Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for PCCP article "Tunnelling splitting patterns in some partially deuterated water trimers"

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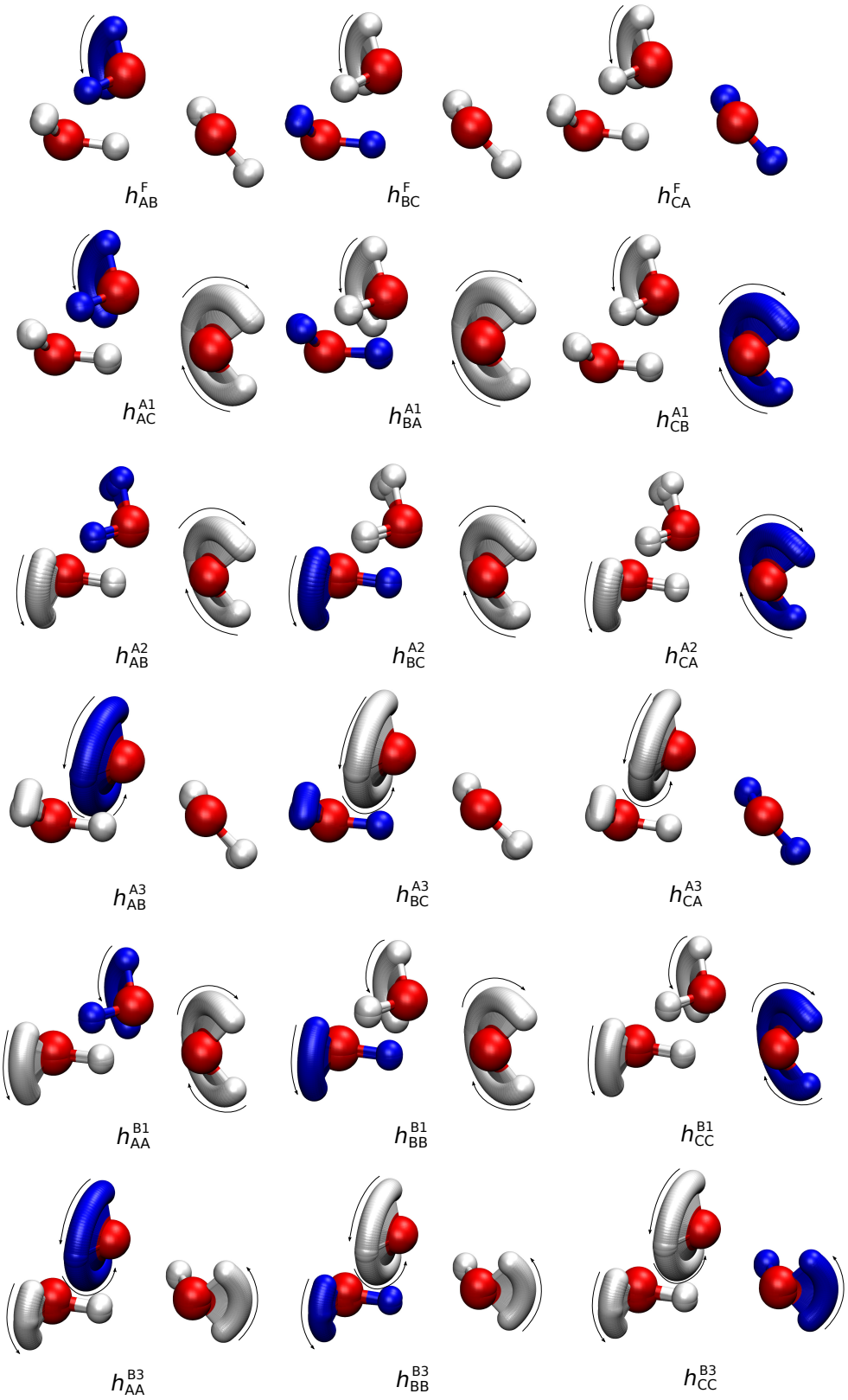

Fig. 1 Minimum action paths of flips and bifurcations connecting symmetry-related structures of $(D_2O)(H_2O)_2$, which are responsible for the formation of the tunnelling splitting spectrum. Sequential snapshots of the trimer along the path are shown, with D atoms in blue and H atoms in red. Pathways are labeled by their corresponding tunnelling matrix elements in Table 3 of the main article, with path labels in the superscript and the initial and final structure labels, A−C, in the subscript. This figure is the reproduced Figure 2 from the main article.

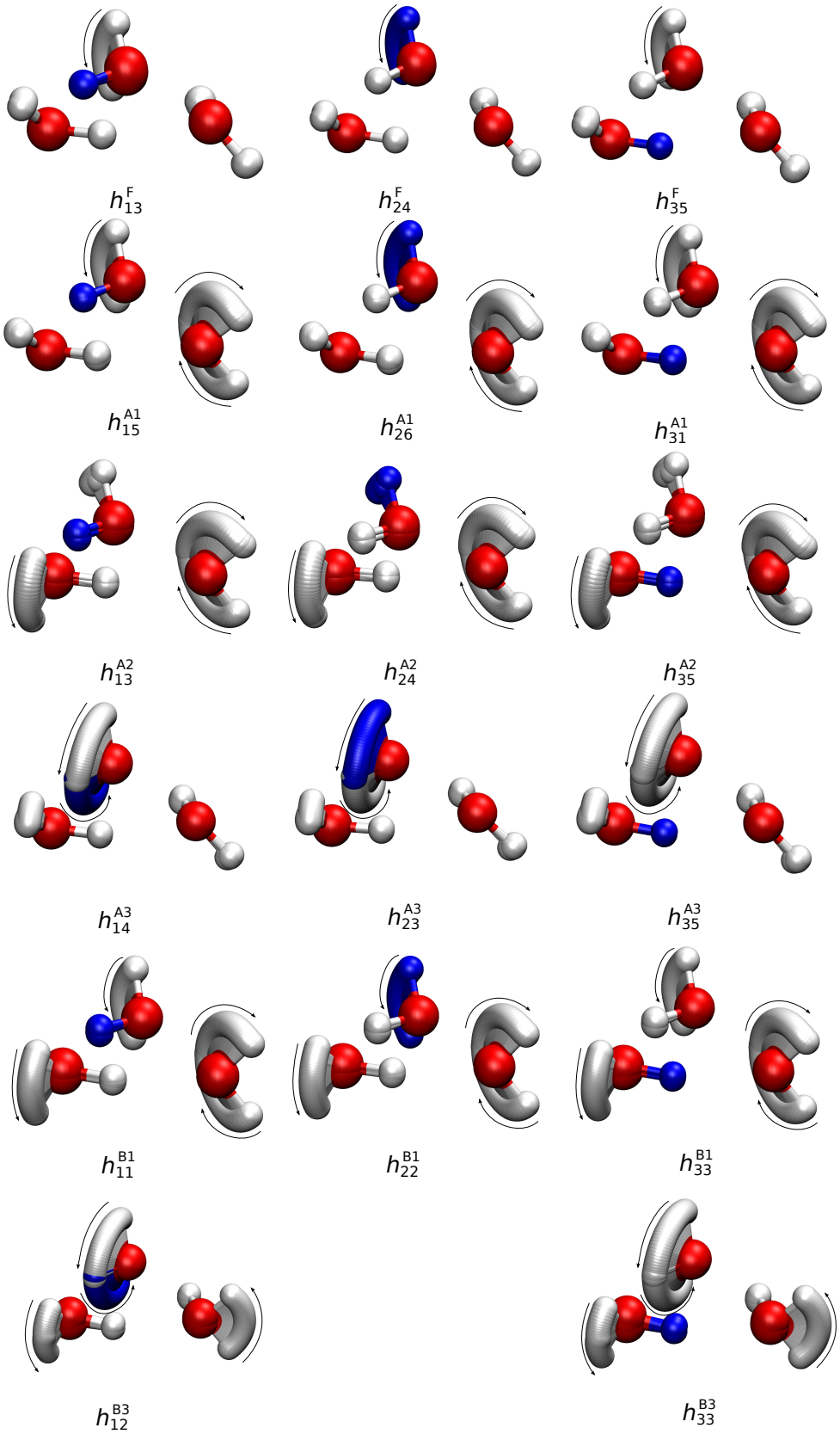

Fig. 2 Part I: Minimum action paths of flips and bifurcations connecting symmetry-related structures of $(HOD)(H_2O)_2$, which are responsible for the formation of the tunnelling splitting spectrum. Sequential snapshots of the trimer along the path are shown, with D atoms in blue and H atoms in red. Pathways are labeled by their corresponding tunnelling matrix elements in Table 4 of the main article, with path labels in the superscript and the initial and final structure labels, $1-6$, in the subscript.

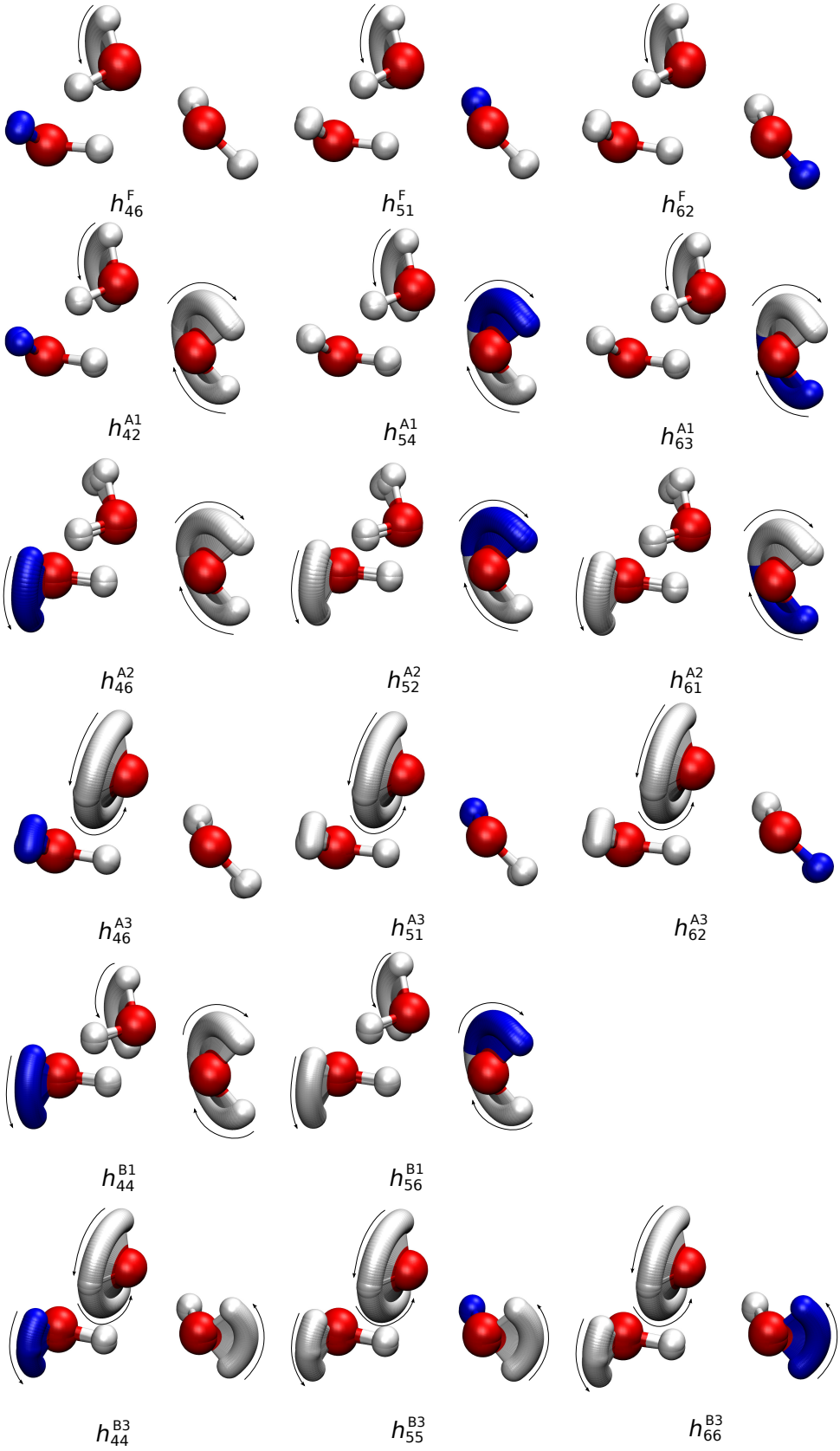

Fig. 3 Part II: Minimum action paths of flips and bifurcations connecting symmetry-related structures of $(HOD)(H_2O)_2$, which are responsible for the formation of the tunnelling splitting spectrum. Sequential snapshots of the trimer along the path are shown, with D atoms in blue and H atoms in red. Pathways are labeled by their corresponding tunnelling matrix elements in Table 4 of the main article, with path labels in the superscript and the initial and final structure labels, $1-6$, in the subscript.

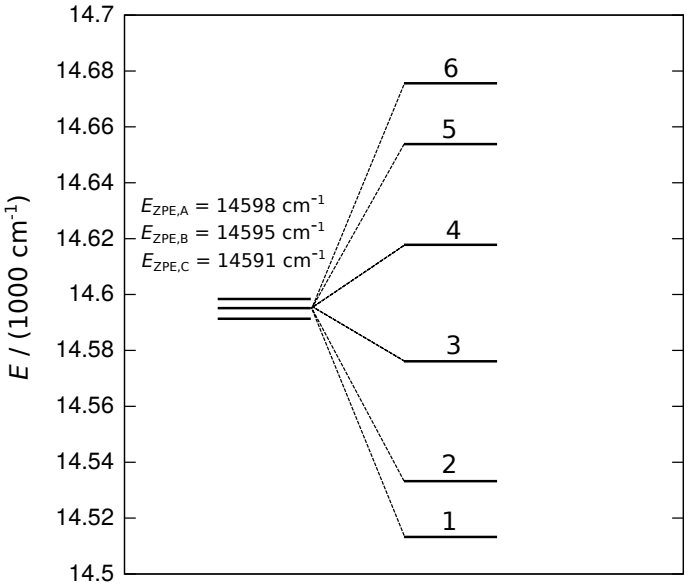

Fig. 4 Ground-state tunnelling splitting spectrum of pseudorotational (flip) states of $(D_2O)(H_2O)_2$. Flip states are labeled 1−6 and their energies are given in Table 1. The left set of levels refers to the non-tunnelling localized zero-point energies given in Table 2 of the main article.

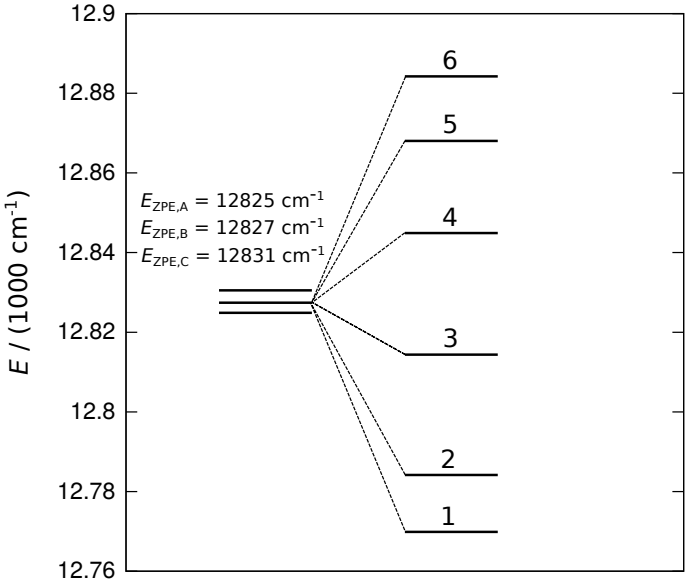

Fig. 5 Ground-state tunnelling splitting spectrum of pseudorotational (flip) states of $(H_2O)(D_2O)_2$. Flip states are labeled 1−6 and their energies are given in Table 2. The left set of levels refers to the non-tunnelling localized zero-point energies given in Table 2 of the main article.

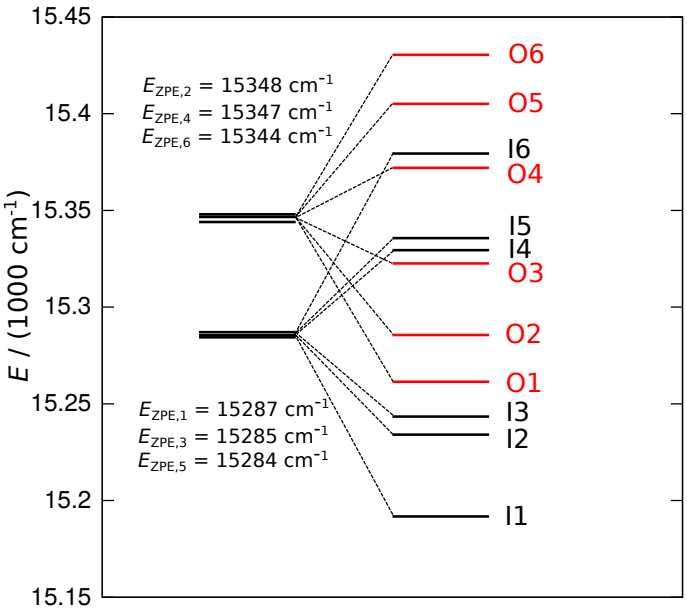

Fig. 6 Ground-state tunnelling splitting spectrum of pseudorotational (flip) states of $(HOD)(H_2O)_2$. Flip states of in-bond H/D substituted isomers are labeled I1−I6, while out-of-bond substituted isomers are labaled O1−O6 and coloured red. Energies of flip states are given in Table 4. The left set of levels refers to the non-tunnelling localized zero-point energies given in Table 2 of the main article.

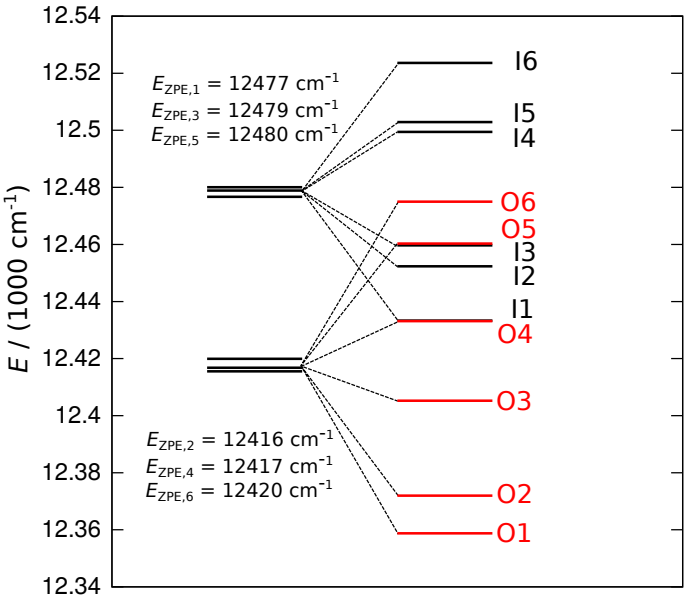

Fig. 7 Ground-state tunnelling splitting spectrum of pseudorotational (flip) states of $(HOD)(D_2O)_2$. Flip states of in-bond H/D substituted isomers are labeled I1−I6, while out-of-bond substituted isomers are labaled O1−O6 and coloured red. Energies of flip states are given in Table 5. The left set of levels refers to the non-tunnelling localized zero-point energies given in Table 2 of the main article.

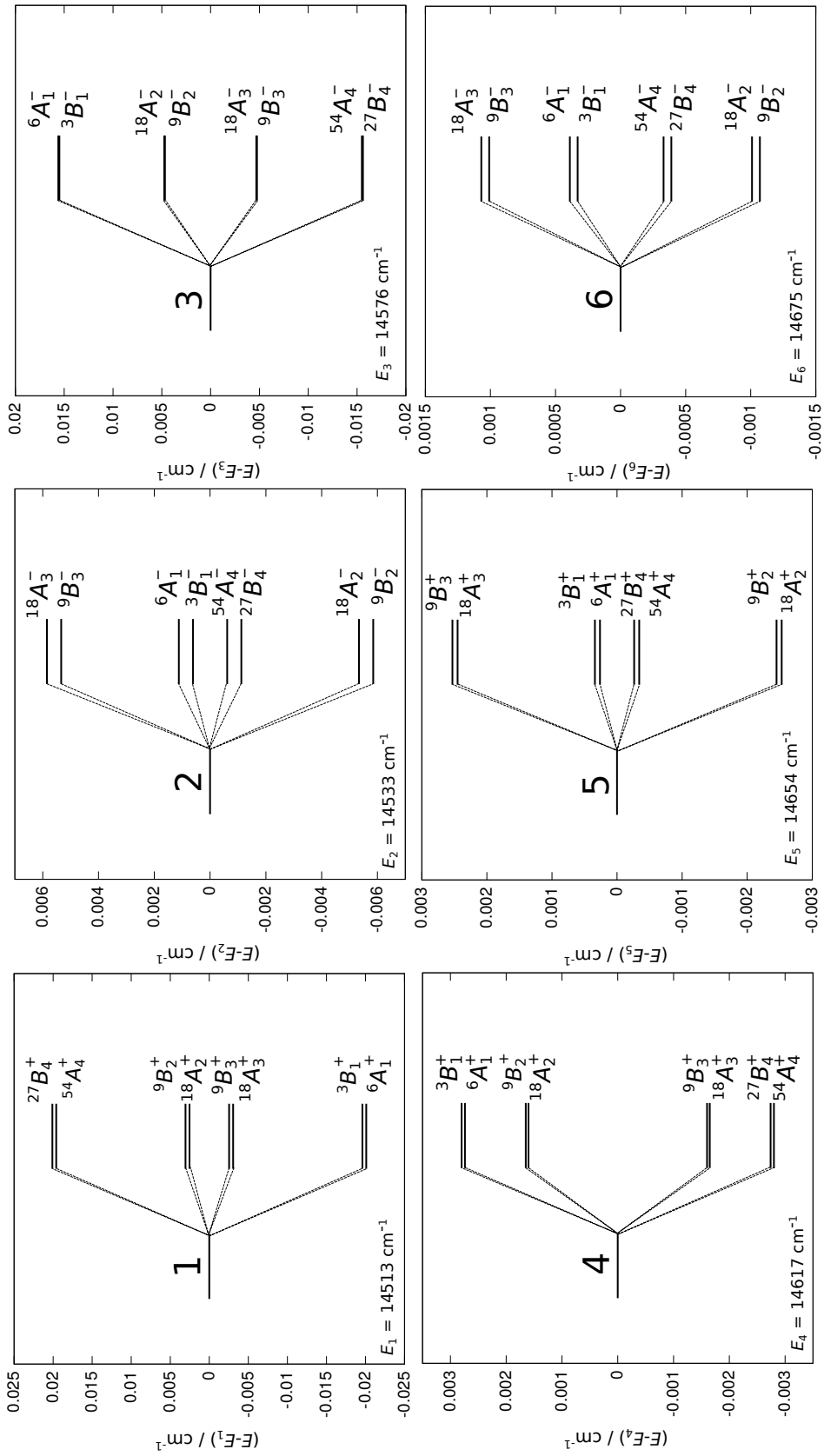

Fig. 8 Fine tunnelling splitting patterns of each pseudorotational (flip) state of $(D_2O)(H_2O)_2$, 1−6, induced by bifurcations. Energies are given in cm^{-1} with respect to the corresponding flip state. Symmetry labels of the G_{16} group and statistical weights are also given. Energy levels are listed in Table 1.

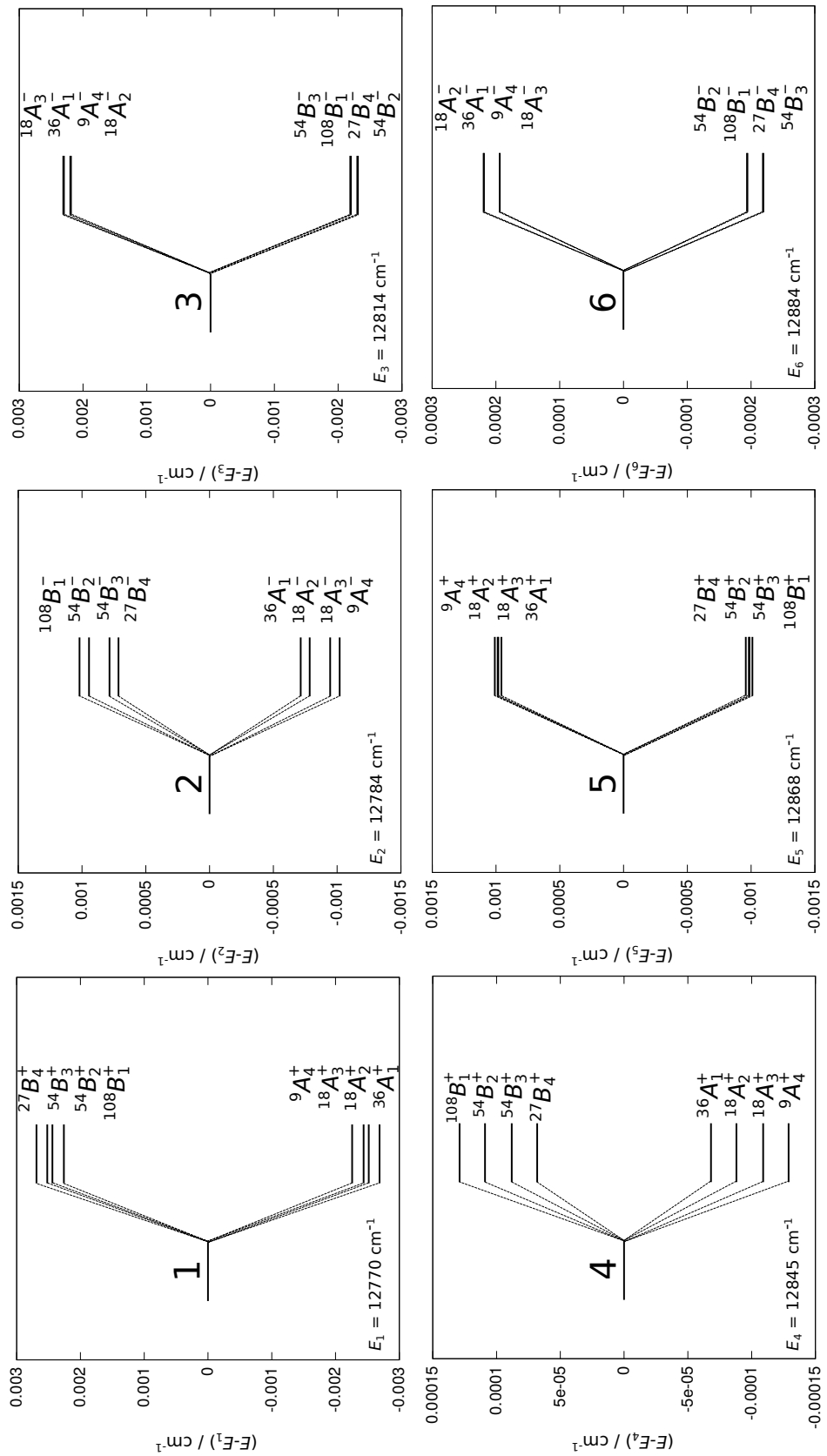

Fig. 9 Fine tunnelling splitting patterns of each pseudorotational (flip) state of $(H_2O)(D_2O)_2$, 1−6, induced by bifurcations. Energies are given in cm^{-1} with respect to the corresponding flip state. Symmetry labels of the G_{16} group and statistical weights are also given. Energy levels are listed in Table 2.

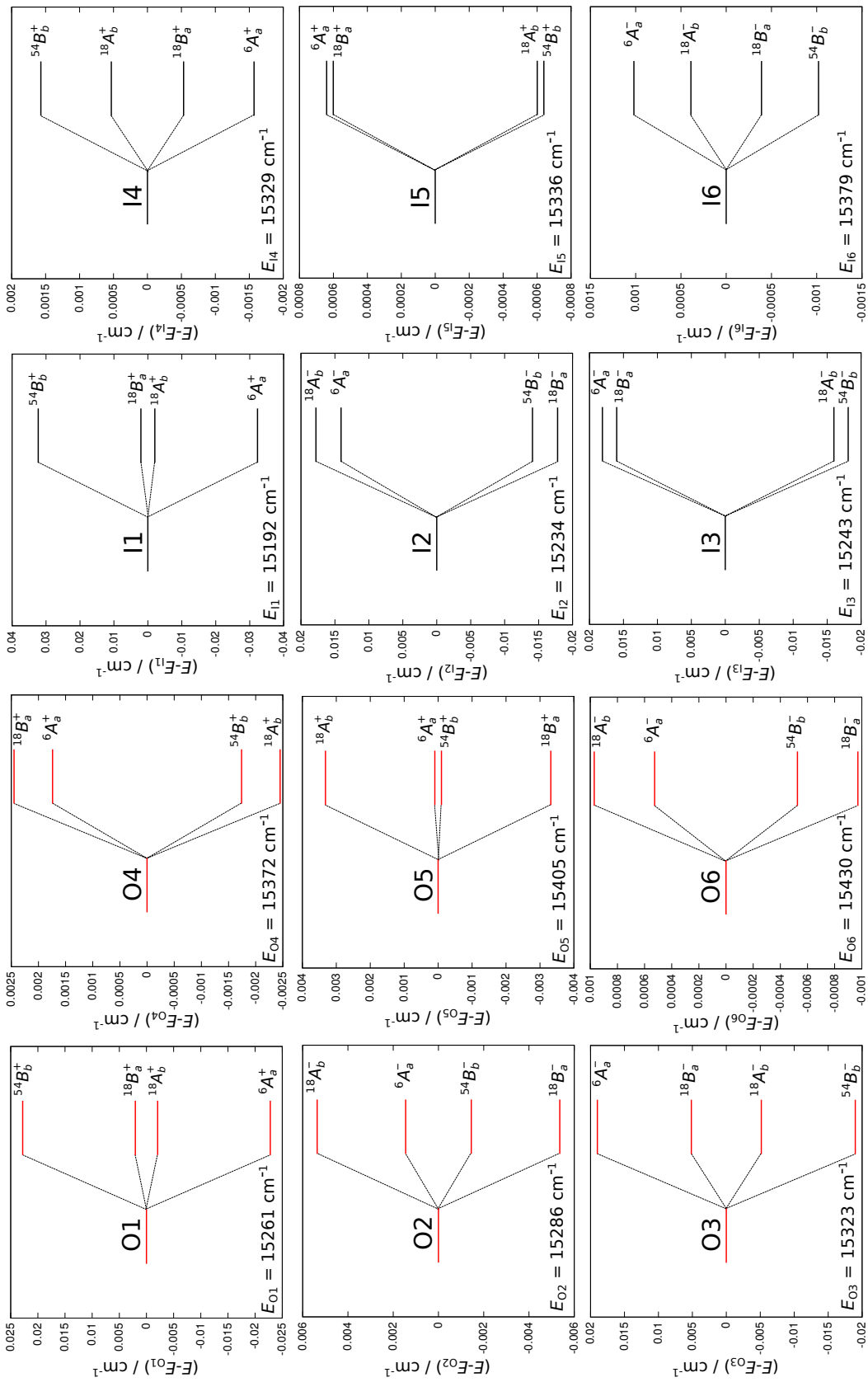

Fig. 10 Fine tunnelling splitting patterns of each pseudorotational (flip) state of $(HOD)(H_2O)_2$, induced by bifurcations. Flip states of in-bond H/D substituted isomers are labeled I1−I6, while out-of-bond substituted isomers are labaled O1−O6 and coloured red. Energies are given in cm^{-1} with respect to the corresponding flip state. Symmetry labels of the G_8 group and statistical weights are also given. Energy levels are listed in Table 4.

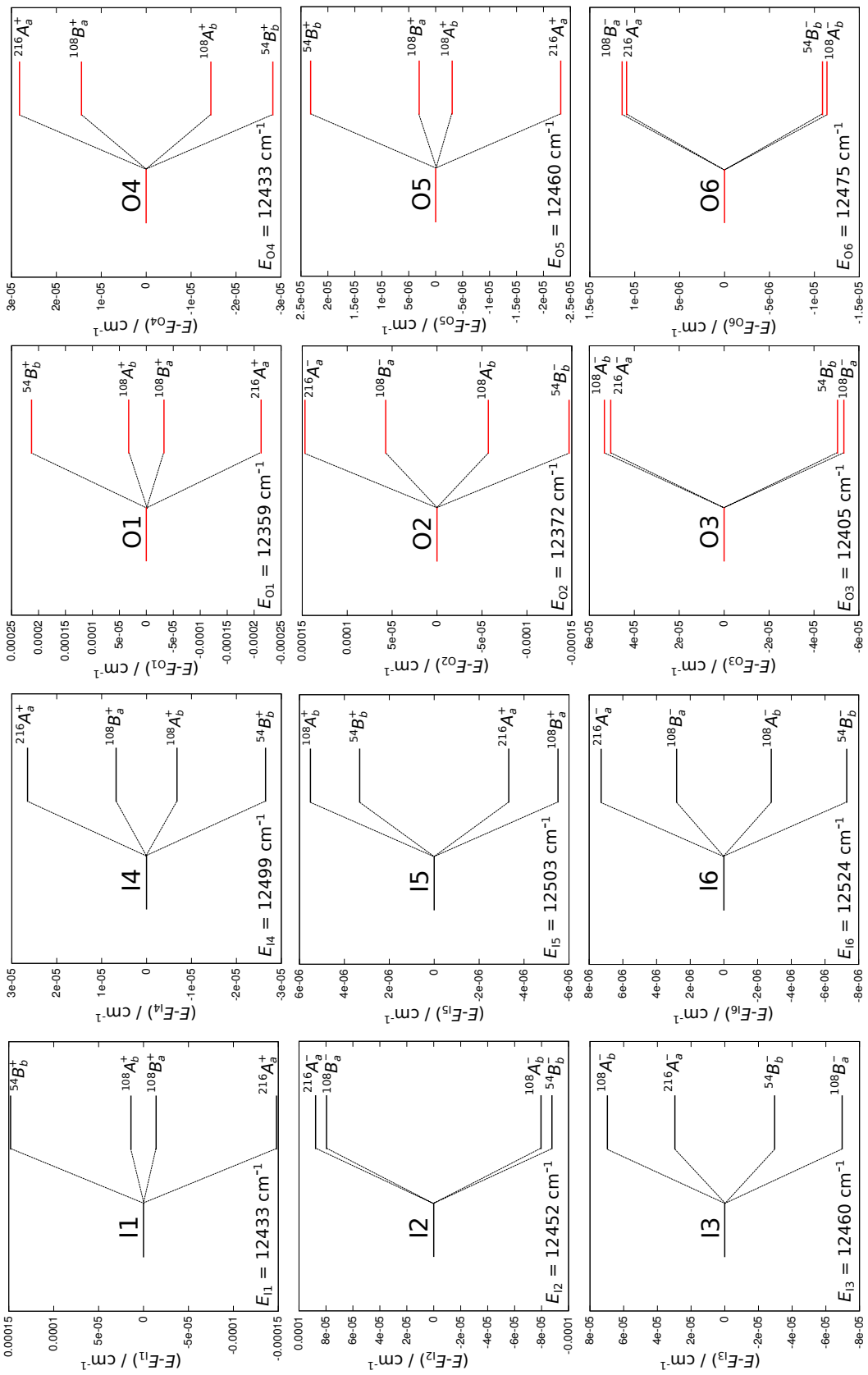

Fig. 11 Fine tunnelling splitting patterns of each pseudorotational (flip) state of $(HOD)(D_2O)_2$, induced by bifurcations. Flip states of in-bond H/D substituted isomers are labeled I1−I6, while out-of-bond substituted isomers are labaled O1−O6 and coloured red. Energies are given in cm^{-1} with respect to the corresponding flip state. Symmetry labels of the G_8 group and statistical weights are also given. Energy levels are listed in Table 5.

Table 1 Tunnelling-splitting pattern of $D_2O(H_2O)_2$ on MB-pol PES [69–71] with regular and scaled flip matrix elements (see text of the main article for details). The energies are given relative to the pseudorotational states 1−6. All energies are given in cm^{-1}. Symmetry labels are given in the first column and are explained in the text of main article.

$D_2O(H_2O)_2$	regular	scaled
6	14675.59	14637.52
$^{18}A_3^-$ (A,B,C)	1.07(−3)	1.13(−3)
$^{9}B_3^-$ (A,B,C)	1.01(−3)	1.07(−3)
$^{6}A_1^-$ (A,B,C)	3.90(−4)	2.93(−4)
$^{3}B_1^-$ (A,B,C)	3.30(−4)	2.34(−4)
$^{54}A_4^-$ (A,B,C)	−3.30(−4)	−2.34(−4)
$^{27}B_4^-$ (A,B,C)	−3.90(−4)	−2.93(−4)
$^{18}A_2^-$ (A,B,C)	−1.01(−3)	−1.07(−3)
$^{9}B_2^-$ (A,B,C)	−1.07(−3)	−1.13(−3)
5	14653.86	14625.60
$^{9}B_3^+$ (A,B,C)	2.53(−3)	2.82(−3)
$^{18}A_3^+$ (A,B,C)	2.45(−3)	2.75(−3)
$^{3}B_1^+$ (A,B,C)	3.41(−4)	1.63(−4)
$^{6}A_1^+$ (A,B,C)	2.62(−4)	8.75(−5)
$^{27}B_4^+$ (A,B,C)	−2.62(−4)	−8.75(−5)
$^{54}A_4^+$ (A,B,C)	−3.41(−4)	−1.64(−4)
$^{9}B_2^+$ (A,B,C)	−2.45(−3)	−2.75(−3)
$^{18}A_2^+$ (A,B,C)	−2.53(−3)	−2.82(−3)
4	14617.81	14608.00
$^{3}B_1^+$ (A,B,C)	2.80(−3)	2.81(−3)
$^{6}A_1^+$ (A,B,C)	2.74(−3)	2.76(−3)
$^{9}B_2^+$ (A,B,C)	1.65(−3)	1.79(−3)
$^{18}A_2^+$ (A,B,C)	1.60(−3)	1.74(−3)
$^{9}B_3^+$ (A,B,C)	−1.60(−3)	−1.74(−3)
$^{18}A_3^+$ (A,B,C)	−1.65(−3)	−1.79(−3)
$^{27}B_4^+$ (A,B,C)	−2.74(−3)	−2.76(−3)
$^{54}A_4^+$ (A,B,C)	−2.80(−3)	−2.81(−3)
3	14576.11	14585.90
$^{6}A_1^-$ (A,B,C)	1.56(−2)	1.54(−2)
$^{3}B_1^-$ (A,B,C)	1.55(−2)	1.53(−2)
$^{18}A_2^-$ (A,B,C)	4.75(−3)	5.08(−3)
$^{9}B_2^-$ (A,B,C)	4.68(−3)	5.00(−3)
$^{18}A_3^-$ (A,B,C)	−4.68(−3)	−5.00(−3)
$^{9}B_3^-$ (A,B,C)	−4.75(−3)	−5.08(−3)
$^{54}A_4^-$ (A,B,C)	−1.55(−2)	−1.53(−2)
$^{27}B_4^-$ (A,B,C)	−1.56(−2)	−1.54(−2)
2	14533.21	14561.48
$^{18}A_3^-$ (A,B,C)	5.85(−3)	6.11(−3)
$^{9}B_3^-$ (A,B,C)	5.34(−3)	5.61(−3)
$^{6}A_1^-$ (A,B,C)	1.12(−3)	1.36(−3)
$^{3}B_1^-$ (A,B,C)	6.12(−4)	8.55(−4)
$^{54}A_4^-$ (A,B,C)	−6.11(−4)	−8.53(−4)
$^{27}B_4^-$ (A,B,C)	−1.12(−3)	−1.36(−3)
$^{18}A_2^-$ (A,B,C)	−5.34(−3)	−5.61(−3)
$^{9}B_2^-$ (A,B,C)	−5.85(−3)	−6.11(−3)
1	14513.24	14551.31
$^{27}B_4^+$ (A,B,C)	2.01(−2)	1.99(−2)
$^{54}A_4^+$ (A,B,C)	1.96(−2)	1.94(−2)
$^{9}B_2^+$ (A,B,C)	3.05(−3)	3.20(−3)
$^{18}A_2^+$ (A,B,C)	2.53(−3)	2.69(−3)
$^{9}B_3^+$ (A,B,C)	−2.53(−3)	−2.69(−3)
$^{18}A_3^+$ (A,B,C)	−3.05(−3)	−3.20(−3)
$^{3}B_1^+$ (A,B,C)	−1.96(−2)	−1.94(−2)
$^{6}A_1^+$ (A,B,C)	−2.01(−2)	−1.99(−2)

Table 2 Tunnelling-splitting pattern of $H_2O(D_2O)_2$ on MB-pol PES [69–71] with regular and scaled flip matrix elements (see text of the main article for details). The energies are given relative to the pseudorotational states 1−6. All energies are given in cm^{-1}. Symmetry labels are given in the first column and are explained in the text of the main article.

$H_2O(D_2O)_2$	regular	scaled
6	12884.23	12857.43
$^{18}A_2^-$ (A,B,C)	2.19(−4)	1.78(−4)
$^{36}A_1^-$ (A,B,C)	2.19(−4)	1.78(−4)
$^{9}A_4^-$ (A,B,C)	1.94(−4)	1.54(−4)
$^{18}A_3^-$ (A,B,C)	1.94(−4)	1.53(−4)
$^{54}B_2^-$ (A,B,C)	−1.94(−4)	−1.53(−4)
$^{108}B_1^-$ (A,B,C)	−1.94(−4)	−1.54(−4)
$^{27}B_4^-$ (A,B,C)	−2.19(−4)	−1.78(−4)
$^{54}B_3^-$ (A,B,C)	−2.19(−4)	−1.78(−4)
5	12868.03	12848.35
$^{9}A_4^+$ (A,B,C)	1.01(−3)	1.01(−3)
$^{18}A_2^+$ (A,B,C)	9.87(−4)	9.87(−4)
$^{18}A_3^+$ (A,B,C)	9.82(−4)	9.80(−4)
$^{36}A_1^+$ (A,B,C)	9.58(−4)	9.58(−4)
$^{27}B_4^+$ (A,B,C)	−9.58(−4)	−9.58(−4)
$^{54}B_2^+$ (A,B,C)	−9.82(−4)	−9.80(−4)
$^{54}B_3^+$ (A,B,C)	−9.87(−4)	−9.87(−4)
$^{108}B_1^+$ (A,B,C)	−1.01(−3)	−1.01(−3)
4	12844.90	12837.77
$^{108}B_1^+$ (A,B,C)	1.29(−4)	1.50(−4)
$^{54}B_2^+$ (A,B,C)	1.09(−4)	1.33(−4)
$^{54}B_3^+$ (A,B,C)	8.81(−5)	1.09(−4)
$^{27}B_4^+$ (A,B,C)	6.81(−5)	9.14(−5)
$^{36}A_1^+$ (A,B,C)	−6.81(−5)	−9.14(−5)
$^{18}A_2^+$ (A,B,C)	−8.81(−5)	−1.09(−4)
$^{18}A_3^+$ (A,B,C)	−1.09(−4)	−1.33(−4)
$^{9}A_4^+$ (A,B,C)	−1.29(−4)	−1.50(−4)
3	12814.38	12821.50
$^{18}A_3^-$ (A,B,C)	2.31(−3)	2.34(−3)
$^{36}A_1^-$ (A,B,C)	2.30(−3)	2.32(−3)
$^{9}A_4^-$ (A,B,C)	2.20(−3)	2.23(−3)
$^{18}A_2^-$ (A,B,C)	2.19(−3)	2.21(−3)
$^{54}B_3^-$ (A,B,C)	−2.19(−3)	−2.21(−3)
$^{108}B_1^-$ (A,B,C)	−2.20(−3)	−2.23(−3)
$^{27}B_4^-$ (A,B,C)	−2.30(−3)	−2.32(−3)
$^{54}B_2^-$ (A,B,C)	−2.31(−3)	−2.34(−3)
2	12784.17	12803.85
$^{108}B_1^-$ (A,B,C)	1.02(−3)	9.98(−4)
$^{54}B_2^-$ (A,B,C)	9.45(−4)	9.30(−4)
$^{54}B_3^-$ (A,B,C)	7.85(−4)	7.66(−4)
$^{27}B_4^-$ (A,B,C)	7.14(−4)	6.97(−4)
$^{36}A_1^-$ (A,B,C)	−7.14(−4)	−6.97(−4)
$^{18}A_2^-$ (A,B,C)	−7.85(−4)	−7.66(−4)
$^{18}A_3^-$ (A,B,C)	−9.45(−4)	−9.30(−4)
$^{9}A_4^-$ (A,B,C)	−1.02(−3)	−9.98(−4)
1	12769.86	12796.66
$^{27}B_4^+$ (A,B,C)	2.69(−3)	2.67(−3)
$^{54}B_3^+$ (A,B,C)	2.52(−3)	2.50(−3)
$^{54}B_2^+$ (A,B,C)	2.44(−3)	2.41(−3)
$^{108}B_1^+$ (A,B,C)	2.26(−3)	2.24(−3)
$^{9}A_4^+$ (A,B,C)	−2.26(−3)	−2.24(−3)
$^{18}A_3^+$ (A,B,C)	−2.44(−3)	−2.41(−3)
$^{18}A_2^+$ (A,B,C)	−2.52(−3)	−2.50(−3)
$^{36}A_1^+$ (A,B,C)	−2.69(−3)	−2.67(−3)

Table 3 Analytic expressions for tunnelling energy levels of $d2$- and $d4$-trimer of each symmetry species in the G_{16} group, relative to the energy of the pseudorotational state, using tunnelling matrix elements in Table 3 of the main article and structure coefficients of pseudorotational states $\beta_{\mathrm{A-C}}$ (see text of the main article for details).

$$
\begin{aligned}
E(A_1^+) = \;& +(\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B1}} + (\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B3}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A2}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A3}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{BA}}^{\mathrm{A1}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{AC}}^{\mathrm{A1}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A2}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A3}} + (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B1}} + (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B3}} \\
& + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A2}} + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A3}} + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{CB}}^{\mathrm{A1}} + (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B1}} + (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B3}} \\
E(A_2^+) = \;& +(\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B1}} + (\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B3}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A2}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A3}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{BA}}^{\mathrm{A1}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{AC}}^{\mathrm{A1}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A2}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A3}} - (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B1}} + (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B3}} \\
& - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A2}} + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A3}} + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{CB}}^{\mathrm{A1}} + (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B1}} - (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B3}} \\
E(A_3^+) = \;& -(\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B1}} + (\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B3}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A2}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A3}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{BA}}^{\mathrm{A1}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{AC}}^{\mathrm{A1}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A2}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A3}} + (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B1}} - (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B3}} \\
& + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A2}} - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A3}} + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{CB}}^{\mathrm{A1}} + (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B1}} + (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B3}} \\
E(A_4^+) = \;& -(\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B1}} + (\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B3}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A2}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A3}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{BA}}^{\mathrm{A1}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{AC}}^{\mathrm{A1}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A2}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A3}} - (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B1}} - (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B3}} \\
& - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A2}} - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A3}} + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{CB}}^{\mathrm{A1}} + (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B1}} - (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B3}} \\
E(B_1^+) = \;& +(\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B1}} - (\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B3}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A2}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A3}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{BA}}^{\mathrm{A1}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{AC}}^{\mathrm{A1}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A2}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A3}} + (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B1}} + (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B3}} \\
& + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A2}} + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A3}} - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{CB}}^{\mathrm{A1}} - (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B1}} + (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B3}} \\
E(B_2^+) = \;& +(\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B1}} - (\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B3}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A2}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A3}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{BA}}^{\mathrm{A1}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{AC}}^{\mathrm{A1}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A2}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A3}} - (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B1}} + (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B3}} \\
& - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A2}} + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A3}} - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{CB}}^{\mathrm{A1}} - (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B1}} - (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B3}} \\
E(B_3^+) = \;& -(\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B1}} - (\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B3}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A2}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A3}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{BA}}^{\mathrm{A1}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{AC}}^{\mathrm{A1}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A2}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A3}} + (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B1}} - (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B3}} \\
& + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A2}} - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A3}} - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{CB}}^{\mathrm{A1}} - (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B1}} + (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B3}} \\
E(B_4^+) = \;& -(\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B1}} - (\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B3}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A2}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A3}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{BA}}^{\mathrm{A1}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{AC}}^{\mathrm{A1}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A2}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A3}} - (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B1}} - (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B3}} \\
& - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A2}} - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A3}} - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{CB}}^{\mathrm{A1}} - (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B1}} - (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B3}} \\
E(A_1^-) = \;& -(\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B1}} - (\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B3}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A2}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A3}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{BA}}^{\mathrm{A1}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{AC}}^{\mathrm{A1}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A2}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A3}} - (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B1}} - (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B3}} \\
& + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A2}} - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A3}} + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{CB}}^{\mathrm{A1}} - (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B1}} - (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B3}} \\
E(A_2^-) = \;& -(\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B1}} - (\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B3}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A2}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A3}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{BA}}^{\mathrm{A1}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{AC}}^{\mathrm{A1}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A2}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A3}} + (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B1}} - (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B3}} \\
& - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A2}} - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A3}} + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{CB}}^{\mathrm{A1}} - (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B1}} + (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B3}} \\
E(A_3^-) = \;& +(\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B1}} - (\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B3}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A2}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A3}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{BA}}^{\mathrm{A1}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{AC}}^{\mathrm{A1}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A2}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A3}} - (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B1}} + (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B3}} \\
& + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A2}} + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A3}} + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{CB}}^{\mathrm{A1}} - (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B1}} - (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B3}} \\
E(A_4^-) = \;& +(\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B1}} - (\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B3}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A2}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A3}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{BA}}^{\mathrm{A1}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{AC}}^{\mathrm{A1}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A2}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A3}} + (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B1}} + (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B3}} \\
& - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A2}} + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A3}} - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{CB}}^{\mathrm{A1}} + (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B1}} + (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B3}} \\
E(B_1^-) = \;& -(\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B1}} + (\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B3}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A2}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A3}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{BA}}^{\mathrm{A1}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{AC}}^{\mathrm{A1}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A2}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A3}} - (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B1}} - (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B3}} \\
& + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A2}} - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A3}} - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{CB}}^{\mathrm{A1}} - (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B1}} - (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B3}} \\
E(B_2^-) = \;& -(\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B1}} + (\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B3}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A2}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A3}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{BA}}^{\mathrm{A1}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{AC}}^{\mathrm{A1}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A2}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A3}} + (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B1}} - (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B3}} \\
& - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A2}} - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A3}} - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{CB}}^{\mathrm{A1}} + (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B1}} + (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B3}} \\
E(B_3^-) = \;& +(\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B1}} + (\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B3}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A2}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A3}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{BA}}^{\mathrm{A1}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{AC}}^{\mathrm{A1}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A2}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A3}} - (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B1}} + (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B3}} \\
& + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A2}} + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A3}} - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{CB}}^{\mathrm{A1}} - (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B1}} - (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B3}} \\
E(B_4^-) = \;& +(\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B1}} + (\beta_\mathrm{A})^2 h_{\mathrm{AA}}^{\mathrm{B3}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A2}} + 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{AB}}^{\mathrm{A3}} - 2\beta_\mathrm{A}\beta_\mathrm{B} h_{\mathrm{BA}}^{\mathrm{A1}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{AC}}^{\mathrm{A1}} - 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A2}} + 2\beta_\mathrm{A}\beta_\mathrm{C} h_{\mathrm{CA}}^{\mathrm{A3}} + (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B1}} + (\beta_\mathrm{B})^2 h_{\mathrm{BB}}^{\mathrm{B3}} \\
& - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A2}} + 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{BC}}^{\mathrm{A3}} - 2\beta_\mathrm{B}\beta_\mathrm{C} h_{\mathrm{CB}}^{\mathrm{A1}} + (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B1}} + (\beta_\mathrm{C})^2 h_{\mathrm{CC}}^{\mathrm{B3}}
\end{aligned}
$$

Table 4 Tunnelling-splitting pattern of $HOD(H_2O)_2$ on MB-pol PES [69–71] with regular and scaled flip matrix elements (see text of the main article for details). The energies are given relative to the pseudorotational states I1−I6 and O1−6, for isomers with D atom in and out of the H-bond, respectively. All energies are given in cm^{-1}. Symmetry labels are given in the first column and are explained in the text of the main article.

$HOD(H_2O)_2$	regular	scaled
O6	15430.46	15390.77
$^{18}A_b^-$ (2,4,6)	9.71(−4)	9.93(−4)
$^{6}A_a^-$ (2,4,6)	5.26(−4)	4.74(−4)
$^{54}B_b^-$ (2,4,6)	−5.26(−4)	−4.74(−4)
$^{18}B_a^-$ (2,4,6)	−9.71(−4)	−9.93(−4)
O5	15405.15	15377.09
$^{18}A_b^+$ (2,4,6)	3.32(−3)	3.50(−3)
$^{6}A_a^+$ (2,4,6)	9.85(−5)	−1.72(−5)
$^{54}B_b^+$ (2,4,6)	−9.87(−5)	1.68(−5)
$^{18}B_a^+$ (2,4,6)	−3.32(−3)	−3.50(−3)
I6	15379.41	15335.33
$^{6}A_a^-$ (1,3,5)	1.02(−3)	9.93(−4)
$^{18}A_b^-$ (1,3,5)	3.90(−4)	4.03(−4)
$^{18}B_a^-$ (1,3,5)	−3.90(−4)	−4.03(−4)
$^{54}B_b^-$ (1,3,5)	−1.02(−3)	−9.94(−4)
O4	15372.06	15360.43
$^{18}B_a^+$ (2,4,6)	2.45(−3)	2.51(−3)
$^{6}A_a^+$ (2,4,6)	1.74(−3)	1.76(−3)
$^{54}B_b^+$ (2,4,6)	−1.74(−3)	−1.76(−3)
$^{18}A_b^+$ (2,4,6)	−2.45(−3)	−2.51(−3)
I5	15335.67	15311.81
$^{6}A_a^+$ (1,3,5)	6.40(−4)	6.12(−4)
$^{18}B_a^+$ (1,3,5)	6.01(−4)	7.33(−4)
$^{18}A_b^+$ (1,3,5)	−6.00(−4)	−7.30(−4)
$^{54}B_b^+$ (1,3,5)	−6.41(−4)	−6.15(−4)
I4	15329.46	15309.25
$^{54}B_b^+$ (1,3,5)	1.57(−3)	1.56(−3)
$^{18}A_b^+$ (1,3,5)	5.32(−4)	8.10(−4)
$^{18}B_a^+$ (1,3,5)	−5.33(−4)	−8.12(−4)
$^{6}A_a^+$ (1,3,5)	−1.57(−3)	−1.56(−3)
O3	15322.57	15334.21
$^{6}A_a^-$ (2,4,6)	1.90(−2)	1.89(−2)
$^{18}B_a^-$ (2,4,6)	5.15(−3)	5.37(−3)
$^{18}A_b^-$ (2,4,6)	−5.15(−3)	−5.37(−3)
$^{54}B_b^-$ (2,4,6)	−1.90(−2)	−1.89(−2)
O2	15285.61	15313.67
$^{18}A_b^-$ (2,4,6)	5.36(−3)	5.56(−3)
$^{6}A_a^-$ (2,4,6)	1.45(−3)	1.59(−3)
$^{54}B_b^-$ (2,4,6)	−1.45(−3)	−1.59(−3)
$^{18}B_a^-$ (2,4,6)	−5.36(−3)	−5.56(−3)
O1	15261.43	15301.13
$^{54}B_b^+$ (2,4,6)	2.28(−2)	2.23(−2)
$^{18}B_a^+$ (2,4,6)	2.05(−3)	2.17(−3)
$^{18}A_b^+$ (2,4,6)	−2.05(−3)	−2.17(−3)
$^{6}A_a^+$ (2,4,6)	−2.28(−2)	−2.23(−2)
I3	15243.41	15263.62
$^{6}A_a^-$ (1,3,5)	1.81(−2)	1.83(−2)
$^{18}B_a^-$ (1,3,5)	1.60(−2)	1.60(−2)
$^{18}A_b^-$ (1,3,5)	−1.61(−2)	−1.60(−2)
$^{54}B_b^-$ (1,3,5)	−1.81(−2)	−1.83(−2)
I2	15234.10	15257.96
$^{18}A_b^-$ (1,3,5)	1.78(−2)	1.77(−2)
$^{6}A_a^-$ (1,3,5)	1.41(−2)	1.40(−2)
$^{54}B_b^-$ (1,3,5)	−1.42(−2)	−1.40(−2)
$^{18}B_a^-$ (1,3,5)	−1.78(−2)	−1.77(−2)
I1	15191.78	15235.86
$^{54}B_b^+$ (1,3,5)	3.23(−2)	3.23(−2)
$^{18}B_a^+$ (1,3,5)	2.05(−3)	2.22(−3)
$^{18}A_b^+$ (1,3,5)	−2.05(−3)	−2.22(−3)
$^{6}A_a^+$ (1,3,5)	−3.23(−2)	−3.23(−2)

Table 5 Tunnelling-splitting pattern of $HOD(D_2O)_2$ on MB-pol PES [69–71] with regular and scaled flip matrix elements (see text of the main article for details). The energies are given relative to the pseudorotational states I1−I6 and O1−6, for isomers with H atom in and out of the H-bond, respectively. All energies are given in cm^{-1}. Symmetry labels are given in the first column and are explained in the text of the main article.

$HOD(D_2O)_2$	regular	scaled
I6	12523.60	12502.42
$^{216}A_a^-$ (1,3,5)	7.29(−6)	7.55(−6)
$^{108}B_a^-$ (1,3,5)	2.81(−6)	3.17(−6)
$^{108}A_b^-$ (1,3,5)	−2.81(−6)	−3.17(−6)
$^{54}B_b^-$ (1,3,5)	−7.29(−6)	−7.55(−6)
I5	12502.87	12491.03
$^{108}A_b^+$ (1,3,5)	5.51(−6)	5.86(−6)
$^{54}B_b^+$ (1,3,5)	3.32(−6)	3.30(−6)
$^{216}A_a^+$ (1,3,5)	−3.32(−6)	−3.30(−6)
$^{108}B_a^+$ (1,3,5)	−5.51(−6)	−5.86(−6)
I4	12499.42	12490.08
$^{216}A_a^+$ (1,3,5)	2.65(−5)	2.62(−5)
$^{108}B_a^+$ (1,3,5)	6.78(−6)	8.49(−6)
$^{108}A_b^+$ (1,3,5)	−6.78(−6)	−8.49(−6)
$^{54}B_b^+$ (1,3,5)	−2.65(−5)	−2.62(−5)
O6	12474.97	12447.72
$^{108}B_a^-$ (2,4,6)	1.14(−5)	1.16(−5)
$^{216}A_a^-$ (2,4,6)	1.09(−5)	1.08(−5)
$^{54}B_b^-$ (2,4,6)	−1.09(−5)	−1.08(−5)
$^{108}A_b^-$ (2,4,6)	−1.14(−5)	−1.16(−5)
O5	12460.32	12439.57
$^{54}B_b^+$ (2,4,6)	2.32(−5)	2.30(−5)
$^{108}B_a^+$ (2,4,6)	3.06(−6)	3.60(−6)
$^{108}A_b^+$ (2,4,6)	−3.06(−6)	−3.60(−6)
$^{216}A_a^+$ (2,4,6)	−2.32(−5)	−2.30(−5)
I3	12459.66	12469.00
$^{108}A_b^-$ (1,3,5)	6.97(−5)	6.96(−5)
$^{216}A_a^-$ (1,3,5)	2.96(−5)	2.96(−5)
$^{54}B_b^-$ (1,3,5)	−2.96(−5)	−2.96(−5)
$^{108}B_a^-$ (1,3,5)	−6.97(−5)	−6.96(−5)
I2	12452.35	12464.19
$^{216}A_a^-$ (1,3,5)	8.77(−5)	8.75(−5)
$^{108}B_a^-$ (1,3,5)	7.96(−5)	7.91(−5)
$^{108}A_b^-$ (1,3,5)	−7.96(−5)	−7.91(−5)
$^{54}B_b^-$ (1,3,5)	−8.77(−5)	−8.75(−5)
I1	12433.32	12454.50
$^{54}B_b^+$ (1,3,5)	1.48(−4)	1.48(−4)
$^{108}A_b^+$ (1,3,5)	1.40(−5)	1.53(−5)
$^{108}B_a^+$ (1,3,5)	−1.40(−5)	−1.53(−5)
$^{216}A_a^+$ (1,3,5)	−1.48(−4)	−1.48(−4)
O4	12433.11	12426.60
$^{216}A_a^+$ (2,4,6)	2.82(−5)	2.67(−5)
$^{108}B_a^+$ (2,4,6)	1.44(−5)	1.58(−5)
$^{108}A_b^+$ (2,4,6)	−1.44(−5)	−1.58(−5)
$^{54}B_b^+$ (2,4,6)	−2.82(−5)	−2.67(−5)
O3	12405.25	12411.76
$^{108}A_b^-$ (2,4,6)	5.33(−5)	5.51(−5)
$^{216}A_a^-$ (2,4,6)	5.05(−5)	5.09(−5)
$^{54}B_b^-$ (2,4,6)	−5.05(−5)	−5.09(−5)
$^{108}B_a^-$ (2,4,6)	−5.33(−5)	−5.51(−5)
O2	12371.99	12392.74
$^{216}A_a^-$ (2,4,6)	1.47(−4)	1.46(−4)
$^{108}B_a^-$ (2,4,6)	5.71(−5)	5.88(−5)
$^{108}A_b^-$ (2,4,6)	−5.71(−5)	−5.88(−5)
$^{54}B_b^-$ (2,4,6)	−1.47(−4)	−1.46(−4)
O1	12358.78	12386.04
$^{54}B_b^+$ (2,4,6)	2.13(−4)	2.12(−4)
$^{108}A_b^+$ (2,4,6)	3.27(−5)	3.46(−5)
$^{108}B_a^+$ (2,4,6)	−3.27(−5)	−3.46(−5)
$^{216}A_a^+$ (2,4,6)	−2.13(−4)	−2.12(−4)

Table 6 Analytic expressions for tunnelling energy levels of $d1$- and $d5$-trimer of each symmetry species in the G_8 group, relative to the energy of the pseudorotational state, using tunnelling matrix elements in Table 4 of the main article and structure coefficients of pseudorotational states β_{1-6} (see text of the main article for details).

$$
\begin{aligned}
E(A_a^+) = \quad & +(\beta_1)^2 h_{11}^{\mathrm{B1}} + 2\beta_1\beta_3 h_{13}^{\mathrm{A2}} + 2\beta_1\beta_3 h_{31}^{\mathrm{A1}} + 2\beta_1\beta_5 h_{15}^{\mathrm{A1}} + 2\beta_1\beta_5 h_{51}^{\mathrm{A3}} + (\beta_3)^2 h_{33}^{\mathrm{B1}} + (\beta_3)^2 h_{33}^{\mathrm{B3}} + 2\beta_3\beta_5 h_{35}^{\mathrm{A2}} + 2\beta_3\beta_5 h_{35}^{\mathrm{A3}} + (\beta_5)^2 h_{55}^{\mathrm{B3}} \\
E(A_b^+) = \quad & -(\beta_1)^2 h_{11}^{\mathrm{B1}} - 2\beta_1\beta_3 h_{13}^{\mathrm{A2}} + 2\beta_1\beta_3 h_{31}^{\mathrm{A1}} - 2\beta_1\beta_5 h_{15}^{\mathrm{A1}} + 2\beta_1\beta_5 h_{51}^{\mathrm{A3}} + (\beta_3)^2 h_{33}^{\mathrm{B1}} - (\beta_3)^2 h_{33}^{\mathrm{B3}} + 2\beta_3\beta_5 h_{35}^{\mathrm{A2}} - 2\beta_3\beta_5 h_{35}^{\mathrm{A3}} + (\beta_5)^2 h_{55}^{\mathrm{B3}} \\
E(B_a^+) = \quad & +(\beta_1)^2 h_{11}^{\mathrm{B1}} + 2\beta_1\beta_3 h_{13}^{\mathrm{A2}} - 2\beta_1\beta_3 h_{31}^{\mathrm{A1}} + 2\beta_1\beta_5 h_{15}^{\mathrm{A1}} - 2\beta_1\beta_5 h_{51}^{\mathrm{A3}} - (\beta_3)^2 h_{33}^{\mathrm{B1}} + (\beta_3)^2 h_{33}^{\mathrm{B3}} - 2\beta_3\beta_5 h_{35}^{\mathrm{A2}} + 2\beta_3\beta_5 h_{35}^{\mathrm{A3}} - (\beta_5)^2 h_{55}^{\mathrm{B3}} \\
E(B_b^+) = \quad & -(\beta_1)^2 h_{11}^{\mathrm{B1}} - 2\beta_1\beta_3 h_{13}^{\mathrm{A2}} - 2\beta_1\beta_3 h_{31}^{\mathrm{A1}} - 2\beta_1\beta_5 h_{15}^{\mathrm{A1}} - 2\beta_1\beta_5 h_{51}^{\mathrm{A3}} - (\beta_3)^2 h_{33}^{\mathrm{B1}} - (\beta_3)^2 h_{33}^{\mathrm{B3}} - 2\beta_3\beta_5 h_{35}^{\mathrm{A2}} - 2\beta_3\beta_5 h_{35}^{\mathrm{A3}} - (\beta_5)^2 h_{55}^{\mathrm{B3}} \\
E(A_a^-) = \quad & -(\beta_1)^2 h_{11}^{\mathrm{B1}} + 2\beta_1\beta_3 h_{13}^{\mathrm{A2}} + 2\beta_1\beta_3 h_{31}^{\mathrm{A1}} + 2\beta_1\beta_5 h_{15}^{\mathrm{A1}} - 2\beta_1\beta_5 h_{51}^{\mathrm{A3}} - (\beta_3)^2 h_{33}^{\mathrm{B1}} - (\beta_3)^2 h_{33}^{\mathrm{B3}} + 2\beta_3\beta_5 h_{35}^{\mathrm{A2}} - 2\beta_3\beta_5 h_{35}^{\mathrm{A3}} - (\beta_5)^2 h_{55}^{\mathrm{B3}} \\
E(A_b^-) = \quad & +(\beta_1)^2 h_{11}^{\mathrm{B1}} - 2\beta_1\beta_3 h_{13}^{\mathrm{A2}} + 2\beta_1\beta_3 h_{31}^{\mathrm{A1}} - 2\beta_1\beta_5 h_{15}^{\mathrm{A1}} - 2\beta_1\beta_5 h_{51}^{\mathrm{A3}} - (\beta_3)^2 h_{33}^{\mathrm{B1}} + (\beta_3)^2 h_{33}^{\mathrm{B3}} + 2\beta_3\beta_5 h_{35}^{\mathrm{A2}} + 2\beta_3\beta_5 h_{35}^{\mathrm{A3}} - (\beta_5)^2 h_{55}^{\mathrm{B3}} \\
E(B_a^-) = \quad & -(\beta_1)^2 h_{11}^{\mathrm{B1}} + 2\beta_1\beta_3 h_{13}^{\mathrm{A2}} - 2\beta_1\beta_3 h_{31}^{\mathrm{A1}} + 2\beta_1\beta_5 h_{15}^{\mathrm{A1}} + 2\beta_1\beta_5 h_{51}^{\mathrm{A3}} + (\beta_3)^2 h_{33}^{\mathrm{B1}} - (\beta_3)^2 h_{33}^{\mathrm{B3}} - 2\beta_3\beta_5 h_{35}^{\mathrm{A2}} - 2\beta_3\beta_5 h_{35}^{\mathrm{A3}} + (\beta_5)^2 h_{55}^{\mathrm{B3}} \\
E(B_b^-) = \quad & +(\beta_1)^2 h_{11}^{\mathrm{B1}} - 2\beta_1\beta_3 h_{13}^{\mathrm{A2}} - 2\beta_1\beta_3 h_{31}^{\mathrm{A1}} - 2\beta_1\beta_5 h_{15}^{\mathrm{A1}} + 2\beta_1\beta_5 h_{51}^{\mathrm{A3}} + (\beta_3)^2 h_{33}^{\mathrm{B1}} + (\beta_3)^2 h_{33}^{\mathrm{B3}} - 2\beta_3\beta_5 h_{35}^{\mathrm{A2}} + 2\beta_3\beta_5 h_{35}^{\mathrm{A3}} + (\beta_5)^2 h_{55}^{\mathrm{B3}}
\end{aligned}
$$