Electronic Supplementary Information for PCCP article "Tunneling splittings in the energetically low-lying structural isomers of the water hexamer: the prism, the cage and the book"

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Table 1 Tunneling matrix elements of the water hexamer prism with deuterated monomers in positions A and D (see Fig. 1 in the main article) on MB-pol PES[1–3] for the rearrangement paths AD, ÃD/D̃A, rot E and rot C (see the main article text for notation) in the vibrational ground state and the five lowest-frequency excited vibrational modes in cm^{-1}.

Mode	ω_e	$h_a/10^{-8}$	$h_g/10^{-9}$	$h_E/10^{-6}$	$h_C/10^{-7}$
GS	0	−4.23	−1.99	−2.66	−1.98
1	61.0	−4.20	−2.26	−3.06	−2.47
2	71.4	−5.24	−3.25	−3.09	−2.27
3	73.1	−4.75	−0.711	−2.67	−2.24
4	108	−2.86	1.16	−2.36	−5.53
5	114	−2.09	2.71	2.15	−2.26

Table 2 Tunneling matrix elements of the water hexamer prism $(H_2{}^{18}O)_6$ on MB-pol PES[1–3] for the rearrangement paths AD, ÃD/D̃A, rot E and rot C (see the main article text for notation) in the vibrational ground state and the five lowest-frequency excited vibrational modes in cm^{-1}.

Mode	ω_e	$h_a/10^{-5}$	$h_g/10^{-6}$	$h_E/10^{-6}$	$h_C/10^{-7}$
GS	0	−2.04	−2.88	−2.52	−1.75
1	59.1	−1.89	−2.97	−2.95	−2.24
2	68.3	−2.43	−3.64	−2.84	−1.97
3	70.4	−0.592	0.0137	−2.59	−1.98
4	105	−0.699	1.25	2.01	−5.22
5	114	−1.06	−0.444	−10.5	−1.73

Table 3 Tunneling matrix elements of the water hexamer-d12 prism $(D_2O)_6$ on MB-pol PES[1–3] for the rearrangement paths AD, ÃD/D̃A, rot E and rot C (see the main article text for notation) in the vibrational ground state and the five lowest-frequency excited vibrational modes in cm^{-1}.

Mode	ω_e	$h_a/10^{-8}$	$h_g/10^{-9}$	$h_E/10^{-10}$	$h_C/10^{-11}$
GS	0	−3.85	−1.91	−3.35	−0.999
1	58.1	−3.67	−1.97	−3.99	−1.51
2	69.0	−4.76	−3.43	−3.46	−0.857
3	71.6	−4.84	−0.852	−2.66	−1.17
4	100	−1.90	1.03	−0.368	−1.23
5	109	−1.62	2.02	41.7	−1.37

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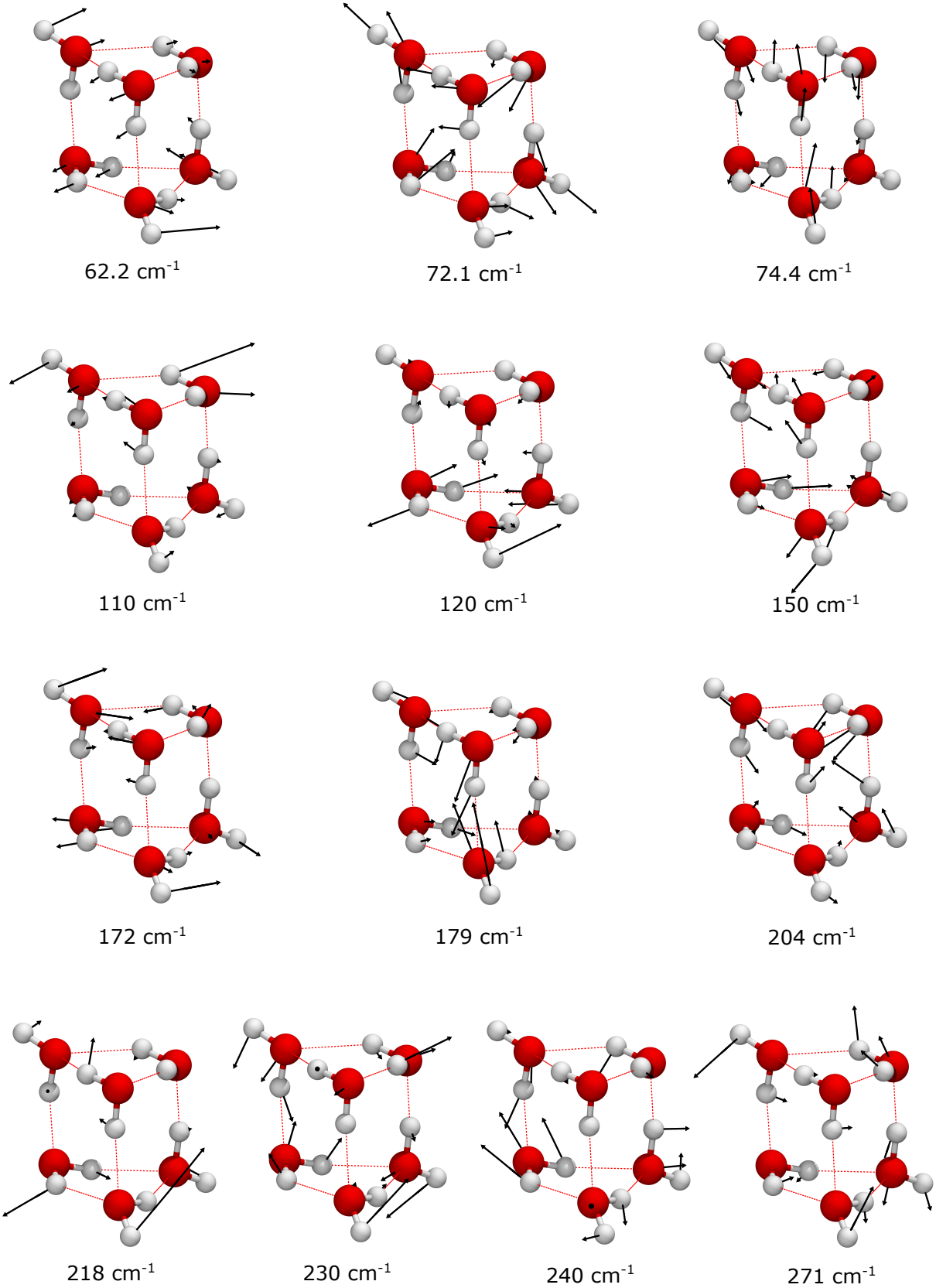

Fig. 1 Normal modes of vibration of the water hexamer prism for the 13 lowest frequencies.

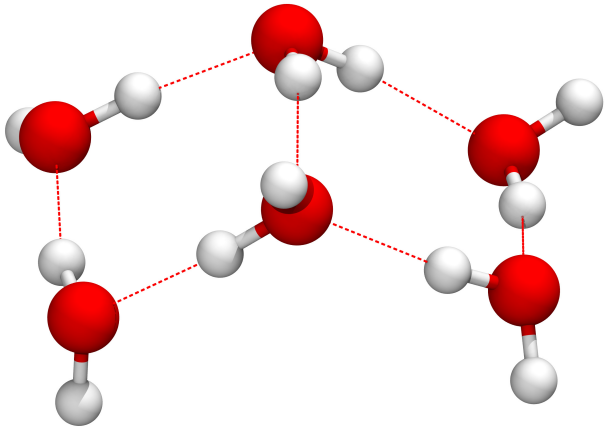

Fig. 2 Equilibrium geometry of a minimum of the water hexamer book, book structure 5, at 200 cm^{-1} above the book structure 1, shown in Fig. 12 (1) in the main article, on MB-pol PES[1–3].

Table 4 Character table of the G_{16} group of the water hexamer book. Class names are defined with the group elements as: $\mathrm{A} \equiv (12)$, $\mathrm{B} \equiv (34)$, $\mathrm{C} \equiv (56)$, $\mathrm{D} \equiv (78)$. Atom labels are defined in Fig. 12 in the main article.

	I	D	C	CD	B	BD	BC	BCD	A	AD	AC	ACD	AB	ABD	ABC	ABCD
A_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
A_2	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1
A_3	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1
A_4	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1
A_5	1	1	1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1
A_6	1	−1	1	−1	−1	1	−1	1	1	−1	1	−1	−1	1	−1	1
A_7	1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1	1	1
A_8	1	−1	−1	1	−1	1	1	−1	1	−1	−1	1	−1	1	1	−1
A_9	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1
A_{10}	1	−1	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1	−1	1
A_{11}	1	1	−1	−1	1	1	−1	−1	−1	−1	1	1	−1	−1	1	1
A_{12}	1	−1	−1	1	1	−1	−1	1	−1	1	1	−1	−1	1	1	−1
A_{13}	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1	1
A_{14}	1	−1	1	−1	−1	1	−1	1	−1	1	−1	1	1	−1	1	−1
A_{15}	1	1	−1	−1	−1	−1	1	1	−1	−1	1	1	1	1	−1	−1
A_{16}	1	−1	−1	1	−1	1	1	−1	−1	1	1	−1	1	−1	−1	1

Table 5 Statistical weights of the vibrational tunneling states in the rotational ground state of the water hexamer book, $(H_2O)_6$ and $(D_2O)_6$, labeled by their symmetry species in the G_{16} group.

irrep	$(H_2O)_6$	$(D_2O)_6$
A_1	16	104976
A_2	48	52488
A_3	48	52488
A_4	144	26224
A_5	48	52488
A_6	144	26224
A_7	144	26224
A_8	432	13122
A_9	48	52488
A_{10}	144	26224
A_{11}	144	26224
A_{12}	432	13122
A_{13}	144	26224
A_{14}	432	13122
A_{15}	432	13122
A_{16}	1296	6561

Table 6 Analytic expressions for the tunnelling energy levels in the water hexamer book for each symmetry species in the G_{16} group, expressed in terms of tunnelling matrix elements in Table 7 of the main article, energies E_i of book structures $i = 1-4$, shown in Fig. 12 in the main article, and coefficients c_i, both given in Table 6 of the main article. See the main article text for details.

$$
\begin{aligned}
E(A_1) = {} & +2c_1c_2h^{12}_{\mathrm{AB}} + 2c_1c_2h^{12}_{\tilde{\mathrm{A}}\mathrm{B}} + 2c_1c_2h^{12}_{\tilde{\mathrm{B}}\mathrm{A}} + 2c_1c_3h^{13}_{\mathrm{CD}} + 2c_1c_3h^{13}_{\tilde{\mathrm{C}}\mathrm{D}} + 2c_1c_3h^{13}_{\tilde{\mathrm{D}}\mathrm{C}} + 2c_2c_4h^{24}_{\mathrm{CD}} + 2c_2c_4h^{24}_{\tilde{\mathrm{C}}\mathrm{D}} + 2c_2c_4h^{24}_{\tilde{\mathrm{D}}\mathrm{C}} \\
& + 2c_3c_4h^{34}_{\mathrm{AB}} + 2c_3c_4h^{34}_{\tilde{\mathrm{A}}\mathrm{B}} + 2c_3c_4h^{34}_{\tilde{\mathrm{B}}\mathrm{A}} + \textstyle\sum_{i=1}^{4}\sum_{\mathrm{X}=\mathrm{A}}^{D} c_i^2 h^{ii}_{\mathrm{rotX}} \\
E(A_2) = {} & +2c_1c_2h^{12}_{\mathrm{AB}} + 2c_1c_2h^{12}_{\tilde{\mathrm{A}}\mathrm{B}} + 2c_1c_2h^{12}_{\tilde{\mathrm{B}}\mathrm{A}} + 2c_1c_3h^{13}_{\mathrm{CD}} + 2c_1c_3h^{13}_{\tilde{\mathrm{C}}\mathrm{D}} - 2c_1c_3h^{13}_{\tilde{\mathrm{D}}\mathrm{C}} + 2c_2c_4h^{24}_{\mathrm{CD}} + 2c_2c_4h^{24}_{\tilde{\mathrm{C}}\mathrm{D}} - 2c_2c_4h^{24}_{\tilde{\mathrm{D}}\mathrm{C}} \\
& + 2c_3c_4h^{34}_{\mathrm{AB}} + 2c_3c_4h^{34}_{\tilde{\mathrm{A}}\mathrm{B}} + 2c_3c_4h^{34}_{\tilde{\mathrm{B}}\mathrm{A}} + \textstyle\sum_{i=1}^{4}\sum_{\mathrm{X}\neq\mathrm{D}} c_i^2 h^{ii}_{\mathrm{rotX}} - \sum_{i=1}^{4} c_i^2 h^{ii}_{\mathrm{rotD}} \\
E(A_3) = {} & +2c_1c_2h^{12}_{\mathrm{AB}} + 2c_1c_2h^{12}_{\tilde{\mathrm{A}}\mathrm{B}} + 2c_1c_2h^{12}_{\tilde{\mathrm{B}}\mathrm{A}} + 2c_1c_3h^{13}_{\mathrm{CD}} - 2c_1c_3h^{13}_{\tilde{\mathrm{C}}\mathrm{D}} + 2c_1c_3h^{13}_{\tilde{\mathrm{D}}\mathrm{C}} + 2c_2c_4h^{24}_{\mathrm{CD}} - 2c_2c_4h^{24}_{\tilde{\mathrm{C}}\mathrm{D}} + 2c_2c_4h^{24}_{\tilde{\mathrm{D}}\mathrm{C}} \\
& + 2c_3c_4h^{34}_{\mathrm{AB}} + 2c_3c_4h^{34}_{\tilde{\mathrm{A}}\mathrm{B}} + 2c_3c_4h^{34}_{\tilde{\mathrm{B}}\mathrm{A}} + \textstyle\sum_{i=1}^{4}\sum_{\mathrm{X}\neq\mathrm{C}} c_i^2 h^{ii}_{\mathrm{rotX}} - \sum_{i=1}^{4} c_i^2 h^{ii}_{\mathrm{rotC}} \\
E(A_4) = {} & +2c_1c_2h^{12}_{\mathrm{AB}} + 2c_1c_2h^{12}_{\tilde{\mathrm{A}}\mathrm{B}} + 2c_1c_2h^{12}_{\tilde{\mathrm{B}}\mathrm{A}} + 2c_1c_3h^{13}_{\mathrm{CD}} - 2c_1c_3h^{13}_{\tilde{\mathrm{C}}\mathrm{D}} - 2c_1c_3h^{13}_{\tilde{\mathrm{D}}\mathrm{C}} + 2c_2c_4h^{24}_{\mathrm{CD}} - 2c_2c_4h^{24}_{\tilde{\mathrm{C}}\mathrm{D}} - 2c_2c_4h^{24}_{\tilde{\mathrm{D}}\mathrm{C}} \\
& + 2c_3c_4h^{34}_{\mathrm{AB}} + 2c_3c_4h^{34}_{\tilde{\mathrm{A}}\mathrm{B}} + 2c_3c_4h^{34}_{\tilde{\mathrm{B}}\mathrm{A}} + \textstyle\sum_{i=1}^{4}\sum_{\mathrm{X}=\mathrm{A,B}} c_i^2 h^{ii}_{\mathrm{rotX}} - \sum_{i=1}^{4}\sum_{\mathrm{Y}=\mathrm{C,D}} c_i^2 h^{ii}_{\mathrm{rotY}} \\
E(A_5) = {} & +2c_1c_2h^{12}_{\mathrm{AB}} + 2c_1c_2h^{12}_{\tilde{\mathrm{A}}\mathrm{B}} - 2c_1c_2h^{12}_{\tilde{\mathrm{B}}\mathrm{A}} + 2c_1c_3h^{13}_{\mathrm{CD}} + 2c_1c_3h^{13}_{\tilde{\mathrm{C}}\mathrm{D}} + 2c_1c_3h^{13}_{\tilde{\mathrm{D}}\mathrm{C}} + 2c_2c_4h^{24}_{\mathrm{CD}} + 2c_2c_4h^{24}_{\tilde{\mathrm{C}}\mathrm{D}} + 2c_2c_4h^{24}_{\tilde{\mathrm{D}}\mathrm{C}} \\
& + 2c_3c_4h^{34}_{\mathrm{AB}} + 2c_3c_4h^{34}_{\tilde{\mathrm{A}}\mathrm{B}} - 2c_3c_4h^{34}_{\tilde{\mathrm{B}}\mathrm{A}} + \textstyle\sum_{i=1}^{4}\sum_{\mathrm{X}\neq\mathrm{B}} c_i^2 h^{ii}_{\mathrm{rotX}} - \sum_{i=1}^{4} c_i^2 h^{ii}_{\mathrm{rotB}} \\
E(A_6) = {} & +2c_1c_2h^{12}_{\mathrm{AB}} + 2c_1c_2h^{12}_{\tilde{\mathrm{A}}\mathrm{B}} - 2c_1c_2h^{12}_{\tilde{\mathrm{B}}\mathrm{A}} + 2c_1c_3h^{13}_{\mathrm{CD}} + 2c_1c_3h^{13}_{\tilde{\mathrm{C}}\mathrm{D}} - 2c_1c_3h^{13}_{\tilde{\mathrm{D}}\mathrm{C}} + 2c_2c_4h^{24}_{\mathrm{CD}} + 2c_2c_4h^{24}_{\tilde{\mathrm{C}}\mathrm{D}} - 2c_2c_4h^{24}_{\tilde{\mathrm{D}}\mathrm{C}} \\
& + 2c_3c_4h^{34}_{\mathrm{AB}} + 2c_3c_4h^{34}_{\tilde{\mathrm{A}}\mathrm{B}} - 2c_3c_4h^{34}_{\tilde{\mathrm{B}}\mathrm{A}} + \textstyle\sum_{i=1}^{4}\sum_{\mathrm{X}=\mathrm{A,C}} c_i^2 h^{ii}_{\mathrm{rotX}} - \sum_{i=1}^{4}\sum_{\mathrm{Y}=\mathrm{B,D}} c_i^2 h^{ii}_{\mathrm{rotY}} \\
E(A_7) = {} & +2c_1c_2h^{12}_{\mathrm{AB}} + 2c_1c_2h^{12}_{\tilde{\mathrm{A}}\mathrm{B}} - 2c_1c_2h^{12}_{\tilde{\mathrm{B}}\mathrm{A}} + 2c_1c_3h^{13}_{\mathrm{CD}} - 2c_1c_3h^{13}_{\tilde{\mathrm{C}}\mathrm{D}} + 2c_1c_3h^{13}_{\tilde{\mathrm{D}}\mathrm{C}} + 2c_2c_4h^{24}_{\mathrm{CD}} - 2c_2c_4h^{24}_{\tilde{\mathrm{C}}\mathrm{D}} + 2c_2c_4h^{24}_{\tilde{\mathrm{D}}\mathrm{C}} \\
& + 2c_3c_4h^{34}_{\mathrm{AB}} + 2c_3c_4h^{34}_{\tilde{\mathrm{A}}\mathrm{B}} - 2c_3c_4h^{34}_{\tilde{\mathrm{B}}\mathrm{A}} + \textstyle\sum_{i=1}^{4}\sum_{\mathrm{X}=\mathrm{A,D}} c_i^2 h^{ii}_{\mathrm{rotX}} - \sum_{i=1}^{4}\sum_{\mathrm{Y}=\mathrm{B,C}} c_i^2 h^{ii}_{\mathrm{rotY}} \\
E(A_8) = {} & +2c_1c_2h^{12}_{\mathrm{AB}} + 2c_1c_2h^{12}_{\tilde{\mathrm{A}}\mathrm{B}} - 2c_1c_2h^{12}_{\tilde{\mathrm{B}}\mathrm{A}} + 2c_1c_3h^{13}_{\mathrm{CD}} - 2c_1c_3h^{13}_{\tilde{\mathrm{C}}\mathrm{D}} - 2c_1c_3h^{13}_{\tilde{\mathrm{D}}\mathrm{C}} + 2c_2c_4h^{24}_{\mathrm{CD}} - 2c_2c_4h^{24}_{\tilde{\mathrm{C}}\mathrm{D}} - 2c_2c_4h^{24}_{\tilde{\mathrm{D}}\mathrm{C}} \\
& + 2c_3c_4h^{34}_{\mathrm{AB}} + 2c_3c_4h^{34}_{\tilde{\mathrm{A}}\mathrm{B}} - 2c_3c_4h^{34}_{\tilde{\mathrm{B}}\mathrm{A}} + \textstyle\sum_{i=1}^{4} c_i^2 h^{ii}_{\mathrm{rotA}} - \sum_{i=1}^{4}\sum_{\mathrm{X}\neq\mathrm{A}} c_i^2 h^{ii}_{\mathrm{rotX}} \\
E(A_9) = {} & +2c_1c_2h^{12}_{\mathrm{AB}} - 2c_1c_2h^{12}_{\tilde{\mathrm{A}}\mathrm{B}} + 2c_1c_2h^{12}_{\tilde{\mathrm{B}}\mathrm{A}} + 2c_1c_3h^{13}_{\mathrm{CD}} + 2c_1c_3h^{13}_{\tilde{\mathrm{C}}\mathrm{D}} + 2c_1c_3h^{13}_{\tilde{\mathrm{D}}\mathrm{C}} + 2c_2c_4h^{24}_{\mathrm{CD}} + 2c_2c_4h^{24}_{\tilde{\mathrm{C}}\mathrm{D}} + 2c_2c_4h^{24}_{\tilde{\mathrm{D}}\mathrm{C}} \\
& + 2c_3c_4h^{34}_{\mathrm{AB}} - 2c_3c_4h^{34}_{\tilde{\mathrm{A}}\mathrm{B}} + 2c_3c_4h^{34}_{\tilde{\mathrm{B}}\mathrm{A}} + \textstyle\sum_{i=1}^{4}\sum_{\mathrm{X}\neq\mathrm{A}} c_i^2 h^{ii}_{\mathrm{rotX}} - \sum_{i=1}^{4} c_i^2 h^{ii}_{\mathrm{rotA}} \\
E(A_{10}) = {} & +2c_1c_2h^{12}_{\mathrm{AB}} - 2c_1c_2h^{12}_{\tilde{\mathrm{A}}\mathrm{B}} + 2c_1c_2h^{12}_{\tilde{\mathrm{B}}\mathrm{A}} + 2c_1c_3h^{13}_{\mathrm{CD}} + 2c_1c_3h^{13}_{\tilde{\mathrm{C}}\mathrm{D}} - 2c_1c_3h^{13}_{\tilde{\mathrm{D}}\mathrm{C}} + 2c_2c_4h^{24}_{\mathrm{CD}} + 2c_2c_4h^{24}_{\tilde{\mathrm{C}}\mathrm{D}} - 2c_2c_4h^{24}_{\tilde{\mathrm{D}}\mathrm{C}} \\
& + 2c_3c_4h^{34}_{\mathrm{AB}} - 2c_3c_4h^{34}_{\tilde{\mathrm{A}}\mathrm{B}} + 2c_3c_4h^{34}_{\tilde{\mathrm{B}}\mathrm{A}} + \textstyle\sum_{i=1}^{4}\sum_{\mathrm{X}=\mathrm{B,C}} c_i^2 h^{ii}_{\mathrm{rotX}} - \sum_{i=1}^{4}\sum_{\mathrm{Y}=\mathrm{A,D}} c_i^2 h^{ii}_{\mathrm{rotY}} \\
E(A_{11}) = {} & +2c_1c_2h^{12}_{\mathrm{AB}} - 2c_1c_2h^{12}_{\tilde{\mathrm{A}}\mathrm{B}} + 2c_1c_2h^{12}_{\tilde{\mathrm{B}}\mathrm{A}} + 2c_1c_3h^{13}_{\mathrm{CD}} - 2c_1c_3h^{13}_{\tilde{\mathrm{C}}\mathrm{D}} + 2c_1c_3h^{13}_{\tilde{\mathrm{D}}\mathrm{C}} + 2c_2c_4h^{24}_{\mathrm{CD}} - 2c_2c_4h^{24}_{\tilde{\mathrm{C}}\mathrm{D}} + 2c_2c_4h^{24}_{\tilde{\mathrm{D}}\mathrm{C}} \\
& + 2c_3c_4h^{34}_{\mathrm{AB}} - 2c_3c_4h^{34}_{\tilde{\mathrm{A}}\mathrm{B}} + 2c_3c_4h^{34}_{\tilde{\mathrm{B}}\mathrm{A}} + \textstyle\sum_{i=1}^{4}\sum_{\mathrm{X}=\mathrm{B,D}} c_i^2 h^{ii}_{\mathrm{rotX}} - \sum_{i=1}^{4}\sum_{\mathrm{Y}=\mathrm{A,C}} c_i^2 h^{ii}_{\mathrm{rotY}} \\
E(A_{12}) = {} & +2c_1c_2h^{12}_{\mathrm{AB}} - 2c_1c_2h^{12}_{\tilde{\mathrm{A}}\mathrm{B}} + 2c_1c_2h^{12}_{\tilde{\mathrm{B}}\mathrm{A}} + 2c_1c_3h^{13}_{\mathrm{CD}} - 2c_1c_3h^{13}_{\tilde{\mathrm{C}}\mathrm{D}} - 2c_1c_3h^{13}_{\tilde{\mathrm{D}}\mathrm{C}} + 2c_2c_4h^{24}_{\mathrm{CD}} - 2c_2c_4h^{24}_{\tilde{\mathrm{C}}\mathrm{D}} - 2c_2c_4h^{24}_{\tilde{\mathrm{D}}\mathrm{C}} \\
& + 2c_3c_4h^{34}_{\mathrm{AB}} - 2c_3c_4h^{34}_{\tilde{\mathrm{A}}\mathrm{B}} + 2c_3c_4h^{34}_{\tilde{\mathrm{B}}\mathrm{A}} + \textstyle\sum_{i=1}^{4} c_i^2 h^{ii}_{\mathrm{rotB}} - \sum_{i=1}^{4}\sum_{\mathrm{X}\neq\mathrm{B}} c_i^2 h^{ii}_{\mathrm{rotX}} \\
E(A_{13}) = {} & +2c_1c_2h^{12}_{\mathrm{AB}} - 2c_1c_2h^{12}_{\tilde{\mathrm{A}}\mathrm{B}} - 2c_1c_2h^{12}_{\tilde{\mathrm{B}}\mathrm{A}} + 2c_1c_3h^{13}_{\mathrm{CD}} + 2c_1c_3h^{13}_{\tilde{\mathrm{C}}\mathrm{D}} + 2c_1c_3h^{13}_{\tilde{\mathrm{D}}\mathrm{C}} + 2c_2c_4h^{24}_{\mathrm{CD}} + 2c_2c_4h^{24}_{\tilde{\mathrm{C}}\mathrm{D}} + 2c_2c_4h^{24}_{\tilde{\mathrm{D}}\mathrm{C}} \\
& + 2c_3c_4h^{34}_{\mathrm{AB}} - 2c_3c_4h^{34}_{\tilde{\mathrm{A}}\mathrm{B}} - 2c_3c_4h^{34}_{\tilde{\mathrm{B}}\mathrm{A}} + \textstyle\sum_{i=1}^{4}\sum_{\mathrm{X}=\mathrm{C,D}} c_i^2 h^{ii}_{\mathrm{rotX}} - \sum_{i=1}^{4}\sum_{\mathrm{Y}=\mathrm{A,B}} c_i^2 h^{ii}_{\mathrm{rotY}} \\
E(A_{14}) = {} & +2c_1c_2h^{12}_{\mathrm{AB}} - 2c_1c_2h^{12}_{\tilde{\mathrm{A}}\mathrm{B}} - 2c_1c_2h^{12}_{\tilde{\mathrm{B}}\mathrm{A}} + 2c_1c_3h^{13}_{\mathrm{CD}} + 2c_1c_3h^{13}_{\tilde{\mathrm{C}}\mathrm{D}} - 2c_1c_3h^{13}_{\tilde{\mathrm{D}}\mathrm{C}} + 2c_2c_4h^{24}_{\mathrm{CD}} + 2c_2c_4h^{24}_{\tilde{\mathrm{C}}\mathrm{D}} - 2c_2c_4h^{24}_{\tilde{\mathrm{D}}\mathrm{C}} \\
& + 2c_3c_4h^{34}_{\mathrm{AB}} - 2c_3c_4h^{34}_{\tilde{\mathrm{A}}\mathrm{B}} - 2c_3c_4h^{34}_{\tilde{\mathrm{B}}\mathrm{A}} + \textstyle\sum_{i=1}^{4} c_i^2 h^{ii}_{\mathrm{rotC}} - \sum_{i=1}^{4}\sum_{\mathrm{X}\neq\mathrm{C}} c_i^2 h^{ii}_{\mathrm{rotX}} \\
E(A_{15}) = {} & +2c_1c_2h^{12}_{\mathrm{AB}} - 2c_1c_2h^{12}_{\tilde{\mathrm{A}}\mathrm{B}} - 2c_1c_2h^{12}_{\tilde{\mathrm{B}}\mathrm{A}} + 2c_1c_3h^{13}_{\mathrm{CD}} - 2c_1c_3h^{13}_{\tilde{\mathrm{C}}\mathrm{D}} + 2c_1c_3h^{13}_{\tilde{\mathrm{D}}\mathrm{C}} + 2c_2c_4h^{24}_{\mathrm{CD}} - 2c_2c_4h^{24}_{\tilde{\mathrm{C}}\mathrm{D}} + 2c_2c_4h^{24}_{\tilde{\mathrm{D}}\mathrm{C}} \\
& + 2c_3c_4h^{34}_{\mathrm{AB}} - 2c_3c_4h^{34}_{\tilde{\mathrm{A}}\mathrm{B}} - 2c_3c_4h^{34}_{\tilde{\mathrm{B}}\mathrm{A}} + \textstyle\sum_{i=1}^{4} c_i^2 h^{ii}_{\mathrm{rotD}} - \sum_{i=1}^{4}\sum_{\mathrm{X}\neq\mathrm{D}} c_i^2 h^{ii}_{\mathrm{rotX}} \\
E(A_{16}) = {} & +2c_1c_2h^{12}_{\mathrm{AB}} - 2c_1c_2h^{12}_{\tilde{\mathrm{A}}\mathrm{B}} - 2c_1c_2h^{12}_{\tilde{\mathrm{B}}\mathrm{A}} + 2c_1c_3h^{13}_{\mathrm{CD}} - 2c_1c_3h^{13}_{\tilde{\mathrm{C}}\mathrm{D}} - 2c_1c_3h^{13}_{\tilde{\mathrm{D}}\mathrm{C}} + 2c_2c_4h^{24}_{\mathrm{CD}} - 2c_2c_4h^{24}_{\tilde{\mathrm{C}}\mathrm{D}} - 2c_2c_4h^{24}_{\tilde{\mathrm{D}}\mathrm{C}} \\
& + 2c_3c_4h^{34}_{\mathrm{AB}} - 2c_3c_4h^{34}_{\tilde{\mathrm{A}}\mathrm{B}} - 2c_3c_4h^{34}_{\tilde{\mathrm{B}}\mathrm{A}} - \textstyle\sum_{i=1}^{4}\sum_{\mathrm{X}=\mathrm{A}}^{D} c_i^2 h^{ii}_{\mathrm{rotX}}
\end{aligned}
$$

References

1 V. Babin, C. Leforestier and F. Paesani, *J. Chem. Theory Comput.*, 2013, **9**, 5395–5403.

2 V. Babin, G. R. Medders and F. Paesani, *J. Chem. Theory Comput.*, 2014, **10**, 1599–1607.

3 S. K. Reddy, S. C. Straight, P. Bajaj, C. Huy Pham, M. Riera, D. R. Moberg, M. A. Morales, C. Knight, A. W. Götz and F. Paesani, *J. Chem. Phys.*, 2016, **145**, 194504.