Supplementary material

Table S1 Displacive mode decomposition and V_A/V_B as a function of mode amplitudes for 15 perovskite structures.

a_p denotes the cell dimension of the cubic aristotype. The mode amplitude is a fraction of a_p. The prime symbol in d' is omitted for tidiness. The three subscripts of d are, in sequence: the relevant atom type, the irrep and the group of digits indicating the linear combination of the corresponding basis modes of the irrep. The V_A/V_B expressions are the same as in Table 3 of the text, with that following the equal sign is in terms of the amplitudes of all the symmetry-adapted modes of X anions condensed in each perovskite structure, and that following the approximately equal sign is in terms of only the tilt mode amplitudes.

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a $a^0a^0a^0$ No. 221 $Pm\bar{3}m$

$a = b = c = a_p$

A: (1*b*) $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

B: (1*a*) 0, 0, 0

X: (3*d*) $\frac{1}{2}$, 0, 0

$$\frac{V_A}{V_B} = 5$$

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b $a^-a^-a^-$ No. 167 $R\bar{3}c$

$a = b \approx \sqrt{2}a_p$, $c \approx 2\sqrt{3}a_p$, hexagonal cell

A: (6*a*) 0, 0, $\frac{1}{4}$

B: (6*b*) 0, 0, 0

X: (18*e*) $x\ (\approx \frac{1}{2}),\ 0,\ \frac{1}{4}$

$$d_{\mathrm{X},R_4^+,123} + \frac{1}{2} = x_{\mathrm{X}}$$

$$\frac{V_{\mathrm{A}}}{V_{\mathrm{B}}} = \frac{6}{1 + 4 \cdot 3 d^2_{\mathrm{X},R_4^+,123}} - 1$$

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c $a^0a^0c^+$ No. 127 *P*4/*mbm*

$a = b \approx \sqrt{2}a_p,\ c \approx a_p$

A: (2*c*) $0,\ \frac{1}{2},\ \frac{1}{2}$

B: (2*a*) 0, 0, 0

X1: (2*b*) $0,\ 0,\ \frac{1}{2}$

X2: (4*g*) $x\ (\approx \frac{1}{4}),\ x + \frac{1}{2},\ 0$

$$\frac{1}{2} d_{\mathrm{X},M_3^+,1} + \frac{1}{4} = x_{\mathrm{X2}}$$

$$\frac{V_{\mathrm{A}}}{V_{\mathrm{B}}} = \frac{6}{1 + 4 d^2_{\mathrm{X},M_3^+,1}} - 1$$

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d $a^0a^0c^-$ No. 140 *I*4/*mcm*

$a = b \approx \sqrt{2}a_p,\ c \approx 2a_p$

A: (4*b*) $0,\ \frac{1}{2},\ \frac{1}{4}$

B: (4*c*) 0, 0, 0

X1: (4*a*) $0,\ 0,\ \frac{1}{4}$

X2: (8*h*) $x\ (\approx \frac{1}{4}),\ x + \frac{1}{2},\ 0$

$$\frac{1}{2}d_{\mathrm{X},R_4^+,1}+\frac{1}{4}=x_{\mathrm{X2}}$$

$$\frac{V_\mathrm{A}}{V_\mathrm{B}}=\frac{6}{1+4d^2_{\mathrm{X},R_4^+,1}}-1$$

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e $a^0b^-b^-$ No. 74 *Imma*

$a \approx \sqrt{2}a_p$, $b \approx 2a_p$, $c \approx \sqrt{2}a_p$

A: (4*e*) $0, \frac{1}{4}, z\ (\approx \frac{1}{2})$

B: (4*a*) 0, 0, 0

X1: (4*e*) $0, \frac{1}{4}, z\ (\approx 0)$

X2: (8*g*) $\frac{1}{4}, y\ (\approx 0), \frac{3}{4}$

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}\begin{pmatrix} d_{\mathrm{A},R_5^+,12} \\ d_{\mathrm{X},R_4^+,12} \\ d_{\mathrm{X},R_5^+,12} \end{pmatrix}+\begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \end{pmatrix}=\begin{pmatrix} z_\mathrm{A} \\ z_{\mathrm{X1}} \\ y_{\mathrm{X2}} \end{pmatrix}$$

$$\frac{V_\mathrm{A}}{V_\mathrm{B}}=\frac{6}{1+8d^2_{\mathrm{X},R_4^+,12}-8d^2_{\mathrm{X},R_5^+,12}}-1$$
$$\approx\frac{6}{1+4\cdot 2d^2_{\mathrm{X},R_4^+,12}}-1$$

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f $a^0b^-c^-$ No. 12 *I*2/*m* (non-standard setting of *C*2/*m*)

$a \approx \sqrt{2}a_p$, $b \approx 2a_p$, $c \approx \sqrt{2}a_p$, $b \approx 90°$

A: (4*i*) $x\ (\approx \frac{1}{4}), 0, z\ (\approx \frac{3}{4})$

B: (4*e*) $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

X1: (4*i*) x ($\approx \frac{1}{4}$), 0, z ($\approx \frac{1}{4}$)

X2: (4*g*) 0, y ($\approx \frac{1}{4}$), 0

X3: (4*h*) $\frac{1}{2}$, y ($\approx \frac{1}{4}$), 0

$$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} d_{\mathrm{A},R_5^+,1} \\ d_{\mathrm{A},R_5^+,2} \\ d_{\mathrm{X},R_4^+,1} \\ d_{\mathrm{X},R_4^+,2} \\ d_{\mathrm{X},R_5^+,1} \\ d_{\mathrm{X},R_5^+,2} \end{pmatrix} + \begin{pmatrix} \frac{1}{4} \\ \frac{3}{4} \\ \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \end{pmatrix} = \begin{pmatrix} x_{\mathrm{A}} \\ z_{\mathrm{A}} \\ x_{\mathrm{X1}} \\ z_{\mathrm{X1}} \\ y_{\mathrm{X2}} \\ y_{\mathrm{X3}} \end{pmatrix}$$

$$\begin{aligned} \frac{V_{\mathrm{A}}}{V_{\mathrm{B}}} &= \frac{6}{1 + 4d^2_{\mathrm{X},R_4^+,1} + 4d^2_{\mathrm{X},R_4^+,2} - 4d^2_{\mathrm{X},R_5^+,1} - 4d^2_{\mathrm{X},R_5^+,2}} - 1 \\ &\approx \frac{6}{1 + 4\left(d^2_{\mathrm{X},R_4^+,1} + d^2_{\mathrm{X},R_4^+,2}\right)} - 1 \end{aligned}$$

g $a^-b^-b^-$ No. 15 *I*2/*a* (non-standard setting of *C*2/*c*)

$a \approx 2a_p$, $b \approx \sqrt{2}a_p$, $c \approx \sqrt{2}a_p$, $a \approx 90°$

A: (4*e*) $\frac{1}{4}$, y (≈ 0), 0

B: (4*b*) 0, $\frac{1}{2}$, 0

X1: (4*e*) $\frac{1}{4}$, y ($\approx \frac{1}{2}$), 0

X2: (8*f*) x (≈ 0), y ($\approx \frac{1}{4}$), z ($\approx \frac{1}{4}$)

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & \frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & -\frac{1}{2} & 0 & -\frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & -\frac{1}{2} & 0 \end{pmatrix} \begin{pmatrix} d_{\mathrm{A},R_5^+,13} \\ d_{\mathrm{X},R_3^+,12} \\ d_{\mathrm{X},R_4^+,13} \\ d_{\mathrm{X},R_4^+,2} \\ d_{\mathrm{X},R_5^+,13} \end{pmatrix} + \begin{pmatrix} 0 \\ \frac{1}{2} \\ 0 \\ \frac{1}{4} \\ \frac{1}{4} \end{pmatrix} = \begin{pmatrix} y_{\mathrm{A}} \\ y_{\mathrm{X1}} \\ x_{\mathrm{X2}} \\ y_{\mathrm{X2}} \\ z_{\mathrm{X2}} \end{pmatrix}$$

$$\frac{V_{\mathrm{A}}}{V_{\mathrm{B}}} = \frac{6}{1-4d^2_{\mathrm{X},R_3^+,12}+8d^2_{\mathrm{X},R_4^+,13}+4d^2_{\mathrm{X},R_4^+,2}-8d^2_{\mathrm{X},R_5^+,13}} - 1$$

$$\approx \frac{6}{1+4\left(2d^2_{\mathrm{X},R_4^+,13}+d^2_{\mathrm{X},R_4^+,2}\right)} - 1$$

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h $a^+b^-b^-$ No. 62 *Pnma*

$a \approx \sqrt{2}a_p$, $b \approx 2a_p$, $c \approx \sqrt{2}a_p$

A: (4*c*) $x\ (\approx \frac{1}{2}), \frac{1}{4}, z\ (\approx 0)$

B: (4*a*) 0, 0, 0

X1: (4*c*) $x\ (\approx 0), \frac{1}{4}, z\ (\approx 0)$

X2: (8*d*) $x\ (\approx \frac{3}{4}), y\ (\approx 0), z\ (\approx \frac{1}{4})$

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & -\frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} d_{\mathrm{A},R_5^+,12} \\ d_{\mathrm{A},X_5^+,1} \\ d_{\mathrm{X},M_2^+,3} \\ d_{\mathrm{X},M_3^+,3} \\ d_{\mathrm{X},R_4^+,12} \\ d_{\mathrm{X},R_5^+,12} \\ d_{\mathrm{X},X_5^+,1} \end{pmatrix} + \begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \\ 0 \\ \frac{3}{4} \\ 0 \\ \frac{1}{4} \end{pmatrix} = \begin{pmatrix} x_{\mathrm{A}} \\ z_{\mathrm{A}} \\ x_{\mathrm{X1}} \\ z_{\mathrm{X1}} \\ x_{\mathrm{X2}} \\ y_{\mathrm{X2}} \\ z_{\mathrm{X2}} \end{pmatrix}$$

$$\frac{V_\mathrm{A}}{V_\mathrm{B}} = \frac{6}{1-4d^2_{\mathrm{X},M_2^+,3}+4d^2_{\mathrm{X},M_3^+,3}+8d^2_{\mathrm{X},R_4^+,12}-8d^2_{\mathrm{X},R_5^+,12}+16\left(d_{\mathrm{X},M_2^+,3}+d_{\mathrm{X},M_3^+,3}\right)\left(d_{\mathrm{X},R_4^+,12}+d_{\mathrm{X},R_5^+,12}\right)d_{\mathrm{X},X_5^+,1}}-1$$

$$\approx \frac{6}{1+4\left(d^2_{\mathrm{X},M_3^+,3}+2d^2_{\mathrm{X},R_4^+,12}\right)}-1$$

i $a^+a^+c^-$ No. 137 $P4_2/nmc$

$a = b \approx 2a_p$, $c \approx 2a_p$

A1: (2*a*) $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$

A2: (2*b*) $\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$

A3: (4*d*) $\frac{1}{4}, \frac{1}{4}, z\ (\approx \frac{1}{4})$

B: (8*e*) 0, 0, 0

X1: (8*g*) $\frac{1}{4}, y\ (\approx 0), z\ (\approx 0)$

X2: (8*g*) $\frac{1}{4}, y\ (\approx \frac{1}{2}), z\ (\approx \frac{1}{2})$

X3: (8*f*) $x\ (\approx \frac{1}{2}), -x, \frac{1}{4}$

$$\begin{pmatrix} -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & \frac{1}{2} & 0 & -\frac{1}{2} & 0 & 0 \end{pmatrix} \begin{pmatrix} d_{\mathrm{A},X_5^+,1256} \\ d_{\mathrm{X},M_3^+,23} \\ d_{\mathrm{X},M_4^+,1} \\ d_{\mathrm{X},M_4^+,23} \\ d_{\mathrm{X},R_4^+,1} \\ d_{\mathrm{X},X_5^+,1256} \end{pmatrix} + \begin{pmatrix} \frac{1}{4} \\ 0 \\ 0 \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} = \begin{pmatrix} z_{\mathrm{A3}} \\ y_{\mathrm{X1}} \\ z_{\mathrm{X1}} \\ y_{\mathrm{X2}} \\ z_{\mathrm{X2}} \\ x_{\mathrm{X3}} \end{pmatrix}$$

$$\frac{V_A}{V_B} = \frac{6}{1+8d^2_{X,M_3^+,23} - 4d^2_{X,M_4^+,1} - 8d^2_{X,M_4^+,23} + 4d^2_{X,R_4^+,1} - 16d_{X,M_4^+,1}\left(d^2_{X,M_3^+,23} - d^2_{X,M_4^+,23}\right) - 16\left(d_{X,M_3^+,23} - d_{X,M_4^+,23}\right)d_{X,R_4^+,1}d_{X,X_5^+,1256}} - 1$$

$$\approx \frac{6}{1+4\left(2d^2_{X,M_3^+,23} + d^2_{X,R_4^+,1}\right)} - 1$$

j $a^0b^+c^-$ No. 63 *Cmcm*

$a \approx 2a_p$, $b \approx 2a_p$, $c \approx 2a_p$

A1: (4*c*) 0, y ($\approx$ 0), $\frac{1}{4}$

A2: (4*c*) 0, y ($\approx \frac{1}{2}$), $\frac{1}{4}$

B: (8*d*) $\frac{1}{4}$, $\frac{1}{4}$, 0

X1: (8*e*) x ($\approx \frac{1}{4}$), 0, 0

X2: (8*f*) 0, y ($\approx \frac{1}{4}$), z ($\approx$ 0)

X3: (8*g*) x ($\approx \frac{1}{4}$), y ($\approx \frac{1}{4}$), $\frac{1}{4}$

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} d_{A,R_5^+,3} \\ d_{A,X_5^+,34} \\ d_{X,M_3^+,1} \\ d_{X,M_4^+,1} \\ d_{X,R_4^+,3} \\ d_{X,R_5^+,3} \\ d_{X,X_5^+,34} \end{pmatrix} + \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{4} \\ \frac{1}{4} \\ 0 \\ \frac{1}{4} \\ \frac{1}{4} \end{pmatrix} = \begin{pmatrix} y_{A1} \\ y_{A2} \\ x_{X1} \\ y_{X2} \\ z_{X2} \\ x_{X3} \\ y_{X3} \end{pmatrix}$$

$$\frac{V_{\mathrm{A}}}{V_{\mathrm{B}}} = \frac{6}{1+4d^2_{\mathrm{X},M_3^+,1} - 4d^2_{\mathrm{X},M_4^+,1} + 4d^2_{\mathrm{X},R_4^+,3} - 4d^2_{\mathrm{X},R_5^+,3} - 8\left(d_{\mathrm{X},M_3^+,1} - d_{\mathrm{X},M_4^+,1}\right)\left(d_{\mathrm{X},R_4^+,3} - d_{\mathrm{X},R_5^+,3}\right)d_{\mathrm{X},X_5^+,34}} - 1$$

$$\approx \frac{6}{1+4\left(d^2_{\mathrm{X},M_3^+,1} + d^2_{\mathrm{X},R_4^+,3}\right)} - 1$$

k $a^+b^-c^-$ No. 11 $P2_1/m$

$a \approx \sqrt{2}a_p$, $b \approx 2a_p$, $c \approx \sqrt{2}a_p$, $b \approx 90°$

A1: (2*e*) x (≈ 0), $\frac{1}{4}$, z (≈ 0)

A2: (2*e*) x ($\approx \frac{1}{2}$), $\frac{1}{4}$, z ($\approx \frac{1}{2}$)

B1: (2*b*) $\frac{1}{2}$, 0, 0

B2: (2*c*) 0, 0, $\frac{1}{2}$

X1: (2*e*) x (≈ 0), $\frac{1}{4}$, z ($\approx \frac{1}{2}$)

X2: (2*e*) x ($\approx \frac{1}{2}$), $\frac{1}{4}$, z (≈ 0)

X3: (4*f*) x ($\approx \frac{1}{4}$), y (≈ 0), z ($\approx \frac{1}{4}$)

X4: (4*f*) x ($\approx \frac{1}{4}$), y (≈ 0), z ($\approx \frac{3}{4}$)

$$
\begin{pmatrix}
\frac{1}{2} & \frac{1}{2} & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & -\frac{1}{2} & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-\frac{1}{2} & -\frac{1}{2} & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-\frac{1}{2} & \frac{1}{2} & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & 1 & 0 \\
0 & 0 & 0 & 0 & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} & 0 & -\frac{1}{2} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & -\frac{1}{2} & 0 & 0 \\
0 & 0 & 0 & 0 & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
d_{\mathrm{A},R_5^+,1} \\ d_{\mathrm{A},R_5^+,2} \\ d_{\mathrm{A},X_5^+,1} \\ d_{\mathrm{A},X_5^+,2} \\ d_{\mathrm{X},M_1^+,3} \\ d_{\mathrm{X},M_2^+,3} \\ d_{\mathrm{X},M_3^+,3} \\ d_{\mathrm{X},M_4^+,3} \\ d_{\mathrm{X},R_4^+,1} \\ d_{\mathrm{X},R_4^+,2} \\ d_{\mathrm{X},R_5^+,1} \\ d_{\mathrm{X},R_5^+,2} \\ d_{\mathrm{X},X_5^+,1} \\ d_{\mathrm{X},X_5^+,2}
\end{pmatrix}
+
\begin{pmatrix}
0 \\ 0 \\ \frac{1}{2} \\ \frac{1}{2} \\ 0 \\ \frac{1}{2} \\ \frac{1}{2} \\ 0 \\ \frac{1}{4} \\ 0 \\ \frac{1}{4} \\ \frac{1}{4} \\ 0 \\ \frac{3}{4}
\end{pmatrix}
=
\begin{pmatrix}
x_{\mathrm{A1}} \\ z_{\mathrm{A1}} \\ x_{\mathrm{A2}} \\ z_{\mathrm{A2}} \\ x_{\mathrm{X1}} \\ z_{\mathrm{X1}} \\ x_{\mathrm{X2}} \\ z_{\mathrm{X2}} \\ x_{\mathrm{X3}} \\ y_{\mathrm{X3}} \\ z_{\mathrm{X3}} \\ x_{\mathrm{X4}} \\ y_{\mathrm{X4}} \\ z_{\mathrm{X4}}
\end{pmatrix}
$$

$$
\begin{aligned}
\frac{V_{\mathrm{A}}}{V_{\mathrm{B}}} = {} & \frac{6}{1+4d_{\mathrm{X},M_1^+,3}^2-4d_{\mathrm{X},M_2^+,3}^2+4d_{\mathrm{X},M_3^+,3}^2-4d_{\mathrm{X},M_4^+,3}^2+4d_{\mathrm{X},R_4^+,1}^2+4d_{\mathrm{X},R_4^+,2}^2-4d_{\mathrm{X},R_5^+,1}^2-4d_{\mathrm{X},R_5^+,2}^2
\\ & \quad +8\begin{pmatrix} \left(d_{\mathrm{X},M_1^+,3}+d_{\mathrm{X},M_2^+,3}+d_{\mathrm{X},M_3^+,3}+d_{\mathrm{X},M_4^+,3}\right)\left(d_{\mathrm{X},R_4^+,1}+d_{\mathrm{X},R_5^+,1}\right) \\ +\left(d_{\mathrm{X},M_1^+,3}-d_{\mathrm{X},M_2^+,3}-d_{\mathrm{X},M_3^+,3}+d_{\mathrm{X},M_4^+,3}\right)\left(d_{\mathrm{X},R_4^+,2}-d_{\mathrm{X},R_5^+,2}\right) \end{pmatrix} d_{\mathrm{X},X_5^+,1}
\\ & \quad -8\begin{pmatrix} \left(d_{\mathrm{X},M_1^+,3}+d_{\mathrm{X},M_2^+,3}-d_{\mathrm{X},M_3^+,3}-d_{\mathrm{X},M_4^+,3}\right)\left(d_{\mathrm{X},R_4^+,1}+d_{\mathrm{X},R_5^+,1}\right) \\ -\left(d_{\mathrm{X},M_1^+,3}-d_{\mathrm{X},M_2^+,3}+d_{\mathrm{X},M_3^+,3}-d_{\mathrm{X},M_4^+,3}\right)\left(d_{\mathrm{X},R_4^+,2}-d_{\mathrm{X},R_5^+,2}\right) \end{pmatrix} d_{\mathrm{X},X_5^+,2}} - 1
\\ \approx {} & \frac{6}{1+4\left(d_{\mathrm{X},M_3^+,3}^2+d_{\mathrm{X},R_4^+,1}^2+d_{\mathrm{X},R_4^+,2}^2\right)} - 1
\end{aligned}
$$

l $a^+a^+a^+$ No. 204 $Im\bar{3}$

$a = b = c \approx 2a_p$

A1: (2*a*) 0, 0, 0

A2: (6*b*) $0, \frac{1}{2}, \frac{1}{2}$

B: (8*c*) $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

X: (24*g*) $0, y\ (\approx \frac{1}{4}), z\ (\approx \frac{1}{4})$

$$\begin{pmatrix} -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} d_{\mathrm{X},M_3^+,123} \\ d_{\mathrm{X},M_4^+,123} \end{pmatrix} + \begin{pmatrix} \frac{1}{4} \\ \frac{1}{4} \end{pmatrix} = \begin{pmatrix} y_{\mathrm{X}} \\ z_{\mathrm{X}} \end{pmatrix}$$

$$\frac{V_{\mathrm{A}}}{V_{\mathrm{B}}} = \frac{6}{1+12d_{\mathrm{X},M_3^+,123}^2 - 12d_{\mathrm{X},M_4^+,123}^2 + 16\left(3d_{\mathrm{X},M_3^+,123}^2 + d_{\mathrm{X},M_4^+,123}^2\right)d_{\mathrm{X},M_4^+,123}} - 1$$

$$\approx \frac{6}{1+4\cdot 3d_{\mathrm{X},M_3^+,123}^2} - 1$$

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m $a^0b^+b^+$ No. 139 $I4/mmm$

$a = b \approx 2a_p$, $c \approx 2a_p$

A1: (2*a*) 0, 0, 0

A2: (2*b*) $0, 0, \frac{1}{2}$

A3: (4*c*) $\frac{1}{2}, 0, 0$

B: (8*f*) $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

X1: (8*h*) $x\ (\approx \frac{1}{4}), x, 0$

X2: (16*n*) 0, *y* (≈ $\frac{1}{4}$), *z* (≈ $\frac{1}{4}$)

$$\begin{pmatrix} \frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & -\frac{1}{2} & 0 \\ -\frac{1}{2} & 0 & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} d_{\mathrm{X},M_3^+,23} \\ d_{\mathrm{X},M_4^+,1} \\ d_{\mathrm{X},M_4^+,23} \end{pmatrix} + \begin{pmatrix} \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \end{pmatrix} = \begin{pmatrix} x_{\mathrm{X1}} \\ y_{\mathrm{X2}} \\ z_{\mathrm{X2}} \end{pmatrix}$$

$$\frac{V_\mathrm{A}}{V_\mathrm{B}} = \frac{6}{1+8d^2_{\mathrm{X},M_3^+,23} - 4d^2_{\mathrm{X},M_4^+,1} - 8d^2_{\mathrm{X},M_4^+,23} - 16d_{\mathrm{X},M_4^+,1}\left(d^2_{\mathrm{X},M_3^+,23} - d^2_{\mathrm{X},M_4^+,23}\right)} - 1$$

$$\approx \frac{6}{1+4\cdot 2d^2_{\mathrm{X},M_3^+,23}} - 1$$

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n $a^+b^+c^+$ No. 71 *Immm*

$a \approx 2a_p$, $b \approx 2a_p$, $c \approx 2a_p$

A1: (2*a*) 0, 0, 0

A2: (2*b*) 0, $\frac{1}{2}$, $\frac{1}{2}$

A3: (2*c*) $\frac{1}{2}$, $\frac{1}{2}$, 0

A4: (2*d*) $\frac{1}{2}$, 0, $\frac{1}{2}$

B: (8*k*) $\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$

X1: (8*l*) 0, *y* (≈ $\frac{1}{4}$), *z* (≈ $\frac{1}{4}$)

X2: (8*m*) *x* (≈ $\frac{1}{4}$), 0, *z* (≈ $\frac{1}{4}$)

X3: (8*n*) *x* (≈ $\frac{1}{4}$), *y* (≈ $\frac{1}{4}$), 0

$$
\begin{pmatrix}
-\frac{1}{2} & 0 & 0 & -\frac{1}{2} & 0 & 0 \\
0 & 0 & \frac{1}{2} & 0 & 0 & -\frac{1}{2} \\
\frac{1}{2} & 0 & 0 & -\frac{1}{2} & 0 & 0 \\
0 & -\frac{1}{2} & 0 & 0 & -\frac{1}{2} & 0 \\
0 & 0 & -\frac{1}{2} & 0 & 0 & -\frac{1}{2} \\
0 & \frac{1}{2} & 0 & 0 & -\frac{1}{2} & 0
\end{pmatrix}
\begin{pmatrix}
d_{\mathrm{X},M_3^+,1} \\ d_{\mathrm{X},M_3^+,2} \\ d_{\mathrm{X},M_3^+,3} \\ d_{\mathrm{X},M_4^+,1} \\ d_{\mathrm{X},M_4^+,2} \\ d_{\mathrm{X},M_4^+,3}
\end{pmatrix}
+
\begin{pmatrix}
\frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4}
\end{pmatrix}
=
\begin{pmatrix}
y_{\mathrm{X1}} \\ z_{\mathrm{X1}} \\ x_{\mathrm{X2}} \\ z_{\mathrm{X2}} \\ x_{\mathrm{X3}} \\ y_{\mathrm{X3}}
\end{pmatrix}
$$

$$
\begin{aligned}
\frac{V_{\mathrm{A}}}{V_{\mathrm{B}}} &= \frac{6}{\begin{array}{l}1+4d_{\mathrm{X},M_3^+,1}^2+4d_{\mathrm{X},M_3^+,2}^2+4d_{\mathrm{X},M_3^+,3}^2-4d_{\mathrm{X},M_4^+,1}^2-4d_{\mathrm{X},M_4^+,2}^2-4d_{\mathrm{X},M_4^+,3}^2 \\ +16d_{\mathrm{X},M_3^+,3}\left(d_{\mathrm{X},M_3^+,2}d_{\mathrm{X},M_4^+,1}+d_{\mathrm{X},M_3^+,1}d_{\mathrm{X},M_4^+,2}\right)+16\left(d_{\mathrm{X},M_3^+,1}d_{\mathrm{X},M_3^+,2}+d_{\mathrm{X},M_4^+,1}d_{\mathrm{X},M_4^+,2}\right)d_{\mathrm{X},M_4^+,3}\end{array}}-1 \\
&\approx \frac{6}{1+4\left(d_{\mathrm{X},M_3^+,1}^2+d_{\mathrm{X},M_3^+,2}^2+d_{\mathrm{X},M_3^+,3}^2\right)}-1
\end{aligned}
$$

o $a^- b^- c^-$ No. 2 $P\bar{1}$

$a \approx \sqrt{2}a_p$, $b \approx \sqrt{2}a_p$, $c \approx \sqrt{2}a_p$, $a \approx 60°$, $b \approx 60°$, $g \approx 60°$

A: (2*i*) x ($\approx \frac{1}{4}$), y ($\approx \frac{1}{4}$), z ($\approx \frac{1}{4}$)

B1: (1*a*) 0, 0, 0

B2: (1*h*) $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

X1: (2*i*) x ($\approx \frac{1}{4}$), y ($\approx \frac{3}{4}$), z ($\approx \frac{1}{4}$)

X2: (2*i*) x ($\approx \frac{1}{4}$), y ($\approx \frac{1}{4}$), z ($\approx \frac{3}{4}$)

X3: (2*i*) x ($\approx \frac{3}{4}$), y ($\approx \frac{1}{4}$), z ($\approx \frac{1}{4}$)

$$
\begin{pmatrix}
-\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{2} & \frac{1}{4} & \frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} & \frac{1}{2} & 0 & -\frac{1}{2} \\
0 & 0 & 0 & -\frac{1}{2} & -\frac{1}{4} & -\frac{1}{2} & \frac{1}{2} & 0 & -\frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} \\
0 & 0 & 0 & \frac{1}{2} & \frac{1}{4} & \frac{1}{2} & -\frac{1}{2} & 0 & -\frac{1}{2} & -\frac{1}{2} & 0 & \frac{1}{2} \\
0 & 0 & 0 & \frac{1}{2} & \frac{1}{4} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\
0 & 0 & 0 & \frac{1}{2} & \frac{1}{4} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\
0 & 0 & 0 & -\frac{1}{2} & -\frac{1}{4} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} & \frac{1}{2} & 0 \\
0 & 0 & 0 & -\frac{1}{2} & \frac{1}{2} & 0 & 0 & -\frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} & \frac{1}{2} \\
0 & 0 & 0 & \frac{1}{2} & -\frac{1}{2} & 0 & 0 & -\frac{1}{2} & -\frac{1}{2} & 0 & \frac{1}{2} & -\frac{1}{2} \\
0 & 0 & 0 & \frac{1}{2} & -\frac{1}{2} & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & -\frac{1}{2} & \frac{1}{2}
\end{pmatrix}
\begin{pmatrix}
d_{\mathrm{A},R_5^+,1} \\ d_{\mathrm{A},R_5^+,2} \\ d_{\mathrm{A},R_5^+,3} \\ d_{\mathrm{X},R_1^+,1} \\ d_{\mathrm{X},R_3^+,1} \\ d_{\mathrm{X},R_3^+,2} \\ d_{\mathrm{X},R_4^+,1} \\ d_{\mathrm{X},R_4^+,2} \\ d_{\mathrm{X},R_4^+,3} \\ d_{\mathrm{X},R_5^+,1} \\ d_{\mathrm{X},R_5^+,2} \\ d_{\mathrm{X},R_5^+,3}
\end{pmatrix}
+
\begin{pmatrix}
\frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \\ \frac{3}{4} \\ \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \\ \frac{3}{4} \\ \frac{3}{4} \\ \frac{1}{4} \\ \frac{1}{4}
\end{pmatrix}
=
\begin{pmatrix}
x_{\mathrm{A}} \\ y_{\mathrm{A}} \\ z_{\mathrm{A}} \\ x_{\mathrm{X1}} \\ y_{\mathrm{X1}} \\ z_{\mathrm{X1}} \\ x_{\mathrm{X2}} \\ y_{\mathrm{X2}} \\ z_{\mathrm{X2}} \\ x_{\mathrm{X3}} \\ y_{\mathrm{X3}} \\ z_{\mathrm{X3}}
\end{pmatrix}
$$

$$
\frac{V_{\mathrm{A}}}{V_{\mathrm{B}}} = \frac{6}{1+12d^2_{\mathrm{X},R_1^+,1} - 3d^2_{\mathrm{X},R_3^+,1} - 4d^2_{\mathrm{X},R_3^+,2} + 4d^2_{\mathrm{X},R_4^+,1} + 4d^2_{\mathrm{X},R_4^+,2} + 4d^2_{\mathrm{X},R_4^+,3} - 4d^2_{\mathrm{X},R_5^+,1} - 4d^2_{\mathrm{X},R_5^+,2} - 4d^2_{\mathrm{X},R_5^+,3}} - 1
$$

$$
\approx \frac{6}{1+4\left(d^2_{\mathrm{X},R_4^+,1} + d^2_{\mathrm{X},R_4^+,2} + d^2_{\mathrm{X},R_4^+,3}\right)} - 1
$$