Hamiltonian formalisms of spin-orbit Jahn-Teller and pseudo-Jahn-Teller problems in trigonal symmetries: Supporting Information

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S.I. SETTING OF E COMPONENT STATES AND e COMPONENT MODES

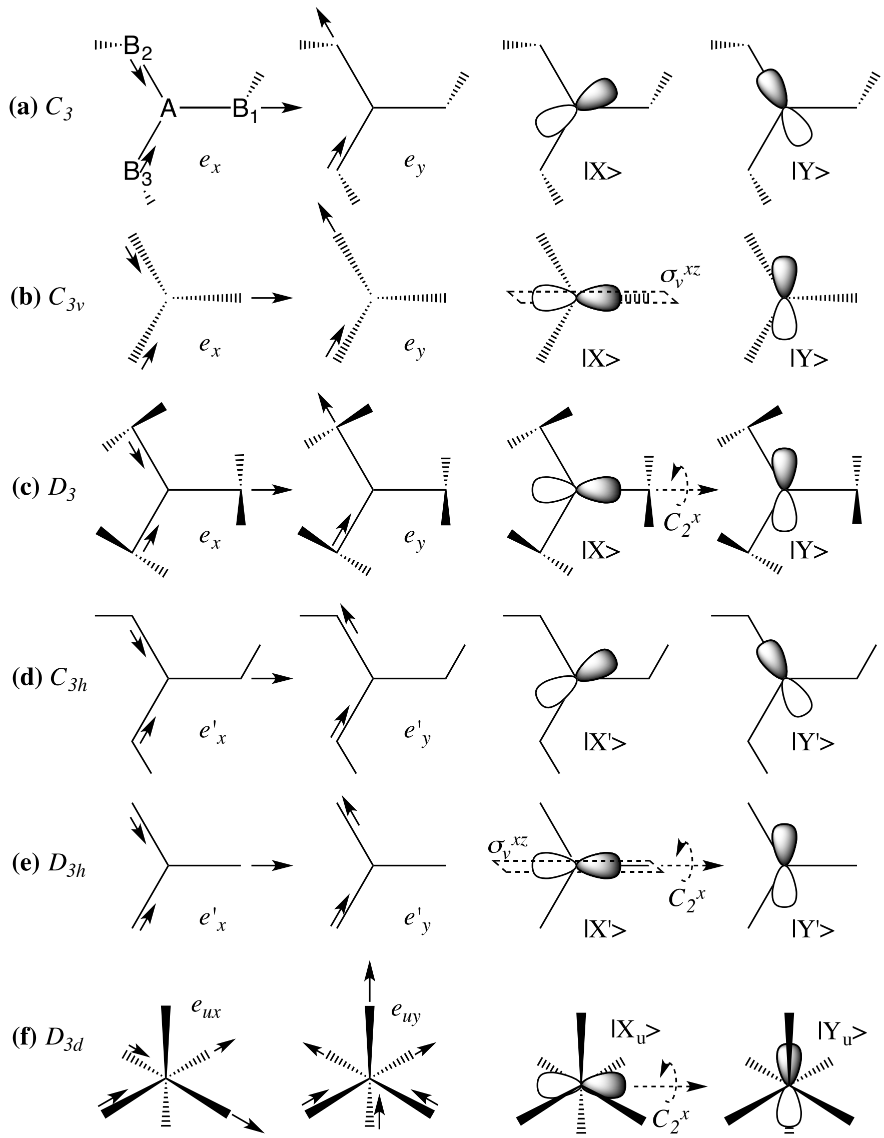

FIG. S.1. Examples of orientations of e and E components in trigonal symmetries, on which the derivations are based. Atomic motions in the modes are represented by solid arrows. With the atom labelling in panel (a), $e_x = \sqrt{\frac{1}{6}}\,(2\Delta r_{AB_1} - \Delta r_{AB_2} - \Delta r_{AB_3})$, and $e_y = \sqrt{\frac{1}{2}}\,(\Delta r_{AB_2} - \Delta r_{AB_3})$. Similar definitions apply to the displayed e modes in the other panels.

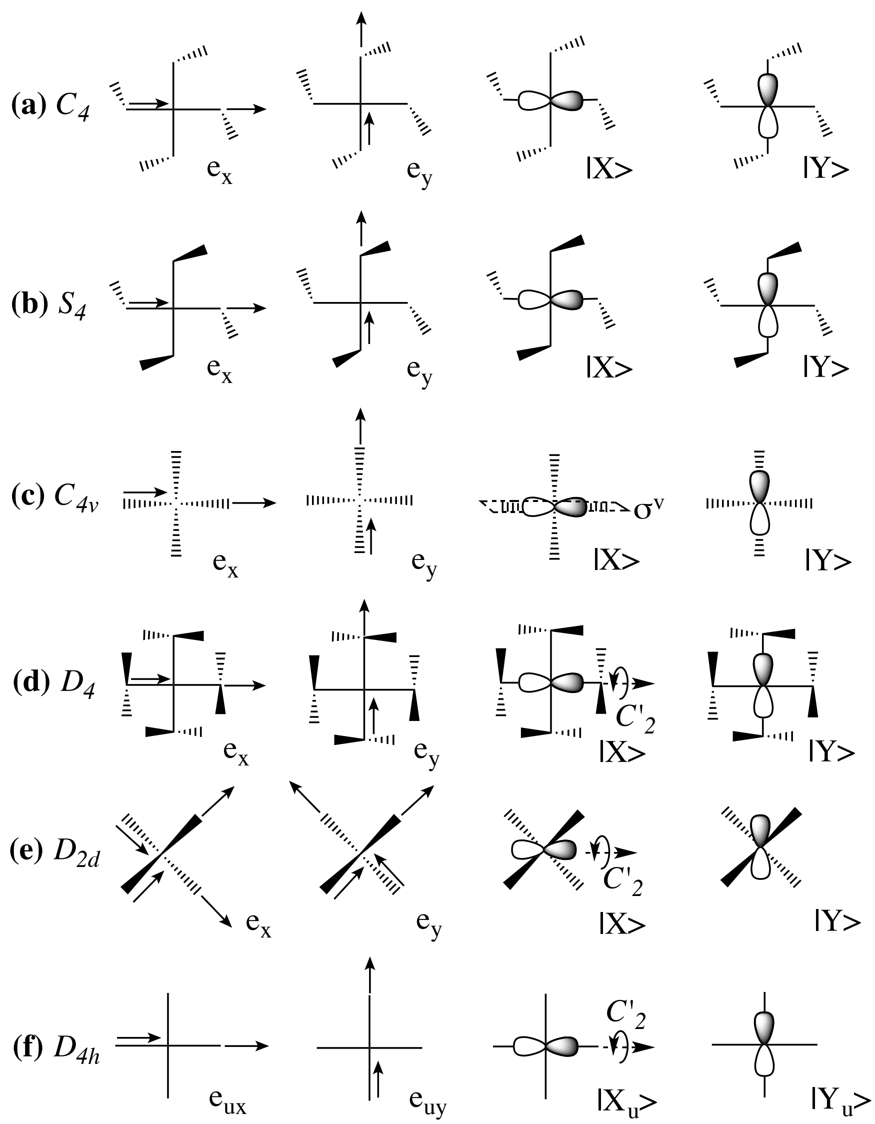

FIG. S.2. Examples of orientations of e and E components in tetragonal symmetries, on which the derivations are based. Atomic motions in the modes are represented by solid arrows. The orientations in C_{4h} symmetry are not shown. They are similar to those in C_4 symmetry.

S.II. SETTING AXES FOR SPIN QUANTIZATIONS

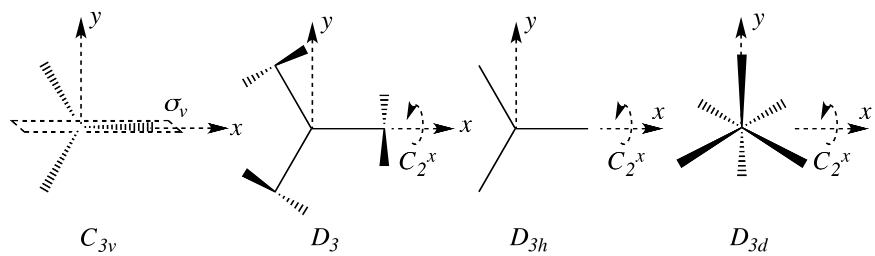

FIG. S.3. Examples of x and y axes for spin quantizations in C_{3v}, D_3, D_{3h}, and D_{3d} symmetries. The z axis is the C_3 axis pointing out of the paper. The x and y axes follow similar definitions in C_{4v}, D_4, D_{2d}, and D_{4h} symmetries.

S.III. EXPANSION FORMULAS IN TRIGONAL SYMMETRIES

All bimodal expansion formulas that feature the symmetry eigenvalues χ^{C_3}, $(\chi^{\sigma_v}_{Re}, \chi^{\sigma_v}_{Im})$, $\left(\chi^{C_2'}_{Re}, \chi^{C_2'}_{Im}\right)$, χ^{σ_h}, and χ^I are summarized in Tables S.I to S.VI. In these tables z is used to represent coordinates of a-type vibrations and the polar coordinates ρ and ϕ for e-type vibrations. For coordinates of vibrational modes of the same type of irreducible representations (irreps), subscripts (1) and (2) are used to differentiate them. *Please do not mistake the parenthesized (1) and (2) for the subscripts 1 and 2 of A-type irreps. The latter denote whether the A-type irreps are symmetric or antisymmetric with respect to $\hat{\sigma}_v$ in C_{3v} symmetry, and with respect to $\hat{C}_2'$ in D_3, D_{3h}, and D_{3d} symmetries.*

Tables S.I and S.II give the bimodal expansions that that are $\hat{C}_3$-eigenfunctions, with $\chi^{C_3} = 1$ and $e^{i\frac{2\pi}{3}}$, respectively. Those are called the root expansions, as they satisfy the symmetry requirements of C_3 symmetry, the *lowest* symmetry in all trigonal symmetries. Expansions with $\chi^{C_3} = e^{-i\frac{2\pi}{3}}$ are simply complex conjugates of those with $\chi^{C_3} = e^{i\frac{2\pi}{3}}$. They are hence not given. Please note that in all expansion throughout this work, the summation indices that appear in the absolute value symbol take all integer values, while the other indices only take nonnegative integer values.

Tables S.III and S.IV summarize the constraints that need to be applied to the root expansions, so that the resultant *branch* expansions feature $(\chi^{\sigma_v}_{Re}, \chi^{\sigma_v}_{Im})$ or $\left(\chi^{C_2'}_{Re}, \chi^{C_2'}_{Im}\right)$. Similarly, Tables S.V and S.VI summarize the constraints that give the *branch* expansions that feature χ^{σ_h} or χ^I.

TABLE S.I. Expansion formulas for $\hat{C}_3$-eigenfunctions of the bimodal vibrational coordinates with eigenvalue 1.

Modes	Expansion formulas
$(a+a)$	$a^r_{I_1,I_2} z^{I_1}_{(1)} z^{I_2}_{(2)} + i a^i_{I_3,I_4} z^{I_3}_{(1)} z^{I_4}_{(2)}$
$(e+a)$	$a^{3m}_{I,2K} z^I \rho^{\lvert 3m\rvert+2K} e^{i3m\phi} = \rho^{\lvert 3m\rvert+2K} \Big[a^{r,3m}_{I_1,2K} z^{I_1} \cos(3m\phi) - a^{i,3m}_{I_2,2K} z^{I_2} \sin(3m\phi)$ $+i \left(a^{r,3m}_{I_1,2K} z^{I_1} \sin(3m\phi) + a^{i,3m}_{I_2,2K} z^{I_2} \cos(3m\phi) \right) \Big]$
$(e+e)$	$a^{m,3n}_{2K_1,2K_2} \rho^{\lvert m\rvert+2K_1}_{(1)} \rho^{\lvert 3n-m\rvert+2K_2}_{(2)} e^{i(m\phi_{(1)}+(3n-m)\phi_{(2)})} = \rho^{\lvert m\rvert+2K_1}_{(1)} \rho^{\lvert 3n-m\rvert+2K_2}_{(2)}$ $\Big[(a^{r,m,3n}_{2K_1,2K_2} \cos(m\phi_{(1)} + (3n-m)\phi_{(2)}) - a^{i,m,3n}_{2K_1,2K_2} \sin(m\phi_{(1)} + (3n-m)\phi_{(2)}))$ $+i(a^{r,m,3n}_{2K_1,2K_2} \sin(m\phi_{(1)} + (3n-m)\phi_{(2)}) + a^{i,m,3n}_{2K_1,2K_2} \cos(m\phi_{(1)} + (3n-m)\phi_{(2)})) \Big]$

TABLE S.II. Expansion formulas for $\hat{C}_3$-eigenfunctions of the bimodal vibrational coordinates with eigenvalue $e^{i\frac{2\pi}{3}}$.

Modes	Expansion formulas
$(a+a)$	not applicable (na)
$(e+a)$	$b^{3n-1}_{I,2K} z^I \rho^{\lvert 3n-1\rvert+2K} e^{i(3n-1)\phi} = \rho^{\lvert 3n-1\rvert+2K} \Big[b^{r,3n-1}_{I_1,2K} z^{I_1} \cos((3n-1)\phi) - b^{i,3n-1}_{I_2,2K} z^{I_2} \sin((3n-1)\phi)$ $+i \left(b^{r,3n-1}_{I_1,2K} z^{I_1} \sin((3n-1)\phi) + b^{i,3n-1}_{I_2,2K} z^{I_2} \cos((3n-1)\phi) \right) \Big]$
$(e+e)$	$b^{m,3n-1}_{2K_1,2K_2} \rho^{\lvert m\rvert+2K_1}_{(1)} \rho^{\lvert 3n-1-m\rvert+2K_2}_{(2)} e^{i(m\phi_{(1)}+(3n-1-m)\phi_{(2)})} = \rho^{\lvert m\rvert+2K_1}_{(1)} \rho^{\lvert 3n-1-m\rvert+2K_2}_{(2)}$ $\Big[b^{r,m,3n-1}_{2K_1,2K_2} \cos(m\phi_{(1)} + (3n-1-m)\phi_{(2)}) - b^{i,m,3n-1}_{2K_1,2K_2} \sin(m\phi_{(1)} + (3n-1-m)\phi_{(2)})$ $+i \left(b^{r,m,3n-1}_{2K_1,2K_2} \sin(m\phi_{(1)} + (3n-1-m)\phi_{(2)}) + b^{i,m,3n-1}_{2K_1,2K_2} \cos(m\phi_{(1)} + (3n-1-m)\phi_{(2)}) \right) \Big]$

TABLE S.III. Constraints on expansions in Table S.I to give the appropriate $\chi_{Re}^{\sigma_v,C_2'}$ and $\chi_{Im}^{\sigma_v,C_2'}$. When $\chi_{Im}^{\sigma_v,C_2'} = 0$, only the real part of the corresponding entry in Table S.I should be considered. When $\chi_{Re}^{\sigma_v,C_2'} = 0$, only the imaginary part of the corresponding entry in Table S.I should be considered.

Modes	$1,(1,0)$	$1,(-1,0)$	$1,(1,-1)$	$1,(0,1)$	$1,(0,-1)$
(a_1+a_1)	nr†	na	na	nr	na
$(a_1+a_2)^{\ddagger}$	I_2 even¶	I_2 odd	I_2 even, I_4 odd	I_4 even	I_4 odd
(a_2+a_2)	I_1, I_2 ee or oo§	I_1, I_2 eo or oe$^{£}$	I_1, I_2 ee or oo, I_3, I_4 eo or oe	I_3, I_4 ee or oo	I_3, I_4 eo or oe
$(e+a_1)$	cos nz$^{\#}$	sin nz	a^r nz	cos nz	sin nz
$(e+a_2)$	I_1 even, I_2 odd	I_1 odd, I_2 even	I_1 even, I_2 odd	I_1 odd, I_2 even	I_1 even, I_2 odd
$(e+e)$	cos nz	sin nz	a^r nz	cos nz	sin nz

† "nr" means "no restriction". ‡ For two modes whose irreps only differ in subscripts, (1)-subscripted coordinates in Table S.I are for the first (a_1 here) and (2)- for the second (a_2 here) mode. ¶ I_2 needs to be even. § I_1 and I_2 need to be both even or both odd. $^{£}$ When I_1 is even, I_2 must be odd, and vice versa. $^{\#}$ Only the terms associated with cosine factors are nonzero.

TABLE S.IV. Constraints on expansions in Table S.II to give the appropriate $\chi_{Re}^{\sigma_v,C_2'}$ and $\chi_{Im}^{\sigma_v,C_2'}$.

Modes	$e^{i\frac{2\pi}{3}},(1,-1)$	$e^{i\frac{2\pi}{3}},(-1,1)$
$(e+a_1)$	b^r nz	b^i nz
$(e+a_2)$	I_1 even, I_2 odd	I_1 odd, I_2 even
$(e+e)$	b^r nz	b^i nz

TABLE S.V. Constraints on expansions in Table S.I to give the appropriate $\left(\chi^{C_3} = 1, \chi^{\sigma_h, I}\right)$. The modes here are given for σ_h. The $'$ and $''$ can be correspondingly replaced by the g and u subscripts for the D_{3d} symmetry.

Vibrational Modes	$(1, 1)$	$(1, -1)$
$(a' + a')$	nr	na
$(a' + a'')^{\dagger}$	I_2, I_4 even	I_2, I_4 odd
$(a'' + a'')$	I_1, I_2 ee or oo I_3, I_4 ee or oo	I_1, I_2 eo or oe I_3, I_4 eo or oe
$(e' + a')$	nr	na
$(e'' + a')$	$3m$ even	$3m$ odd
$(e' + a'')$	I even	I odd
$(e'' + a'')$	$3m, I$ ee or oo	$3m, I$ eo or oe
$(e' + e')$	nr	na
$(e'' + e')$	m even	m odd
$(e'' + e'')$	$3n$ even	$3n$ odd

† For two modes whose irreps only differ in subscripts, (1)-subscripted coordinates in Table S.I are for the first (a' here) and (2)- for the second (a'' here) mode. This rule applies in all constraints tables.

TABLE S.VI. Constraints on expansions in Table S.II to give the appropriate $\left(\chi^{C_3} = e^{i\frac{2\pi}{3}}, \chi^{\sigma_h, I}\right)$. The modes here are given for σ_h. The $'$ and $''$ can be correspondingly replaced by the g and u subscripts for the D_{3d} symmetry.

Vibrational Modes	$(e^{i\frac{2\pi}{3}}, 1)$	$(e^{i\frac{2\pi}{3}}, -1)$
$(e' + a')$	nr	na
$(e'' + a')$	$3n$ odd	$3n$ even
$(e' + a'')$	I even	I odd
$(e'' + a'')$	$3n$ even,I odd $3n$ odd, I even	$3n$ even,I even $3n$ odd, I odd
$(e' + e')$	nr	na
$(e'' + e')$	m even	m odd
$(e'' + e'')$	$3n$ odd	$3n$ even

S.IV. EXPANSION FORMULAS IN TETRAGONAL SYMMETRIES

All bimodal expansion formulas that feature the symmetry eigenvalues χ^{C_4}, $(\chi^{\sigma_v}_{Re}, \chi^{\sigma_v}_{Im})$, $\left(\chi^{C_2'}_{Re}, \chi^{C_2'}_{Im}\right)$, χ^{σ_h}, and χ^{I} are summarized in Tables S.VII to S.XV. In these tables z is used to represent coordinates of a-type vibrations, w for b-type vibrations, and the polar coordinates ρ and ϕ for e-type vibrations. For coordinates of vibrational modes of the same type of irreducible representations (irreps), subscripts (1) and (2) are used to differentiate them. *Please do not mistake the parenthesized (1) and (2) for the subscripts 1 and 2 of A- and B-type irreps. The latter denote whether the A- and B-type irreps are symmetric or antisymmetric with respect to $\hat{\sigma}_v$ in C_{4v} symmetry, and with respect to $\hat{C}_2'$ in D_{2d}, D_4, and D_{4h} symmetries.*

Tables S.VII and S.IX give the bimodal expansions that that are $\hat{C}_4$-eigenfunctions, with $\chi^{C_4} = 1$, -1, and i, respectively. Those are called the root expansions, as they satisfy the symmetry requirements of C_4 symmetry, the *lowest* symmetry in all tetragonal symmetries. Expansions with $\chi^{C_4} = -i$ are simply complex conjugates of those with $\chi^{C_4} = i$. They are hence not given. Please note that in all expansion throughout this work, the summation indices that appear in the absolute value symbol take all integer values, while the other indices only take nonnegative integer values. Please note that C_4 and S_4 are isomorphic point groups. The C_4-eigenvalues are also S_4-eigenvalues and the root expansion formulas are also applicable for S_4 symmetry.

Tables S.X and S.XII summarize the constraints that need to be applied to the root expansions, so that the resultant *branch* expansions feature $(\chi^{\sigma_v}_{Re}, \chi^{\sigma_v}_{Im})$ or $\left(\chi^{C_2'}_{Re}, \chi^{C_2'}_{Im}\right)$. Similarly, Tables S.XIII and S.XV summarize the constraints that give the *branch* expansions that feature χ^{I}.

TABLE S.VII. Expansion formulas for $\hat{C}_4$-eigenfunctions of the bimodal vibrational coordinates with eigenvalue 1.

Modes	Expansion formulas
$(a+a)$	$a^r_{I_1,I_2} z^{I_1}_{(1)} z^{I_2}_{(2)} + i a^i_{I_3,I_4} z^{I_3}_{(1)} z^{I_4}_{(2)}$
$(a+b)$	$a^r_{I_1,2J} z^{I_1} w^{2J} + i a^i_{I_2,2J} z^{I_2} w^{2J}$
$(b+b)$	$a^r_{2J_1+1,2J_2+1} w^{2J_1+1}_{(1)} w^{2J_2+1}_{(2)} + i a^i_{2J_1+1,2J_2+1} w^{2J_1+1}_{(1)} w^{2J_2+1}_{(2)}$ $+ a^r_{2J_1,2J_2} w^{2J_1}_{(1)} w^{2J_2}_{(2)} + i a^i_{2J_1,2J_2} w^{2J_1}_{(1)} w^{2J_2}_{(2)}$
$(e+a)$	$a^{4m}_{I,2K} z^I \rho^{\lvert 4m\rvert+2K} e^{i4m\phi} = \rho^{\lvert 4m\rvert+2K}[a^{r,4m}_{I_1,2K} z^{I_1}\cos(4m\phi) - a^{i,4m}_{I_2,2K} z^{I_2}\sin(4m\phi)$ $+ i a^{r,4m}_{I_1,2K} z^{I_1}\sin(4m\phi) + i a^{i,4m}_{I_2,2K} z^{I_2}\cos(4m\phi)]$
$(e+b)$	$a^{2m}_{2I,2K} w^{mod(m,2)+2I} \rho^{\lvert 2m\rvert+2K} e^{i2m\phi} = w^{mod(m,2)+2I}\rho^{\lvert 2m\rvert+2K}\left[a^{r,2m}_{2I,2K}\cos(2m\phi)\right.$ $\left. - a^{i,2m}_{2I,2K}\sin(2m\phi) + i a^{r,2m}_{2I,2K}\sin(2m\phi) + i a^{i,2m}_{2I,2K}\cos(2m\phi)\right]$
$(e+e)$	$a^{m_1,4n}_{2K_1,2K_2} \rho^{\lvert m_1\rvert+2K_1}_{(1)} \rho^{\lvert 4n-m_1\rvert+2K_2}_{(2)} e^{i(m_1\phi_{(1)}+(4n-m_1)\phi_{(2)})} = \rho^{\lvert m_1\rvert+2K_1}_{(1)} \rho^{\lvert 4n-m_1\rvert+2K_2}_{(2)}$ $\left[(a^{r,m_1,4n}_{2K_1,2K_2}\cos(m_1\phi_{(1)}+(4n-m_1)\phi_{(2)}) - a^{i,m_1,4n}_{2K_1,2K_2}\sin(m_1\phi_{(1)}+(4n-m_1)\phi_{(2)}))\right.$ $\left. + i(a^{r,m_1,4n}_{2K_1,2K_2}\sin(m_1\phi_{(1)}+(4n-m_1)\phi_{(2)}) + a^{i,m_1,4n}_{2K_1,2K_2}\cos(m_1\phi_{(1)}+(4n-m_1)\phi_{(2)}))\right]$

TABLE S.VIII. Expansion formulas for $\hat{C}_4$-eigenfunctions of the bimodal vibrational coordinates with eigenvalue -1.

Modes	Expansion formulas
$(a+a)$	na
$(a+b)$	$b^r_{I_1,2J+1} z^{I_1} w^{2J+1} + i b^i_{I_2,2J+1} z^{I_2} w^{2J+1}$
$(b+b)$	$b^r_{2J_1+1,2J_2} w^{2J_1+1}_{(1)} w^{2J_2}_{(2)} + i b^i_{2J_1+1,2J_2} w^{2J_1+1}_{(1)} w^{2J_2}_{(2)} + b^r_{2J_1,2J_2+1} w^{2J_1}_{(1)} w^{2J_2+1}_{(2)} + i b^i_{2J_1,2J_2+1} w^{2J_1}_{(1)} w^{2J_2+1}_{(2)}$
$(e+a)$	$b^{4n+2}_{I,2K} z^I \rho^{\lvert 4n+2\rvert+2K} e^{i(4n+2)\phi} = \rho^{\lvert 4n+2\rvert+2K}\left[b^{r,4n+2}_{I_1,2K} z^{I_1}\cos((4n+2)\phi) - b^{i,4n+2}_{I_2,2K} z^{I_2}\sin((4n+2)\phi)\right.$ $\left. + i b^{r,4n+2}_{I_1,2K} z^{I_1}\sin((4n+2)\phi) + i b^{i,4n+2}_{I_2,2K} z^{I_2}\cos((4n+2)\phi)\right]$
$(e+b)$	$b^{2m}_{2I,2K} w^{mod(m,2)+2I+1} \rho^{\lvert 2m\rvert+2K} e^{i2m\phi} = w^{mod(m,2)+2I+1}\rho^{\lvert 2m\rvert+2K}\left[b^{r,2m}_{2I,2K}\cos(2m\phi) - b^{i,2m}_{2I,2K}\sin(2m\phi)\right.$ $\left. + i b^{r,2m}_{2I,2K}\sin(2m\phi) + i b^{i,2m}_{2I,2K}\cos(2m\phi)\right]$
$(e+e)$	$b^{m_1,4n+2}_{2K_1,2K_2} \rho^{\lvert m_1\rvert+2K_1}_{(1)} \rho^{\lvert 4n+2-m_1\rvert+2K_2}_{(2)} e^{i(m_1\phi_{(1)}+(4n+2-m_1)\phi_{(2)})} = \rho^{\lvert m_1\rvert+2K_1}_{(1)} \rho^{\lvert 4n+2-m_1\rvert+2K_2}_{(2)}$ $\left[(b^{r,m_1,4n+2}_{2K_1,2K_2}\cos(m_1\phi_{(1)}+(4n+2-m_1)\phi_{(2)}) - b^{i,m_1,4n+2}_{2K_1,2K_2}\sin(m_1\phi_{(1)}+(4n+2-m_1)\phi_{(2)}))\right.$ $\left. + i(b^{r,m_1,4n+2}_{2K_1,2K_2}\sin(m_1\phi_{(1)}+(4n+2-m_1)\phi_{(2)}) + b^{i,m_1,4n+2}_{2K_1,2K_2}\cos(m_1\phi_{(1)}+(4n+2-m_1)\phi_{(2)}))\right]$

TABLE S.IX. Expansion formulas for $\hat{C}_4$-eigenfunctions of the bimodal vibrational coordinates with eigenvalue i.

Modes	Expansion formulas
$(\gamma+\gamma)^{\dagger}$	na
$(e+a)$	$c^{4n+1}_{I,2K} z^I \rho^{\|4n-1\|+2K} e^{i(4n-1)\phi} = \rho^{\|4n-1\|+2K} \left[c^{r,4n-1}_{I_1,2K} z^{I_1} \cos((4n-1)\phi) - c^{i,4n-1}_{I_2,2K} z^{I_2} \sin((4n-1)\phi) \right]$ $+i\rho^{\|4n-1\|+2K} \left[c^{r,4n-1}_{I_1,2K} z^{I_1} \sin((4n-1)\phi) + c^{i,4n-1}_{I_2,2K} z^{I_2} \cos((4n-1)\phi) \right]$
$(e+b)$	$c^{2n-1}_{2I,2K} w^{mod(n,2)+2I} \rho^{\|2n-1\|+2K} e^{i(2n-1)\phi}$ $= w^{mod(n,2)+2I} \rho^{\|2n-1\|+2K} \left[c^{r,2n-1}_{2I,2K} \cos((2n-1)\phi) - c^{i,2n-1}_{2I,2K} \sin((2n-1)\phi) \right]$ $+iw^{mod(n,2)+2I} \rho^{\|2n-1\|+2K} \left[c^{r,2n-1}_{2I,2K} \sin((2n-1)\phi) + c^{i,2n-1}_{2I,2K} \cos((2n-1)\phi) \right]$
$(e+e)$	$c^{m_1,4n-1}_{2K_1,2K_2} \rho^{\|m_1\|+2K_1}_{(1)} \rho^{\|4n-1-m_1\|+2K_2}_{(2)} e^{i(m_1\phi_{(1)}+(4n-1-m_1)\phi_{(2)})} = \rho^{\|m_1\|+2K_1}_{(1)} \rho^{\|4n-1-m_1\|+2K_2}_{(2)}$ $\Big[(c^{r,m_1,4n-1}_{2K_1,2K_2} \cos(m_1\phi_{(1)} + (4n-1-m_1)\phi_{(2)}) - c^{i,m_1,4n-1}_{2K_1,2K_2} \sin(m_1\phi_{(1)} + (4n-1-m_1)\phi_{(2)}))$ $+i(c^{r,m_1,4n-1}_{2K_1,2K_2} \sin(m_1\phi_{(1)} + (4n-1-m_1)\phi_{(2)}) + c^{i,m_1,4n-1}_{2K_1,2K_2} \cos(m_1\phi_{(1)} + (4n-1-m_1)\phi_{(2)})) \Big]$

† Including $(a+a)$, $(b+b)$, and $(a+b)$.

TABLE S.X. Constraints on expansions in Table S.VII to give the appropriate $\chi_{Re}^{\sigma_v,C_2'}$ and $\chi_{Im}^{\sigma_v,C_2'}$. When $\chi_{Im}^{\sigma_v,C_2'} = 0$ ($\chi_{Re}^{\sigma_v,C_2'} = 0$), only the real (imaginary) part of the corresponding entry in Table S.VII should be considered.

Modes	$(1,(1,0))$	$(1,(-1,0))$	$(1,(1,-1))$	$(1,(0,1))$	$(1,(0,-1))$
(a_1+a_1)	nr[†]	na	na	nr	na
(a_1+a_2)[‡]	I_2 even[¶]	I_2 odd	I_2 even, I_4 odd	I_4 even	I_4 odd
(a_2+a_2)	I_1, I_2 ee or oo[§]	I_1, I_2 eo or oe[£]	I_1, I_2 ee or oo, I_3, I_4 eo or oe	I_3, I_4 ee or oo	I_3, I_4 eo or oe
$(a_1+b_1), (a_1+b_2)$	nr	na	na	nr	na
$(a_2+b_1), (a_2+b_2)$	I_1 even	I_1 odd	I_1 even, I_2 odd	I_2 even	I_2 odd
$(b_1+b_1), (b_2+b_2)$	nr	na	na	nr	na
(b_1+b_2)	a_{ee} nz[$]	a_{oo} nz[$]	a_{ee}^r, a_{oo}^i nz	a_{ee} nz	a_{oo} nz
$(e+a_1), (e+b_1)$,	cos nz[#]	sin nz	a^r nz	cos nz	sin nz
$(e+a_2)$	I_1 even, I_2 odd	I_1 odd, I_2 even	I_1 even, I_2 odd	I_1 odd, I_2 even	I_1 even, I_2 odd
$(e+b_2)$	cos nz if m even, sin nz if m odd	sin nz if m even, cos nz if m odd	a^r nz if m even, a^i nz if m odd	cos nz if m even, sin nz if m odd	sin nz if m even, cos nz if m odd
$(e+e)$	cos nz	sin nz	a^r nz	cos nz	sin nz

[†] "nr" means "no restriction". [‡] For two modes whose irreps only differ in subscripts, (1)-subscripted coordinates in Table S.VII are for the first (a_1 here) and (2)- for the second (a_2 here) mode. [¶] I_2 needs to be even. [§] I_1 and I_2 need to be both even or both odd. [£] When I_1 is even, I_2 must be odd, and vice versa. [$] a_{ee} means $a_{2J_1,2J_2}$. a_{oo} means $a_{2J_1+1,2J_2+1}$. "nz" means only these coefficients are nonzero. [#] Only the terms associated with cos factors are nonzero.

TABLE S.XI. Constraints on expansions in Table S.VIII to give the appropriate $\chi^{\sigma_v}_{Re,C_2'}$ and $\chi^{\sigma_v,C_2'}_{Im}$. When $\chi^{\sigma_v,C_2'}_{Im} = 0$ ($\chi^{\sigma_v,C_2'}_{Re} = 0$), only the real (imaginary) part of the corresponding entry in Table S.VIII should be considered.

Modes	$(-1,(1,0))$	$(-1,(-1,0))$	$(-1,(1,-1))$	$(-1,(0,1))$	$(-1,(0,-1))$
(a_1+b_1)	nr	na	na	nr	na
(a_1+b_2)	na	nr	na	na	nr
(a_2+b_1)	I_1 even	I_1 odd	I_1 even, I_2 odd	I_2 even	I_2 odd
(a_2+b_2)	I_1 odd	I_1 even	I_1 odd, I_2 even	I_2 odd	I_2 even
(b_1+b_1)	nr	na	na	nr	na
(b_1+b_2)	b_{oe} nz	b_{eo} nz	b^r_{oe}, b^i_{eo} nz	b_{oe} nz	b_{eo} nz
(b_2+b_2)	na	nr	na	na	nr
$(e+a_1), (e+b_1)$	cos nz	sin nz	b^r nz	cos nz	sin nz
$(e+a_2)$	I_1 even, I_2 odd	I_1 odd, I_2 even	I_1 even, I_2 odd	I_1 odd, I_2 even	I_1 even, I_2 odd
$(e+b_2)$	cos nz if m odd, sin nz if m even	sin nz if m odd, cos nz if m even	b^r nz if m odd, b^i nz if m even	sin nz if m odd, cos nz if m even	cos nz if m odd, sin nz if m even
$(e+e)$	cos nz	sin nz	b^r nz	cos nz	sin nz

TABLE S.XII. Constraints on expansions in Table S.IX to give the appropriate $\chi^{\sigma_v}_{Re}$ and $\chi^{\sigma_v}_{Im}$.

Modes	$(i,(1,-1))$	$(i,(-1,1))$
$(e+a_1)$, $(e+b_1)$	c^r nz	c^i nz
$(e+a_2)$	I_1 even, I_2 odd	I_1 odd, I_2 even
$(e+b_2)$	c^r (c^i) nz if n even (odd)	c^r (c^i) nz if n odd (even)
$(e+e)$	c^r nz	c^i nz

TABLE S.XIII. Constraints on expansions in Table S.VII in the main text to give the appropriate $\left(\chi^{C_4} = 1, \chi^{I}\right)$.

Vibrational Modes	$(1,1)$	$(1,-1)$
$(a_g + a_g)$	nr	na
$(a_g + a_u)$	I_2 even	I_2 odd
$(a_u + a_u)$	I_1, I_2 ee or oo I_3, I_4 ee or oo	I_1, I_2 eo or oe I_3, I_4 eo or oe
$(a_g + b_g)$, $(a_g + b_u)$	nr	na
$(a_u + b_g)$, $(a_u + b_u)$	I_1 even	I_1 odd
$(b_g + b_g)$, $(b_u + b_u)$	nr	na
$(b_g + b_u)$	a_{ee} nz	a_{oo} nz
$(e_g + a_g)$, $(e_u + a_g)$	nr	na
$(e_g + a_u)$, $(e_u + a_u)$	I even	I odd
$(e_g + b_g)$, $(e_u + b_g)$	nr	na
$(e_g + b_u)$, $(e_u + b_u)$	m even	m odd
$(e_g + e_g)$, $(e_u + e_u)$	nr	na
$(e_g + e_u)$	m_1 even	m_1 odd

TABLE S.XIV. Constraints on expansions in Table S.VIII in the main text to give the appropriate $\left(\chi^{C_4} = -1, \chi^I\right)$.

Vibrational Modes	$(-1, 1)$	$(-1, -1)$
$(a_g + b_g)$	nr	na
$(a_g + b_u)$	na	nr
$(a_u + b_g)$	I_1 even	I_1 odd
$(a_u + b_u)$	I_1 odd	I_1 even
$(b_g + b_g)$	nr	na
$(b_g + b_u)$	b_{oe} nz	b_{eo} nz
$(b_u + b_u)$	na	nr
$(e_u + a_g)$, $(e_g + a_g)$	nr	na
$(e_u + a_u)$, $(e_g + a_u)$	I even	I odd
$(e_u + b_g)$, $(e_g + b_g)$	nr	na
$(e_u + b_u)$, $(e_g + b_u)$	m odd	m even
$(e_u + e_u)$	nr	na
$(e_u + e_g)$	m_1 even	m_1 odd
$(e_g + e_g)$	nr	na

TABLE S.XV. Constraints on expansions in Table S.IX in the main text to give the appropriate $\left(\chi^{C_4} = i, \chi^{I}\right)$.

Vibrational Modes	$(i,1)$	$(i,-1)$
$(e_g + a_g)$	nr	na
$(e_g + a_u)$	I even	I odd
$(e_u + a_g)$	na	nr
$(e_u + a_u)$	I odd	I even
$(e_g + b_g)$	nr	na
$(e_g + b_u)$	n even	n odd
$(e_u + b_g)$	na	nr
$(e_u + b_u)$	n odd	n even
$(e_g + e_g)$	nr	na
$(e_g + e_u)$	m_1 odd	m_1 even
$(e_u + e_u)$	na	nr