & -p_z \\ -p_x & p_y & -p_z \end{pmatrix}$ 4×Fe4[+ −] $\begin{pmatrix} -p_x & p_y & -p_z \\ p_x & p_y & -p_z \end{pmatrix}$ 4×Fe5[+ −] $\begin{pmatrix} p_x & -p_y & p_z \\ -p_x & -p_y & p_z \end{pmatrix}$ 4×Fe6[+ −] $\begin{pmatrix} -p_x & -p_y & p_z \\ p_x & -p_y & p_z \end{pmatrix}$ 4×Fe7[+ −] $\begin{pmatrix} -p_x & p_y & p_z \\ p_x & p_y & p_z \end{pmatrix}$ 4×Fe8[+ −] $\begin{pmatrix} p_x & p_y & p_z \\ -p_x & p_y & p_z \end{pmatrix}$	4×Fe1[+ −] $\begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$ 4×Fe2[+ −] $\begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$ 4×Fe3[+ −] $\begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$ 4×Fe4[+ −] $\begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$ 4×Fe5[+ −] $\begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$ 4×Fe6[+ −] $\begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$ 4×Fe7[+ −] $\begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$ 4×Fe8[+ −] $\begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$	• **Electric behavior**: Antiferroelectric • **Connection between opposite-moment sites**: $\mathcal{M}_{[100]}$ • **Magnetoelectric term**: $\mathcal{H}_{ME} = 0$ • **Notes**: No spin splitting occurs.
$PrMn_2O_5$	*Pbam* (D_{2h})	C_s	P_cc ($m.1'$)	2×Mn_1^{4+} [+ −] $\begin{pmatrix} 0 & 0 & -p_{z1} \\ -\mathcal{Q}_{xy1} & -\mathcal{Q}_{y1} & 0 \\ 0 & 0 & p_{z1} \end{pmatrix}$ 2×Mn_2^{4+} [+ −] $\begin{pmatrix} 0 & 0 & p_{z1} \\ \mathcal{Q}_{xy1} & -\mathcal{Q}_{y1} & 0 \\ 0 & 0 & -p_{z1} \end{pmatrix}$ 1×Mn_1^{3+} [+ −] $\begin{pmatrix} -p_{x2} & p_{y2} & 0 \\ -\mathcal{Q}_{xy2} & -\mathcal{Q}_{y2} & 0 \\ -p_{x2} & p_{y2} & 0 \end{pmatrix}$ 1×Mn_2^{3+} [+ −] $\begin{pmatrix} p_{x2} & -p_{y2} & 0 \\ p_{x2} & -p_{y2} & 0 \end{pmatrix}$ 1×Mn_3^{3+} [+ −] $\begin{pmatrix} p_{x2} & p_{y2} & 0 \\ \mathcal{Q}_{xy2} & -\mathcal{Q}_{y2} & 0 \\ p_{x2} & p_{y2} & 0 \end{pmatrix}$ 1×Mn_4^{3+} [+ −] $\begin{pmatrix} -p_{x2} & -p_{y2} & 0 \\ -p_{x2} & -p_{y2} & 0 \end{pmatrix}$	2×Mn^{4+}[+ −] $\begin{pmatrix} \mathcal{Q}_{x1} & -\mathcal{Q}_{xy1} & 0 \\ -\mathcal{Q}_{xy1} & -\mathcal{Q}_{y1} & 0 \\ 0 & 0 & -\mathcal{Q}_{x1} + \mathcal{Q}_{y1} \end{pmatrix} \begin{pmatrix} \mathcal{Q}_{x1} & -\mathcal{Q}_{xy1} & 0 \\ -\mathcal{Q}_{xy1} & -\mathcal{Q}_{y1} & 0 \\ 0 & 0 & -\mathcal{Q}_{x1} + \mathcal{Q}_{y1} \end{pmatrix}$ 2×Mn^{4+}[+ −] $\begin{pmatrix} \mathcal{Q}_{x1} & \mathcal{Q}_{xy1} & 0 \\ \mathcal{Q}_{xy1} & -\mathcal{Q}_{y1} & 0 \\ 0 & 0 & -\mathcal{Q}_{x1} + \mathcal{Q}_{y1} \end{pmatrix} \begin{pmatrix} \mathcal{Q}_{x1} & \mathcal{Q}_{xy1} & 0 \\ \mathcal{Q}_{xy1} & -\mathcal{Q}_{y1} & 0 \\ 0 & 0 & -\mathcal{Q}_{x1} + \mathcal{Q}_{y1} \end{pmatrix}$ 1×Mn^{3+}[+ −] $\begin{pmatrix} \mathcal{Q}_{x2} & -\mathcal{Q}_{xy2} & 0 \\ -\mathcal{Q}_{xy2} & -\mathcal{Q}_{y2} & 0 \\ 0 & 0 & -\mathcal{Q}_{x2} + \mathcal{Q}_{y2} \end{pmatrix} \begin{pmatrix} \mathcal{Q}_{x2} & -\mathcal{Q}_{xy2} & 0 \\ -\mathcal{Q}_{xy2} & -\mathcal{Q}_{y2} & 0 \\ 0 & 0 & -\mathcal{Q}_{x2} + \mathcal{Q}_{y2} \end{pmatrix}$ 1×Mn^{3+}[+ −] $\begin{pmatrix} \mathcal{Q}_{x2} & -\mathcal{Q}_{xy2} & 0 \\ -\mathcal{Q}_{xy2} & -\mathcal{Q}_{y2} & 0 \\ 0 & 0 & -\mathcal{Q}_{x2} + \mathcal{Q}_{y2} \end{pmatrix} \begin{pmatrix} \mathcal{Q}_{x2} & -\mathcal{Q}_{xy2} & 0 \\ -\mathcal{Q}_{xy2} & -\mathcal{Q}_{y2} & 0 \\ 0 & 0 & -\mathcal{Q}_{x2} + \mathcal{Q}_{y2} \end{pmatrix}$ 1×Mn^{3+}[+ −] $\begin{pmatrix} \mathcal{Q}_{x2} & \mathcal{Q}_{xy2} & 0 \\ \mathcal{Q}_{xy2} & -\mathcal{Q}_{y2} & 0 \\ 0 & 0 & -\mathcal{Q}_{x2} + \mathcal{Q}_{y2} \end{pmatrix} \begin{pmatrix} \mathcal{Q}_{x2} & \mathcal{Q}_{xy2} & 0 \\ \mathcal{Q}_{xy2} & -\mathcal{Q}_{y2} & 0 \\ 0 & 0 & -\mathcal{Q}_{x2} + \mathcal{Q}_{y2} \end{pmatrix}$ 1×Mn^{3+}[+ −] $\begin{pmatrix} \mathcal{Q}_{x2} & \mathcal{Q}_{xy2} & 0 \\ \mathcal{Q}_{xy2} & -\mathcal{Q}_{y2} & 0 \\ 0 & 0 & -\mathcal{Q}_{x2} + \mathcal{Q}_{y2} \end{pmatrix} \begin{pmatrix} \mathcal{Q}_{x2} & \mathcal{Q}_{xy2} & 0 \\ \mathcal{Q}_{xy2} & -\mathcal{Q}_{y2} & 0 \\ 0 & 0 & -\mathcal{Q}_{x2} + \mathcal{Q}_{y2} \end{pmatrix}$	• **Electric behavior**: Antiferroelectric • **Connection between opposite-moment sites**: $\mathcal{M}_{[001]}$ • **Magnetoelectric term**: $\mathcal{H}_{ME} = 0$ • **Notes**: The manganese valences are different.
HoNiGe	*Pnma* (D_{2h})	C_s	P_cc ($m.1'$)	2×Ho1[+ −] $\begin{pmatrix} p_x & 0 & p_z \\ p_x & 0 & p_z \end{pmatrix}$ 2×Ho2[+ −] $\begin{pmatrix} -p_x & 0 & p_z \\ -p_x & 0 & p_z \end{pmatrix}$ 2×Ho3[+ −] $\begin{pmatrix} -p_x & 0 & -p_z \\ -p_x & 0 & -p_z \end{pmatrix}$ 2×Ho4[+ −] $\begin{pmatrix} p_x & 0 & -p_z \\ p_x & 0 & -p_z \end{pmatrix}$	2×Ho1[+ −] $\begin{pmatrix} \mathcal{Q}_x & 0 & \mathcal{Q}_{xz} \\ 0 & -\mathcal{Q}_y & 0 \\ \mathcal{Q}_{xz} & 0 & -\mathcal{Q}_x + \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} \mathcal{Q}_x & 0 & \mathcal{Q}_{xz} \\ 0 & -\mathcal{Q}_y & 0 \\ \mathcal{Q}_{xz} & 0 & -\mathcal{Q}_x + \mathcal{Q}_y \end{pmatrix}$ 2×Ho2[+ −] $\begin{pmatrix} \mathcal{Q}_x & 0 & -\mathcal{Q}_{xz} \\ 0 & -\mathcal{Q}_y & 0 \\ -\mathcal{Q}_{xz} & 0 & -\mathcal{Q}_x + \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} \mathcal{Q}_x & 0 & -\mathcal{Q}_{xz} \\ 0 & -\mathcal{Q}_y & 0 \\ -\mathcal{Q}_{xz} & 0 & -\mathcal{Q}_x + \mathcal{Q}_y \end{pmatrix}$ 2×Ho3[+ −] $\begin{pmatrix} \mathcal{Q}_x & 0 & \mathcal{Q}_{xz} \\ 0 & -\mathcal{Q}_y & 0 \\ \mathcal{Q}_{xz} & 0 & -\mathcal{Q}_x + \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} \mathcal{Q}_x & 0 & \mathcal{Q}_{xz} \\ 0 & -\mathcal{Q}_y & 0 \\ \mathcal{Q}_{xz} & 0 & -\mathcal{Q}_x + \mathcal{Q}_y \end{pmatrix}$ 2×Ho4[+ −] $\begin{pmatrix} \mathcal{Q}_x & 0 & -\mathcal{Q}_{xz} \\ 0 & -\mathcal{Q}_y & 0 \\ -\mathcal{Q}_{xz} & 0 & -\mathcal{Q}_x + \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} \mathcal{Q}_x & 0 & -\mathcal{Q}_{xz} \\ 0 & -\mathcal{Q}_y & 0 \\ -\mathcal{Q}_{xz} & 0 & -\mathcal{Q}_x + \mathcal{Q}_y \end{pmatrix}$	• **Electric behavior**: Antiferroelectric • **Connection between opposite-moment sites**: $\mathcal{M}_{[010]}$ • **Magnetoelectric term**: $\mathcal{H}_{ME} = 0$ • **Notes**: No spin splitting occurs. Magnetic moments and dipoles lie within the plane.
$AgCrS_2$	$R3m$ (C_{3v})	C_s	C_cm ($m.1'$)	2×Cr1[+ −] $\begin{pmatrix} -p_x & 0 & p_z \\ -p_x & 0 & p_z \end{pmatrix}$ 2×Cr2[+ −] $\begin{pmatrix} -p_x & 0 & p_z \\ -p_x & 0 & p_z \end{pmatrix}$	4×Cr1[+ −] $\begin{pmatrix} \mathcal{Q}_x & 0 & -\mathcal{Q}_{xz} \\ 0 & -\mathcal{Q}_y & 0 \\ -\mathcal{Q}_{xz} & 0 & -\mathcal{Q}_x + \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} \mathcal{Q}_x & 0 & -\mathcal{Q}_{xz} \\ 0 & -\mathcal{Q}_y & 0 \\ -\mathcal{Q}_{xz} & 0 & -\mathcal{Q}_x + \mathcal{Q}_y \end{pmatrix}$ 4×Cr2[+ −] $\begin{pmatrix} \mathcal{Q}_x & 0 & -\mathcal{Q}_{xz} \\ 0 & -\mathcal{Q}_y & 0 \\ -\mathcal{Q}_{xz} & 0 & -\mathcal{Q}_x + \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} \mathcal{Q}_x & 0 & -\mathcal{Q}_{xz} \\ 0 & -\mathcal{Q}_y & 0 \\ -\mathcal{Q}_{xz} & 0 & -\mathcal{Q}_x + \mathcal{Q}_y \end{pmatrix}$	• **Electric behavior**: Ferroelectric • **Connection between opposite-moment sites**: $\mathcal{M}_{[010]}$ • **Magnetoelectric term**: $\mathcal{H}_{ME} = 0$ • **Notes**: Dipolar and quadrupolar terms are equal between pairs; therefore, no SS occurs.

Comp	Crystal symmetry (space and point group)	Site point group	Magnetic symmetry (space and point group)	Related dipoles	Related quadrupoles	Comments/$\mathcal{M}_{\hat{e}}$
$BaFe_2Se_3$	$Pnma$ (D_{2h})	C_1	C_am ($m1'$)	4×Fe1[+ −] $\begin{pmatrix} -p_x & -p_y & -p_z \\ -p_x & p_y & -p_z \end{pmatrix}$ 4×Fe2[+ −] $\begin{pmatrix} -p_x & p_y & -p_z \\ -p_x & -p_y & -p_z \end{pmatrix}$ 4×Fe3[+ −] $\begin{pmatrix} p_x & -p_y & -p_z \\ p_x & p_y & -p_z \end{pmatrix}$ 4×Fe4[+ −] $\begin{pmatrix} p_x & p_y & -p_z \\ p_x & -p_y & -p_z \end{pmatrix}$ 4×Fe5[+ −] $\begin{pmatrix} p_x & p_y & p_z \\ p_x & -p_y & p_z \end{pmatrix}$ 4×Fe6[+ −] $\begin{pmatrix} p_x & -p_y & p_z \\ p_x & p_y & p_z \end{pmatrix}$ 4×Fe7[+ −] $\begin{pmatrix} -p_x & -p_y & p_z \\ -p_x & p_y & p_z \end{pmatrix}$ 4×Fe8[+ −] $\begin{pmatrix} -p_x & p_y & p_z \\ -p_x & -p_y & p_z \end{pmatrix}$	4×Fe1[+ −] $\begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$ 4×Fe2[+ −] $\begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$ 4×Fe3[+ −] $\begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$ 4×Fe4[+ −] $\begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$ 4×Fe5[+ −] $\begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$ 4×Fe6[+ −] $\begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & \mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ \mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$ 4×Fe7[+ −] $\begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$ 4×Fe8[+ −] $\begin{pmatrix} -\mathcal{Q}_x & -\mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & \mathcal{Q}_y & -\mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} -\mathcal{Q}_x & \mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & \mathcal{Q}_y & \mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & \mathcal{Q}_{yz} & \mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$	• **Electric behavior**: Antiferroelectric • **Connection between opposite-moment sites**: $\mathcal{M}_{[010]}$ • **Magnetoelectric term**: $\mathcal{H}_{ME} = 0$ • **Notes**: —
$La_{1.5}Ca_{0.5}CoO_4$	$Cmm2$ (C_{2v})	C_{2v}	P_cC ($m.1'$)	2×Co1[+ −] $\begin{pmatrix} -p_x & 0 & 0 \\ -p_x & 0 & 0 \end{pmatrix}$ 2×Co2[+ −] $\begin{pmatrix} -p_x & 0 & -p_z \\ -p_x & 0 & -p_z \end{pmatrix}$	2×Co1[+ −] $\begin{pmatrix} \mathcal{Q}_x & 0 & 0 \\ 0 & \mathcal{Q}_y & 0 \\ 0 & 0 & -\mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} \mathcal{Q}_x & 0 & 0 \\ 0 & \mathcal{Q}_y & 0 \\ 0 & 0 & -\mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$ 2×Co2[+ −] $\begin{pmatrix} \mathcal{Q}_x & 0 & -\mathcal{Q}_{xz} \\ 0 & \mathcal{Q}_y & 0 \\ -\mathcal{Q}_{xz} & 0 & -\mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} \mathcal{Q}_x & 0 & -\mathcal{Q}_{xz} \\ 0 & \mathcal{Q}_y & 0 \\ -\mathcal{Q}_{xz} & 0 & -\mathcal{Q}_x - \mathcal{Q}_y \end{pmatrix}$	• **Electric behavior**: Ferroelectric • **Connection between opposite-moment sites**: $\mathcal{M}_{[010]}$ • **Magnetoelectric term**: $\mathcal{H}_{ME} = 0$ • **Notes**: Two cobalt sites are non-magnetic.
Li_2FeGeS_4	Pn (C_s)	C_1	C_ac ($m.1'$)	4×Fe1[+ −] $\begin{pmatrix} p_x & -p_y & p_z \\ p_x & p_y & p_z \end{pmatrix}$ 4×Fe2[+ −] $\begin{pmatrix} p_x & p_y & p_z \\ p_x & -p_y & p_z \end{pmatrix}$	4×Fe1[+ −] $\begin{pmatrix} \mathcal{Q}_x & -\mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & -\mathcal{Q}_y & \mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & \mathcal{Q}_{yz} & -\mathcal{Q}_x + \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} \mathcal{Q}_x & \mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & -\mathcal{Q}_y & -\mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & -\mathcal{Q}_x + \mathcal{Q}_y \end{pmatrix}$ 4×Fe2[+ −] $\begin{pmatrix} \mathcal{Q}_x & \mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ \mathcal{Q}_{xy} & -\mathcal{Q}_y & -\mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & -\mathcal{Q}_{yz} & -\mathcal{Q}_x + \mathcal{Q}_y \end{pmatrix} \begin{pmatrix} \mathcal{Q}_x & -\mathcal{Q}_{xy} & -\mathcal{Q}_{xz} \\ -\mathcal{Q}_{xy} & -\mathcal{Q}_y & \mathcal{Q}_{yz} \\ -\mathcal{Q}_{xz} & \mathcal{Q}_{yz} & -\mathcal{Q}_x + \mathcal{Q}_y \end{pmatrix}$	• **Electric behavior**: Ferroelectric • **Connection between opposite-moment sites**: $\mathcal{M}_{[010]}$ • **Magnetoelectric term**: $\mathcal{H}_{ME} = 0$ • **Notes**: —