Supplementary Information to

Rovibrational quantum dynamical computations for deuterated isotopologues of the methane-water dimer

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S1. TABLES

TABLE S1: Vibrational states of $CH_4 \cdot H_2O$ (HH) with $J = 0$: energy levels, irrep labels of the G_{48} molecular symmetry group, and coupled-rotor decomposition.

Label	E [cm^{-1}]	$\Gamma^{\pm}$	Coupled-rotor states ($J = 0$)	
			dominant	minor
HH–J0.1	219.6	A_1^+	$[0, 0_{00}]$	$[3, 0_{00}]$
HH–J0.2–4	4.2	F_2^+	$[1, 0_{00}]$	$[2, 0_{00}]$
HH–J0.5	6.6	A_2^-	$[0, 1_{01}]$	
HH–J0.6–8	10.3	F_1^-	$[1, 1_{01}]$	$[2, 1_{01}]$
HH–J0.9–11	30.1	F_2^+	$[1, 1_{11}]$	$[1, 0_{00}]$ & $[2, 0_{00}]$
HH–J0.12–14	31.6	F_2^-	$[1, 1_{10}]$	$[1, 1_{01}]$ & $[2, 1_{10}]$
HH–J0.15–17	31.7	F_1^-	$[1, 1_{10}]$	$[1, 1_{01}]$ & $[2, 1_{10}]$
HH–J0.18–19	35.1	E^-	$[2, 1_{10}]$	$[2, 1_{01}]$
HH–J0.20–22	35.5	F_1^+	$[1, 1_{11}]$	
HH–J0.23–24	35.7	E^+	$[2, 0_{00}]$ & $[2, 1_{11}]$	
HH–J0.25	36.1	A_1^+(SM)	$[0, 0_{00}]$	$[0, 1_{11}]$ & $[3, 0_{00}]$

TABLE S2: Vibrational states of $CH_4 \cdot D_2O$ (HD) with $J = 0$. See also caption to Table S1.

Label	E [cm^{-1}]	$\Gamma^{\pm}$	Coupled-rotor states ($J = 0$)	
			dominant	minor
HD–J0.1	202.8	A_1^+	$[0, 0_{00}]$	$[0, 2_{02}]$ & $[3, 0_{00}]$
HD–J0.2	1.0	A_2^-	$[0, 1_{01}]$	$[3, 1_{01}]$
HD–J0.3–5	3.0	F_2^+	$[1, 0_{00}]$	$[1, 2_{02}]$ & $[2, 0_{00}]$
HD–J0.6–8	4.0	F_1^-	$[1, 1_{01}]$	$[2, 1_{01}]$
HD–J0.9–11	19.7	F_1^-	$[1, 1_{10}]$	
HD–J0.12–14	19.7	F_2^-	$[1, 1_{10}]$	
HD–J0.15–17	20.4	F_2^+	$[1, 1_{11}]$	$[1, 2_{11}]$
HD–J0.18–20	20.6	F_1^+	$[1, 1_{11}]$	$[1, 2_{11}]$
HD–J0.21–22	22.7	E^-	$[2, 1_{10}]$	
HD–J0.23–24	23.5	E^+	$[2, 1_{11}]$	

TABLE S3: Vibrational states of $CD_4 \cdot H_2O$ (DH) with $J = 0$. See also caption to Table S1.

Label	E [cm^{-1}]	$\Gamma^{\pm}$	Coupled-rotor states ($J = 0$)	
			dominant	minor
DH–J0.1	204.6	A_1^+	$[0, 0_{00}]$	$[3, 0_{00}]$
DH–J0.2–4	0.8	F_2^+	$[1, 0_{00}]$	$[2, 0_{00}]$
DH–J0.5	5.7	A_2^-	$[0, 1_{01}]$	$[3, 1_{01}]$
DH–J0.6–8	6.4	F_1^-	$[1, 1_{01}]$	$[2, 1_{01}]$
DH–J0.9–11	26.0	F_1^-	$[1, 1_{10}]$	$[2, 1_{10}]$ & $[3, 1_{10}]$ & $[1, 1_{01}]$
DH–J0.12–14	26.1	F_2^-	$[1, 1_{10}]$	$[2, 1_{10}]$
DH–J0.15–16	26.4	E^+	$[1, 0_{00}]$ & $[1, 1_{11}]$	$[2, 0_{00}]$ & $[2, 1_{11}]$
DH–J0.17–18	26.6	E^-	$[2, 1_{10}]$	
DH–J0.19–21	27.3	F_2^+	$[2, 0_{00}]$	$[1, 1_{11}]$ & $[2, 1_{11}]$
DH–J0.22–24	28.9	F_1^+	$[1, 1_{11}]$	$[2, 1_{11}]$

TABLE S4: Vibrational states of $CD_4 \cdot D_2O$ (DD) with $J = 0$. See also caption to Table S1.

Label	E [cm^{-1}]	$\Gamma^{\pm}$	Coupled-rotor states ($J = 0$)	
			dominant	minor
DD–J0.1	184.8	A_1^+	$[0, 0_{00}]$	$[0, 2_{02}]$ & $[3, 0_{00}]$
DD–J0.2–4	0.5	F_2^+	$[1, 0_{00}]$	$[2, 0_{00}]$ & $[1, 2_{02}]$
DD–J0.5	0.9	A_2^-	$[0, 1_{01}]$	$[3, 1_{01}]$
DD–J0.6–8	1.3	F_1^-	$[1, 1_{01}]$	$[2, 1_{01}]$
DD–J0.9–11	15.5	F_1^-	$[1, 1_{10}]$	$[2, 1_{10}]$
DD–J0.12–14	15.5	F_2^-	$[1, 1_{10}]$	$[2, 1_{10}]$
DD–J0.15–16	15.9	E^-	$[2, 1_{10}]$	
DD–J0.17–19	16.2	F_2^+	$[1, 1_{11}]$	
DD–J0.20–22	16.2	F_1^+	$[1, 1_{11}]$	$[1, 2_{11}]$
DD–J0.23–24	16.6	E^+	$[2, 1_{11}]$	

TABLE S5: Rovibrational states of $CH_4 \cdot H_2O$ (HH) with $J = 1$: energy levels, irrep labels of the G_{48} group for the the parent vibrational state, and coupled-rotor decomposition.

Label	E [cm^{-1}]	Vib. parent	Coupled-rotor states ($J = 1$)	
			dominant	minor
HH–J1.1	0.3	$A_1^+[0.0]$	$[0, 0_{00}]$	
HH–J1.2–4	4.5	$F_2^+[4.2]$	$[1, 0_{00}]$	$[2, 0_{00}]$
HH–J1.5	6.9	$A_2^-[6.6]$	$[0, 1_{01}]$	
HH–J1.6–11	7.5	$F_2^+[30.1]$, $F_1^+[35.5]$	$[1, 0_{00}]$	$[2, 0_{00}]$
HH–J1.12–14	10.6	$F_1^-[10.3]$	$[1, 1_{01}]$	$[2, 1_{01}]$
HH–J1.15–16	12.0	$E^+[35.7]$	$[2, 0_{00}]$	
HH–J1.17–22	13.9	$F_2^-[31.6]$, $F_1^-[31.7]$	$[1, 1_{01}]$	$[2, 1_{01}]$ & $[3, 1_{01}]$
HH–J1.23–24	17.9	$E^-[35.1]$	$[2, 1_{01}]$	
HH–J1.25–26	25.5	$A_2^-[6.6]$	$[0, 1_{10}]$	$[2, 1_{01}]$
HH–J1.27–32	28.6	$F_1^-[10.3]$	$[1, 1_{10}]$	$[1, 1_{01}]$ & $[2, 1_{10}]$
HH–J1.33–34	28.9	$A_1^+[0.0]$	$[0, 1_{11}]$	$[0, 2_{11}]$
HH–J1.35–37	30.4	$F_2^+[30.1]$	$[1, 1_{11}]$	$[2, 0_{00}]$
HH–J1.38–43	30.6	$F_2^+[4.2]$	$[1, 1_{11}]$	$[1, 0_{00}]$ & $[2, 0_{00}]$
HH–J1.44–46	31.9	$F_2^-[31.6]$	$[1, 1_{10}]$	$[1, 1_{01}]$ & $[2, 1_{10}]$
HH–J1.47–49	32.0	$F_1^-[31.7]$	$[1, 1_{10}]$	$[1, 1_{01}]$ & $[2, 1_{10}]$
HH–J1.50–51	35.4	$E^-[35.1]$	$[2, 1_{10}]$	
HH–J1.52–54	35.8	$F_1^+[35.5]$	$[1, 1_{11}]$	
HH–J1.55–56	36.0	$E^+[35.7]$	$[2, 0_{00}]$	$[2, 1_{11}]$

TABLE S6: Rovibrational states of $CH_4 \cdot D_2O$ (HD) with $J = 1$. See also caption to Table S5.

Label	E [cm^{-1}]	Vib. parent	Coupled-rotor states ($J = 1$)	
			dominant	minor
HD–J1.1	0.3	$A_1^+[0.0]$	$[0, 0_{00}]$	$[0, 2_{02}]$
HD–J1.2	1.3	$A_2^-[1.0]$	$[0, 1_{01}]$	$[3, 1_{01}]$
HD–J1.3–5	3.3	$F_2^+[3.0]$	$[1, 0_{00}]$	$[2, 0_{00}]$ & $[1, 2_{02}]$
HD–J1.6–8	4.2	$F_1^-[4.0]$	$[1, 1_{01}]$	
HD–J1.9–14	6.9	$F_2^+[20.4]$, $F_1^+[20.6]$	$[1, 0_{00}]$	$[1, 2_{02}]$
HD–J1.15–20	7.9	$F_1^-[19.7]$, $F_2^-[19.7]$	$[1, 1_{01}]$	
HD–J1.21–22	10.1	$E^+[23.5]$	$[2, 0_{00}]$	
HD–J1.23–24	11.0	$E^-[22.7]$	$[2, 1_{01}]$	
HD–J1.25–26	13.5	$A_2^-[1.0]$	$[0, 1_{10}]$	
HD–J1.27–28	14.3	$A_1^+[0.0]$	$[0, 1_{11}]$	$[0, 2_{11}]$
HD–J1.29–34	16.2	$F_1^-[4.0]$	$[1, 1_{10}]$	$[2, 1_{10}]$
HD–J1.35–40	17.0	$F_2^+[3.0]$	$[1, 1_{11}]$	$[2, 1_{11}]$ & $[1, 2_{11}]$
HD–J1.41–43	20.0	$F_1^-[19.7]$	$[1, 1_{10}]$	$[2, 1_{10}]$
HD–J1.44–46	20.0	$F_2^-[19.7]$	$[1, 1_{10}]$	$[2, 1_{10}]$
HD–J1.47–49	20.7	$F_2^+[20.4]$	$[1, 1_{11}]$	$[1, 2_{11}]$
HD–J1.50–52	20.9	$F_1^+[20.6]$	$[1, 1_{11}]$	$[1, 2_{11}]$
HD–J1.53–54	23.0	$E^-[22.7]$	$[2, 1_{10}]$	
HD–J1.55–56	23.8	$E^+[23.5]$	$[2, 1_{11}]$	

TABLE S7: Rovibrational states of $CD_4 \cdot H_2O$ (DH) with $J = 1$. See also caption to Table S5.

Label	E [cm^{-1}]	Vib. parent	Coupled-rotor states ($J = 1$)	
			dominant	minor
DH–J1.1	0.3	$A_1^+[0.0]$	$[0, 0_{00}]$	
DH–J1.2–4	1.0	$F_2^+[0.8]$	$[1, 0_{00}]$	$[2, 0_{00}]$
DH–J1.5–6	3.2	$F_2^+[27.2]$, $F_1^+[28.9]$	$[1, 0_{00}]$	$[2, 0_{00}]$
DH–J1.7–10	3.2	$E^+[26.4]$ & $F_2^+[27.2]$, $F_1^+[28.9]$	$[1, 0_{00}]$	
DH–J1.11–12	3.9	$F_2^+[27.2]$	$[2, 0_{00}]$	
DH–J1.13	6.0	$A_2^-[5.7]$	$[0, 1_{01}]$	$[3, 1_{01}]$
DH–J1.14–16	6.7	$F_1^-[6.4]$	$[1, 1_{01}]$	$[2, 1_{01}]$
DH–J1.17–22	8.9	$F_1^-[26.0]$, $F_2^-[26.2]$	$[1, 1_{01}]$	$[2, 1_{01}]$ & $[3, 1_{01}]$
DH–J1.23–24	9.6	$E^-[26.6]$	$[2, 1_{01}]$	
DH–J1.25–26	23.7	$A_2^-[5.7]$	$[0, 1_{10}]$	
DH–J1.27–32	24.1	$F_1^-[6.4]$	$[1, 1_{10}]$	$[2, 1_{10}]$
DH–J1.33–36	26.1	$F_2^+[0.8]$	$[0, 1_{10}]$	
DH–J1.37–38,41	26.3	$F_1^-[26.0]$	$[1, 1_{10}]$	$[3, 1_{10}]$ & $[2, 1_{10}]$
DH–J1.39–40	26.3	$F_2^+[0.8]$	$[0, 1_{10}]$	
DH–J1.41–44	26.4	$F_2^-[26.2]$	$[1, 1_{10}]$	$[2, 1_{10}]$
DH–J1.45–46	26.7	$A_1^+[0.0]$	$[0, 1_{11}]$	
DH–J1.47–48	26.7	$E^+[26.4]$	$[1, 0_{00}]$ & $[1, 1_{11}]$	$[2, 0_{00}]$ & $[2, 1_{11}]$
DH–J1.49–50	26.8	$E^-[26.6]$	$[2, 1_{10}]$	
DH–J1.51–53	27.9	$F_2^+[27.2]$	$[2, 0_{00}]$ & $[1, 1_{11}]$	$[2, 1_{11}]$
DH–J1.54–56	29.3	$F_1^+[28.9]$	$[1, 1_{11}]$	

TABLE S8: Rovibrational states of $CD_4 \cdot D_2O$ (DD) with $J = 1$. See also caption to Table S5.

Label	E [cm^{-1}]	Vib. parent	Coupled-rotor states ($J = 1$)	
			dominant	minor
DD–J1.1	0.2	$A_1^+[0.0]$	$[0, 0_{00}]$	$[0, 2_{02}]$
DD–J1.2–4	0.8	$F_2^+[0.5]$	$[1, 0_{00}]$	$[2, 0_{00}]$ & $[1, 2_{02}]$
DD–J1.5	1.1	$A_2^-[0.9]$	$[0, 1_{01}]$	$[2, 1_{01}]$
DD–J1.6–8	1.6	$F_1^-[1.3]$	$[1, 1_{01}]$	$[2, 1_{01}]$
DD–J1.9–14	3.0	$F_2^+[16.2]$, $F_1^+[16.3]$	$[1, 0_{00}]$	$[2, 0_{00}]$
DD–J1.15–16	3.5	$E^+[16.6]$	$[2, 0_{00}]$	
DD–J1.17–22	3.9	$F_1^-[15.5]$, $F_2^-[15.5]$	$[1, 1_{01}]$	$[2, 1_{01}]$
DD–J1.23–24	4.4	$E^-[15.9]$	$[2, 1_{01}]$	
DD–J1.25–26	12.9	$A_2^-[0.9]$	$[0, 1_{10}]$	
DD–J1.27–32	13.3	$F_1^-[1.3]$	$[1, 1_{10}]$	$[2, 1_{10}]$
DD–J1.33–34	13.7	$A_1^+[0.0]$	$[0, 1_{11}]$	$[0, 2_{11}]$
DD–J1.35–40	14.1	$F_2^+[0.5]$	$[1, 1_{11}]$	$[2, 1_{11}]$
DD–J1.41–43	15.7	$F_1^-[15.5]$	$[1, 1_{10}]$	$[2, 1_{10}]$
DD–J1.44–46	15.7	$F_2^-[15.5]$	$[1, 1_{10}]$	$[2, 1_{10}]$
DD–J1.47–48	16.2	$E^-[15.9]$	$[2, 1_{10}]$	
DD–J1.49–51	16.4	$F_2^+[16.2]$	$[1, 1_{11}]$	
DD–J1.42–54	16.5	$F_1^+[16.3]$	$[1, 1_{11}]$	
DD–J1.55–56	16.9	$E^+[16.6]$	$[2, 1_{11}]$	

TABLE S9: Rovibrational states of $CH_4 \cdot H_2O$ (HH) with $J = 2$. See also caption to Table S5.

Label	E [cm^{-1}]	Vib. parent	Coupled-rotor states ($J = 2$)	
			dominant	minor
HH–J2.1	0.9	$A_1^+[0.0]$	$[0, 0_{00}]$	
HH–J2.2–4	5.0	$F_2^+[4.2]$	$[1, 0_{00}]$	$[2, 0_{00}]$
HH–J2.5	7.5	$A_2^-[6.6]$	$[0, 1_{01}]$	
HH–J2.6–11	8.1	$F_2^+[30.1]$, $F_1^+[35.5]$	$[1, 0_{00}]$	$[2, 0_{00}]$
HH–J2.12–14	11.2	$F_1^-[10.3]$	$[1, 1_{01}]$	$[2, 1_{01}]$
HH–J2.15–16	12.6	$E^+[35.7]$	$[2, 0_{00}]$	
HH–J2.17–22	14.5	$F_2^-[31.6]$, $F_1^-[31.7]$	$[1, 1_{01}]$	$[2, 1_{01}]$ & $[3, 1_{01}]$
HH–J2.23–24	18.5	$E^-[35.1]$	$[2, 1_{01}]$	
HH–J2.25–26	22.6	many Γ^+ states	$[2, 0_{00}]$	
HH–J2.27–32	25.4	many Γ^+ states	$[2, 0_{00}]$	
HH–J2.33–34	26.1	$A_2^-[6.6]$	$[0, 1_{10}]$	$[0, 1_{01}]$
HH–J2.35–36	28.8	many Γ^- states	$[2, 1_{01}]$	
HH–J2.37–42	29.2	$F_1^-[10.3]$	$[1, 1_{10}]$	$[1, 1_{01}]$ & $[2, 1_{10}]$
HH–J2.43–44	29.5	$A_1^+[0.0]$	$[0, 1_{11}]$	
HH–J2.45–47	30.9	$F_2^+[30.1]$	$[1, 1_{11}]$	$[1, 0_{00}]$ & $[2, 0_{00}]$
HH–J2.48–53	31.2	$F_2^+[4.2]$	$[1, 1_{11}]$	$[2, 0_{00}]$
HH–J2.54–59	31.6	many Γ^- states	$[2, 1_{01}]$	$[3, 1_{01}]$
HH–J2.60–62	32.5	$F_2^-[31.6]$	$[1, 1_{10}]$	$[1, 1_{01}]$
HH–J2.63–65	32.6	$F_1^-[31.7]$	$[1, 1_{10}]$	$[1, 1_{01}]$ & $[2, 1_{10}]$
HH–J2.66–71	33.0	$F_2^-[31.6]$, $F_1^-[31.7]$	$[1, 1_{10}]$	$[2, 1_{10}]$
HH–J2.72–73	36.0	$E^-[35.1]$	$[2, 1_{10}]$	
HH–J2.74–75	36.1	$E^-[35.1]$	$[2, 1_{10}]$	
HH–J2.76–78	36.4	$F_1^+[35.5]$	$[1, 1_{11}]$	
HH–J2.79–80	36.5	$E^+[35.7]$	$[2, 0_{00}]$	
HH–J2.81–86	36.6	$F_1^+[35.5]$	$[1, 1_{11}]$	
HH–J2.87	36.9	A_1^+(SM)$[36.1]$	$[0, 0_{00}]$ & $[0, 1_{11}]$	$[3, 0_{00}]$
HH–J2.88–89	38.2	$E^+[35.7]$	$[2, 1_{11}]$	

TABLE S10: Rovibrational states of $CH_4 \cdot D_2O$ (HD) with $J = 2$. See also caption to Table S5.

Label	E [cm^{-1}]	Vib. parent	Coupled-rotor states ($J = 2$)	
			dominant	minor
HD–J2.1	0.8	$A_1^+[0.0]$	$[0, 0_{00}]$	$[0, 2_{02}]$
HD–J2.2	1.9	$A_2^-[1.0]$	$[0, 1_{01}]$	
HD–J2.3–5	3.8	$F_2^+[3.0]$	$[1, 0_{00}]$	$[2, 0_{00}]$ & $[1, 2_{02}]$
HD–J2.6–8	4.8	$F_1^-[4.0]$	$[1, 1_{01}]$	$[2, 1_{01}]$
HD–J2.9–14	7.4	$F_2^+[20.4]$, $F_1^+[20.6]$	$[1, 0_{00}]$	$[1, 2_{02}]$
HD–J2.15–20	8.4	$F_1^-[19.7]$, $F_2^-[19.7]$	$[1, 1_{01}]$	$[2, 1_{01}]$
HD–J2.21–22	10.7	$E^+[22.7]$	$[2, 0_{00}]$	
HD–J2.23–24	11.6	$E^-[23.5]$	$[2, 1_{01}]$	
HD–J2.25–26	14.0	$A_2^-[1.0]$	$[0, 1_{10}]$	
HD–J2.27–28	14.9	$A_1^+[0.0]$	$[0, 11_1]$	$[0, 2_{11}]$
HD–J2.29–34	16.8	$F_1^-[4.0]$	$[1, 1_{10}]$	$[2, 1_{10}]$
HD–J2.35–40	17.6	$F_2^+[3.0]$	$[1, 1_{11}]$	$[2, 1_{11}]$ & $[1, 2_{11}]$
HD–J2.41–46	20.4	$F_1^-[19.7]$, $F_2^-[19.7]$	$[1, 1_{10}]$	
HD–J2.47–49	20.6	$F_1^-[19.7]$	$[1, 1_{10}]$	$[2, 1_{10}]$
HD–J2.50–52	20.6	$F_2^-[19.7]$	$[1, 1_{10}]$	$[2, 1_{10}]$
HD–J2.53–54,57	21.2	$F_2^+[20.4]$	$[1, 1_{11}]$	
HD–J2.55–56,58	21.2	$F_2^+[20.4]$, $F_1^+[20.6]$	$[1, 1_{11}]$	$[1, 2_{11}]$
HD–J2.59–61	21.3	$F_2^+[20.4]$, $F_1^+[20.6]$	$[1, 1_{11}]$	$[1, 2_{11}]$
HD–J2.62–64	21.5	$F_1^+[20.6]$	$[1, 1_{11}]$	$[1, 2_{11}]$
HD–J2.65–66	21.8	many Γ^+ states	$[2, 0_{00}]$	
HD–J2.67–68	22.8	many Γ^- states	$[2, 1_{01}]$	
HD–J2.69–72	23.6	$E^-[23.5]$	$[2, 1_{10}]$	
HD–J2.73–74	24.1	$E^+[22.7]$	$[2, 1_{11}]$	
HD–J2.75–76	24.3	$E^+[22.7]$	$[2, 1_{11}]$	
HD–J2.77–82	24.3	many Γ^+ states	$[2, 0_{00}]$	$[2, 2_{02}]$
HD–J2.83–88	25.3	many Γ^- states	$[2, 1_{01}]$	

TABLE S11: Rovibrational states of $CD_4 \cdot H_2O$ (DH) with $J = 2$. See also caption to Table S5.

Label	E [cm^{-1}]	Vib. parent	Coupled-rotor states ($J = 2$)	
			dominant	minor
DH–J2.1	0.8	$A_1^+[0.0]$	$[0, 0_{00}]$	
DH–J2.2–4	1.5	$F_2^+[0.8]$	$[1, 0_{00}]$	$[2, 0_{00}]$
DH–J2.5–6	3.7	$F_2^+[27.2]$, $F_1^+[28.9]$	$[1, 0_{00}]$	$[2, 0_{00}]$
DH–J2.7–10	3.7	$E^+[26.4]$ & $F_2^+[27.2]$, $F_1^+[28.9]$	$[1, 0_{00}]$	
DH–J2.11–12	4.4	$F_2^+[27.2]$	$[2, 0_{00}]$	
DH–J2.13	6.5	$A_2^-[5.7]$	$[0, 1_{01}]$	$[3, 1_{01}]$
DH–J2.14–16	7.2	$F_1^-[6.4]$	$[1, 1_{01}]$	$[2, 1_{01}]$
DH–J2.17–22	9.4	$F_1^-[26.0]$, $F_2^-[26.2]$	$[1, 1_{01}]$	$[2, 1_{01}]$, $[3, 1_{01}]$
DH–J2.23–24	10.1	$E^-[26.6]$	$[2, 1_{01}]$	
DH–J2.25–26	11.0	many Γ^+ states	$[2, 0_{00}]$	
DH–J2.27–32	11.6	many Γ^+ states	$[2, 0_{00}]$	$[4, 0_{00}]$
DH–J2.33–34	16.7	many Γ^- states	$[2, 1_{01}]$	
DH–J2.35–40	17.3	many Γ^- states	$[2, 1_{01}]$	$[3, 1_{01}]$
DH–J2.41–42	24.2	$A_2^-[5.7]$	$[0, 1_{10}]$	
DH–J2.43–48	24.6	$F_1^-[6.4]$	$[1, 1_{10}]$ & $[2, 1_{10}]$	
DH–J2.49–52	26.6	$F_2^+[0.8]$	$[1, 1_{11}]$	$[2, 0_{00}]$
DH–J2.53–54,57	26.8	$F_1^-[26.0]$	$[1, 1_{10}]$	
DH–J2.55–56	26.8	$F_2^+[0.8]$	$[1, 1_{11}]$	$[2, 0_{00}]$
DH–J2.57–60,64	26.9	$F_2^-[26.2]$	$[1, 1_{10}]$	$[2, 1_{10}]$
DH–J2.62–63	27.0	$F_1^-[26.0]$, $F_2^-[26.2]$	$[1, 1_{10}]$	$[2, 1_{10}]$
DH–J2.65–66	27.0	$F_1^-[26.0]$, $F_2^-[26.2]$	$[1, 1_{10}]$	$[2, 1_{10}]$
DH–J2.67–68	27.2	$A_1^+[0.0]$	$[0, 1_{11}]$	
DH–J2.69–70	27.2	$E^+[26.4]$	$[1, 0_{00}]$	$[2, 0_{00}]$
DH–J2.71–72	27.3	$E^-[26.6]$	$[2, 1_{10}]$	
DH–J2.73–74	27.3	$E^-[26.6]$	$[2, 1_{10}]$	
DH–J2.75–77	28.4	$F_2^+[27.2]$	$[2, 0_{00}]$	$[1, 1_{11}]$ & $[2, 1_{11}]$
DH–J2.78–79	29.4	$F_2^+[27.2]$	$[2, 1_{11}]$	
DH–J2.80–82	29.8	$F_1^+[28.9]$	$[1, 1_{11}]$	$[2, 1_{11}]$
DH–J2.83–88	30.1	$F_2^+[27.2]$, $F_1^+[28.9]$	$[1, 1_{11}]$	

TABLE S12: Rovibrational states of $CD_4 \cdot D_2O$ (DD) with $J = 2$. See also caption to Table S5.

Label	E [cm^{-1}]	Vib. parent	Coupled-rotor states ($J = 2$)	
			dominant	minor
DD–J2.1	0.7	$A_1^+[0.0]$	$[0, 0_{00}]$	$[0, 2_{02}]$
DD–J2.2–4	1.2	$F_2^+[0.5]$	$[1, 0_{00}]$	$[2, 0_{00}]$ & $[1, 2_{02}]$
DD–J2.5	1.6	$A_2^-[0.9]$	$[0, 1_{01}]$	$[3, 1_{01}]$
DD–J2.6–8	2.1	$F_1^-[1.3]$	$[1, 1_{01}]$	$[2, 1_{01}]$
DD–J2.9–14	3.5	$F_2^+[16.2]$, $F_1^+[16.3]$	$[1, 0_{00}]$	$[2, 0_{00}]$
DD–J2.15–16	4.0	$E^+[16.6]$	$[2, 0_{00}]$	
DD–J2.17–22	4.4	$F_1^-[15.5]$, $F_2^-[15.5]$	$[1, 1_{01}]$	$[1, 1_{10}]$ & $[3, 1_{01}]$
DD–J2.23–24	4.8	$E^-[15.9]$	$[2, 1_{01}]$	
DD–J2.25–26	10.9	many Γ^+ states	$[2, 0_{00}]$	
DD–J2.27–32	11.3	many Γ^+ states	$[2, 0_{00}]$	$[3, 0_{00}]$
DD–J2.33–34	11.7	many Γ^- states	$[2, 1_{01}]$	
DD–J2.35–40	12.2	many Γ^- states	$[2, 1_{01}]$ & $[3, 1_{01}]$	
DD–J2.41–42	13.4	$A_2^-[0.9]$	$[0, 1_{10}]$	
DD–J2.43–48	13.8	$F_1^-[1.3]$	$[1, 1_{10}]$	$[2, 1_{10}]$
DD–J2.49–50	14.2	$A_1^+[0.0]$	$[0, 1_{11}]$	$[0, 2_{11}]$
DD–J2.51–56	14.6	$F_2^+[0.5]$	$[1, 1_{11}]$	
DD–J2.57–62	16.0	$F_1^-[15.5]$, $F_2^-[15.5]$	$[1, 1_{10}]$	$[2, 1_{10}]$
DD–J2.63–65	16.3	$F_1^-[15.5]$	$[1, 1_{10}]$	$[2, 1_{10}]$
DD–J2.66–68	16.3	$F_2^-[15.5]$	$[1, 1_{10}]$	$[2, 1_{10}]$
DD–J2.69–70	16.4	$E^-[15.9]$	$[2, 1_{10}]$	
DD–J2.71–72	16.6	$E^-[15.9]$	$[2, 1_{10}]$	
DD–J2.73–78	16.8	$F_2^+[16.2]$, $F_1^+[16.3]$	$[1, 1_{11}]$	
DD–J2.79–81	17.0	$F_2^+[16.2]$	$[1, 1_{11}]$	
DD–J2.82–84	17.0	$F_1^+[16.3]$	$[1, 1_{11}]$	
DD–J2.85–86	17.2	$E^+[16.6]$	$[2, 1_{11}]$	
DD–J2.87–88	17.4	$E^+[16.6]$	$[2, 1_{11}]$	

TABLE S13: Sum of the energies of the methane and the water rotors in $CH_4 \cdot H_2O$ (HH).

$CH_4 \cdot H_2O$			j^M	0	1	2	3	4	5	6
j^W	k_a	k_c	E [cm^{-1}]	0.0	10.2	30.5	61.1	101.8	152.7	213.8
0	0	0	0.0	0.0	10.2	30.5	61.1	101.8	152.7	213.8
1	0	1	23.2	23.2	33.4	53.8	84.3	125.1	176.0	237.0
1	1	1	35.5	35.5	45.7	66.1	96.6	137.3	188.2	249.3
1	1	0	40.4	40.4	50.6	71.0	101.5	142.2	193.1	254.2
2	0	2	68.5	68.5	78.7	99.1	129.6	170.3	221.2	282.3
2	1	2	77.1	77.1	87.3	107.7	138.2	178.9	229.8	290.9
2	1	1	91.8	91.8	102.0	122.3	152.9	193.6	244.5	305.6
2	2	1	128.7	128.7	138.8	159.2	189.7	230.5	281.4	342.5
2	2	0	129.8	129.8	140.0	160.4	190.9	231.7	282.6	343.7
3	0	3	133.9	133.9	144.0	164.4	194.9	235.7	286.6	347.7
3	1	3	138.8	138.8	149.0	169.3	199.9	240.6	291.5	352.6
3	1	2	168.0	168.0	178.2	198.5	229.1	269.8	320.7	381.8
3	2	2	198.4	198.4	208.5	228.9	259.5	300.2	351.1	412.2
3	2	1	203.9	203.9	214.1	234.5	265.0	305.8	356.7	417.8
3	3	1	272.7	272.7	282.9	303.3	333.8	374.5	425.4	486.5
3	3	0	272.9	272.9	283.1	303.4	334.0	374.7	425.6	486.7

TABLE S14: Sum of the energies of the methane and the water rotors in $CH_4 \cdot D_2O$ (HD).

$CH_4 \cdot D_2O$			j^M	0	1	2	3	4	5	6
j^W	k_a	k_c	E [cm^{-1}]	0.0	10.2	30.5	61.1	101.8	152.7	213.8
0	0	0	0.0	0.0	10.2	30.5	61.1	101.8	152.7	213.8
1	0	1	11.9	11.9	22.1	42.5	73.0	113.7	164.6	225.7
1	1	1	19.6	19.6	29.8	50.1	80.7	121.4	172.3	233.4
1	1	0	21.9	21.9	32.1	52.5	83.0	123.7	174.6	235.7
2	0	2	35.3	35.3	45.5	65.8	96.4	137.1	188.0	249.1
2	1	2	41.1	41.1	51.3	71.7	102.2	142.9	193.8	254.9
2	1	1	48.1	48.1	58.2	78.6	109.1	149.9	200.8	261.9
2	2	1	71.1	71.1	81.3	101.7	132.2	172.9	223.8	284.9
2	2	0	71.6	71.6	81.7	102.1	132.7	173.4	224.3	285.4
3	0	3	69.4	69.4	79.5	99.9	130.5	171.2	222.1	283.2
3	1	3	73.2	73.2	83.3	103.7	134.2	175.0	225.9	287.0
3	1	2	86.9	86.9	97.1	117.5	148.0	188.8	239.7	300.8
3	2	2	106.9	106.9	117.0	137.4	168.0	208.7	259.6	320.7
3	2	1	109.0	109.0	119.2	139.5	170.1	210.8	261.7	322.8
3	3	1	151.3	151.3	161.5	181.9	212.4	253.2	304.1	365.1
3	3	0	151.4	151.4	161.6	181.9	212.5	253.2	304.1	365.2

TABLE S15: Sum of the energies of the methane and the water rotors in $CD_4 \cdot H_2O$ (DH).

$CD_4 \cdot H_2O$			j^M	0	1	2	3	4	5	6
j^W	k_a	k_c	E [cm^{-1}]	0.0	5.1	15.4	30.9	51.5	77.2	108.1
0	0	0	0.0	0.0	5.1	15.4	30.9	51.5	77.2	108.1
1	0	1	23.2	23.2	28.4	38.7	54.1	74.7	100.4	131.3
1	1	1	35.5	35.5	40.7	51.0	66.4	87.0	112.7	143.6
1	1	0	40.4	40.4	45.6	55.9	71.3	91.9	117.6	148.5
2	0	2	68.5	68.5	73.7	84.0	99.4	120.0	145.7	176.6
2	1	2	77.1	77.1	82.3	92.5	108.0	128.6	154.3	185.2
2	1	1	91.8	91.8	96.9	107.2	122.7	143.3	169.0	199.9
2	2	1	128.7	128.7	133.8	144.1	159.5	180.1	205.8	236.7
2	2	0	129.8	129.8	135.0	145.3	160.7	181.3	207.0	237.9
3	0	3	133.9	133.9	139.0	149.3	164.7	185.3	211.0	241.9
3	1	3	138.8	138.8	143.9	154.2	169.7	190.3	216.0	246.9
3	1	2	168.0	168.0	173.1	183.4	198.9	219.4	245.2	276.1
3	2	2	198.4	198.4	203.5	213.8	229.2	249.8	275.6	306.4
3	2	1	203.9	203.9	209.1	219.4	234.8	255.4	281.1	312.0
3	3	1	272.7	272.7	277.9	288.2	303.6	324.2	349.9	380.8
3	3	0	272.9	272.9	278.1	288.3	303.8	324.4	350.1	381.0

TABLE S16: Sum of the energies of the methane and the water rotors in $CD_4 \cdot D_2O$ (DD).

$CD_4 \cdot D_2O$			j^M	0	1	2	3	4	5	6
j^W	k_a	k_c	E [cm^{-1}]	0.0	5.1	15.4	30.9	51.5	77.2	108.1
0	0	0	0.0	0.0	5.1	15.4	30.9	51.5	77.2	108.1
1	0	1	11.9	11.9	17.1	27.4	42.8	63.4	89.1	120.0
1	1	1	19.6	19.6	24.8	35.0	50.5	71.1	96.8	127.7
1	1	0	21.9	21.9	27.1	37.4	52.8	73.4	99.1	130.0
2	0	2	35.3	35.3	40.4	50.7	66.2	86.8	112.5	143.4
2	1	2	41.1	41.1	46.3	56.6	72.0	92.6	118.3	149.2
2	1	1	48.1	48.1	53.2	63.5	78.9	99.5	125.2	156.1
2	2	1	71.1	71.1	76.3	86.6	102.0	122.6	148.3	179.2
2	2	0	71.6	71.6	76.7	87.0	102.4	123.0	148.8	179.6
3	0	3	69.4	69.4	74.5	84.8	100.2	120.8	146.6	177.4
3	1	3	73.2	73.2	78.3	88.6	104.0	124.6	150.3	181.2
3	1	2	86.9	86.9	92.1	102.4	117.8	138.4	164.1	195.0
3	2	2	106.9	106.9	112.0	122.3	137.7	158.3	184.1	214.9
3	2	1	109.0	109.0	114.1	124.4	139.9	160.5	186.2	217.1
3	3	1	151.3	151.3	156.5	166.8	182.2	202.8	228.5	259.4
3	3	0	151.4	151.4	156.5	166.8	182.3	202.9	228.6	259.5

TABLE S17: Coupling energy, E_c defined in Section III, of the rotors for the studied methane-water isotopologues with $J = 0$. The second column contains the analytic solution in $2\mu R^2$ units, the remaining columns give the numerical value of E_c in cm^{-1} for the equilibrium distance, $R = R_{eq} = 6.5$ bohr, and for an arbitrarily chosen large value, $R = 100$ bohr. The reduced masses are $\mu_{HH} = 8.481697$ u, $\mu_{HD} = 8.903115$ u, $\mu_{DH} = 9.489256$ u, and $\mu_{DD} = 10.01987$ u.

$J = 0$		$CH_4 \cdot H_2O$		$CH_4 \cdot D_2O$		$CD_4 \cdot H_2O$		$CD_4 \cdot D_2O$	
j	$E_c \cdot 2\mu R^2$	R_{eq}	R_{100}	R_{eq}	R_{100}	R_{eq}	R_{100}	R_{eq}	R_{100}
0	0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1	2	0.336	0.001	0.320	0.001	0.300	0.001	0.284	0.001
2	6	1.008	0.004	0.960	0.004	0.901	0.004	0.853	0.004
3	12	2.016	0.009	1.920	0.008	1.802	0.008	1.706	0.007
4	20	3.360	0.014	3.201	0.014	3.003	0.013	2.844	0.012
5	30	5.040	0.021	4.801	0.020	4.505	0.019	4.266	0.018

TABLE S18: Coupling energy, E_c in cm^{-1}, for $J = 1$. See also caption to Table S17.

$J = 1$		$CH_4 \cdot H_2O$		$CH_4 \cdot D_2O$		$CD_4 \cdot H_2O$		$CD_4 \cdot D_2O$	
j	$E_c \cdot 2\mu R^2$	R_{eq}	R_{100}	R_{eq}	R_{100}	R_{eq}	R_{100}	R_{eq}	R_{100}
0	2	0.336	0.001	0.320	0.001	0.300	0.001	0.284	0.001
1	6	1.008	0.004	0.960	0.004	0.901	0.004	0.853	0.004
	2	0.336	0.001	0.320	0.001	0.300	0.001	0.284	0.001
	0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	12	2.016	0.009	1.920	0.008	1.802	0.008	1.706	0.007
	6	1.008	0.004	0.960	0.004	0.901	0.004	0.853	0.004
	2	0.336	0.001	0.320	0.001	0.300	0.001	0.284	0.001
3	20	3.360	0.014	3.201	0.014	3.003	0.013	2.844	0.012
	12	2.016	0.009	1.920	0.008	1.802	0.008	1.706	0.007
	6	1.008	0.004	0.960	0.004	0.901	0.004	0.853	0.004
4	30	5.040	0.021	4.801	0.020	4.505	0.019	4.266	0.018
	20	3.360	0.014	3.201	0.014	3.003	0.013	2.844	0.012
	12	2.016	0.009	1.920	0.008	1.802	0.008	1.706	0.007
5	42	7.056	0.030	6.722	0.028	6.306	0.027	5.972	0.025
	30	5.040	0.021	4.801	0.020	4.505	0.019	4.266	0.018
	20	3.360	0.014	3.201	0.014	3.003	0.013	2.844	0.012

TABLE S19: Coupling energy, E_c in cm^{-1}, for $J = 2$. See also caption to Table S17.

$J = 2$		$CH_4 \cdot H_2O$		$CH_4 \cdot D_2O$		$CD_4 \cdot H_2O$		$CD_4 \cdot D_2O$	
j	$E_c \cdot 2\mu R^2$	R_{eq}	R_{100}	R_{eq}	R_{100}	R_{eq}	R_{100}	R_{eq}	R_{100}
0	6	1.008	0.004	0.960	0.004	0.901	0.004	0.853	0.004
1	12	2.016	0.009	1.920	0.008	1.802	0.008	1.706	0.007
	6	1.008	0.004	0.960	0.004	0.901	0.004	0.853	0.004
	2	0.336	0.001	0.320	0.001	0.300	0.001	0.284	0.001
2	20	3.360	0.014	3.201	0.014	3.003	0.013	2.844	0.012
	12	2.016	0.009	1.920	0.008	1.802	0.008	1.706	0.007
	6	1.008	0.004	0.960	0.004	0.901	0.004	0.853	0.004
	2	0.336	0.001	0.320	0.001	0.300	0.001	0.284	0.001
	0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
3	30	5.040	0.021	4.801	0.020	4.505	0.019	4.266	0.018
	20	3.360	0.014	3.201	0.014	3.003	0.013	2.844	0.012
	12	2.016	0.009	1.920	0.008	1.802	0.008	1.706	0.007
	6	1.008	0.004	0.960	0.004	0.901	0.004	0.853	0.004
	2	0.336	0.001	0.320	0.001	0.300	0.001	0.284	0.001
4	42	7.056	0.030	6.722	0.028	6.306	0.027	5.972	0.025
	30	5.040	0.021	4.801	0.020	4.505	0.019	4.266	0.018
	20	3.360	0.014	3.201	0.014	3.003	0.013	2.844	0.012
	12	2.016	0.009	1.920	0.008	1.802	0.008	1.706	0.007
	6	1.008	0.004	0.960	0.004	0.901	0.004	0.853	0.004
5	56	9.407	0.040	8.962	0.038	8.409	0.036	7.963	0.034
	42	7.056	0.030	6.722	0.028	6.306	0.027	5.972	0.025
	30	5.040	0.021	4.801	0.020	4.505	0.019	4.266	0.018
	20	3.360	0.014	3.201	0.014	3.003	0.013	2.844	0.012
	12	2.016	0.009	1.920	0.008	1.802	0.008	1.706	0.007

S2. CHARACTER TABLES

TABLE S20: Character table of the C_{2v}(M) molecular symmetry group.

C_{2v}(M)	E	(ab)	E^*	[(ab)]*
n_{cl}	1	1	1	1
A_1	1	1	1	1
A_2	1	1	−1	−1
B_1	1	−1	−1	1
B_2	1	−1	1	−1

TABLE S21: Character table of the T_d(M) molecular symmetry group.

T_d(M)	E	(123)	(14)(23)	[(1423)]*	[(23)]*
n_{cl}	1	8	3	6	6
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
F_1	3	0	−1	1	−1
F_2	3	0	−1	−1	1

TABLE S22: Character table of the molecular symmetry group of $CH_4{\cdot}H_2O$, G_{48} (the table is taken from Ref. [1] but with explicit notation for space inversion).

G_{48}	E	(123)	(14)(23)	[(1423)(ab)]*	[(23)(ab)]*	(ab)	(123)(ab)	(14)(23)(ab)	[(1423)]*	[(23)]*
n_{cl}	1	8	3	6	6	1	8	3	6	6
A_1^+	1	1	1	1	1	1	1	1	1	1
A_2^+	1	1	1	−1	−1	1	1	1	−1	−1
E^+	2	−1	2	0	0	2	−1	2	0	0
F_1^+	3	0	−1	1	−1	3	0	−1	1	−1
F_2^+	3	0	−1	−1	1	3	0	−1	−1	1
A_1^-	1	1	1	1	1	−1	−1	−1	−1	−1
A_2^-	1	1	1	−1	−1	−1	−1	−1	1	1
E^-	2	−1	2	0	0	−2	1	−2	0	0
F_1^-	3	0	−1	1	−1	−3	0	1	−1	1
F_2^-	3	0	−1	−1	1	−3	0	1	1	−1

TABLE S23: Characters and irrep decomposition of the $[[j^{\mathrm{M}}, j^{\mathrm{W}}_{k_\mathrm{a}k_\mathrm{c}}]_j, \Lambda]_J$ coupled-rotor functions which dominate the ZPV(GM) splitting manifold with $J = 1$ and Γ^+ symmetry in the G_{48} group (see also Figure 3).

Γ	E	(123)	(14)(23)	[(1423)(ab)]*	[(23)(ab)]*	(ab)	(123)(ab)	(14)(23)(ab)	[(1423)]*	[(23)]*	Irreps
	1	8	3	6	6	1	8	3	6	6	
$[[0, 0_{00}]_0, 1]_1$	1	1	1	−1	−1	1	1	1	−1	−1	A_2^+
$[[0, 1_{11}]_1, 0]_1$	1	1	1	−1	−1	1	1	1	−1	−1	A_2^+
$[[0, 1_{11}]_1, 1]_1$	1	1	1	1	1	1	1	1	1	1	A_1^+
$[[0, 1_{11}]_1, 2]_1$	1	1	1	−1	−1	1	1	1	−1	−1	A_2^+
$[[1, 0_{00}]_1, 0]_1$	3	0	−1	1	−1	3	0	−1	1	−1	F_1^+
$[[1, 0_{00}]_1, 1]_1$	3	0	−1	−1	1	3	0	−1	−1	1	F_2^+
$[[1, 0_{00}]_1, 2]_1$	3	0	−1	1	−1	3	0	−1	1	−1	F_1^+
$[[1, 1_{11}]_0, 1]_1$	3	0	−1	1	−1	3	0	−1	1	−1	F_1^+
$[[1, 1_{11}]_1, 0]_1$	3	0	−1	−1	1	3	0	−1	−1	1	F_2^+
$[[1, 1_{11}]_1, 1]_1$	3	0	−1	1	−1	3	0	−1	1	−1	F_1^+
$[[1, 1_{11}]_1, 2]_1$	3	0	−1	−1	1	3	0	−1	−1	1	F_2^+
$[[1, 1_{11}]_2, 1]_1$	3	0	−1	1	−1	3	0	−1	1	−1	F_1^+
$[[1, 1_{11}]_2, 2]_1$	3	0	−1	−1	1	3	0	−1	−1	1	F_2^+
$[[1, 1_{11}]_2, 3]_1$	3	0	−1	1	−1	3	0	−1	1	−1	F_1^+
$[[2, 0_{00}]_2, 1]_1$	5	−1	1	1	−1	5	−1	1	1	−1	$E^+ \oplus F_1^+$
$[[2, 0_{00}]_2, 2]_1$	5	−1	1	−1	1	5	−1	1	−1	1	$E^+ \oplus F_2^+$
$[[2, 0_{00}]_2, 3]_1$	5	−1	1	1	−1	5	−1	1	1	−1	$E^+ \oplus F_1^+$
$[[2, 1_{11}]_1, 0]_1$	5	−1	1	1	−1	5	−1	1	1	−1	$E^+ \oplus F_1^+$
$[[2, 1_{11}]_1, 1]_1$	5	−1	1	−1	1	5	−1	1	−1	1	$E^+ \oplus F_2^+$
$[[2, 1_{11}]_1, 2]_1$	5	−1	1	1	−1	5	−1	1	1	−1	$E^+ \oplus F_1^+$
$[[2, 1_{11}]_2, 1]_1$	5	−1	1	−1	1	5	−1	1	−1	1	$E^+ \oplus F_2^+$
$[[2, 1_{11}]_2, 2]_1$	5	−1	1	1	−1	5	−1	1	1	−1	$E^+ \oplus F_1^+$
$[[2, 1_{11}]_2, 3]_1$	5	−1	1	−1	1	5	−1	1	−1	1	$E^+ \oplus F_2^+$

TABLE S24: Characters and irrep decomposition of the $[[j^{\mathrm{M}}, j^{\mathrm{W}}_{k_\mathrm{a}k_\mathrm{c}}]_j, \Lambda]_J$ coupled-rotor functions which dominate the ZPV(GM) splitting manifold with $J = 1$ and Γ^- symmetry in the G_{48} group (see also Figure 4).

Γ	E	(123)	(14)(23)	[(1423)(ab)]*	[(23)(ab)]*	(ab)	(123)(ab)	(14)(23)(ab)	[(1423)]*	[(23)]*	Irreps
	1	8	3	6	6	1	8	3	6	6	
$[[0,1_{01}]_1,0]_1$	1	1	1	1	1	−1	−1	−1	−1	−1	A_1^-
$[[0,1_{01}]_1,1]_1$	1	1	1	−1	−1	−1	−1	−1	1	1	A_2^-
$[[0,1_{01}]_1,2]_1$	1	1	1	1	1	−1	−1	−1	−1	−1	A_1^-
$[[0,1_{10}]_1,0]_1$	1	1	1	−1	−1	−1	−1	−1	1	1	A_2^-
$[[0,1_{10}]_1,1]_1$	1	1	1	1	1	−1	−1	−1	−1	−1	A_1^-
$[[0,1_{10}]_1,2]_1$	1	1	1	−1	−1	−1	−1	−1	1	1	A_2^-
$[[1,1_{01}]_0,1]_1$	3	0	−1	−1	1	−3	0	1	1	−1	F_2^-
$[[1,1_{01}]_1,0]_1$	3	0	−1	1	−1	−3	0	1	−1	1	F_1^-
$[[1,1_{01}]_1,1]_1$	3	0	−1	−1	1	−3	0	1	1	−1	F_2^-
$[[1,1_{01}]_1,2]_1$	3	0	−1	1	−1	−3	0	1	−1	1	F_1^-
$[[1,1_{01}]_2,1]_1$	3	0	−1	−1	1	−3	0	1	1	−1	F_2^-
$[[1,1_{01}]_2,2]_1$	3	0	−1	1	−1	−3	0	1	−1	1	F_1^-
$[[1,1_{01}]_2,3]_1$	3	0	−1	−1	1	−3	0	1	1	−1	F_2^-
$[[1,1_{10}]_0,1]_1$	3	0	−1	1	−1	−3	0	1	−1	1	F_1^-
$[[1,1_{10}]_1,0]_1$	3	0	−1	−1	1	−3	0	1	1	−1	F_2^-
$[[1,1_{10}]_1,1]_1$	3	0	−1	1	−1	−3	0	1	−1	1	F_1^-
$[[1,1_{10}]_1,2]_1$	3	0	−1	−1	1	−3	0	1	1	−1	F_2^-
$[[1,1_{10}]_2,1]_1$	3	0	−1	1	−1	−3	0	1	−1	1	F_1^-
$[[1,1_{10}]_2,2]_1$	3	0	−1	−1	1	−3	0	1	1	−1	F_2^-
$[[1,1_{10}]_2,3]_1$	3	0	−1	1	−1	−3	0	1	−1	1	F_1^-
$[[2,1_{01}]_1,0]_1$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2,1_{01}]_1,1]_1$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2,1_{01}]_1,2]_1$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2,1_{01}]_2,1]_1$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2,1_{01}]_2,2]_1$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2,1_{01}]_2,3]_1$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2,1_{01}]_3,2]_1$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2,1_{01}]_3,3]_1$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2,1_{01}]_3,4]_1$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2,1_{10}]_1,0]_1$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2,1_{10}]_1,1]_1$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2,1_{10}]_1,2]_1$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2,1_{10}]_2,1]_1$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2,1_{10}]_2,2]_1$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2,1_{10}]_2,3]_1$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2,1_{10}]_3,2]_1$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2,1_{10}]_3,3]_1$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2,1_{10}]_3,4]_1$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$

TABLE S25: Characters and irrep decomposition of the $[[j^{\mathrm{M}}, j^{\mathrm{W}}_{k_\mathrm{a}k_\mathrm{c}}]_j, \Lambda]_J$ coupled-rotor functions which dominate the ZPV(GM) splitting manifold with $J = 2$ and Γ^+ symmetry in the G_{48} group (see also Figure 3).

Γ	E	(123)	(14)(23)	[(1423)(ab)]*	[(23)(ab)]*	(ab)	(123)(ab)	(14)(23)(ab)	[(1423)]*	[(23)]*	Irreps
	1	8	3	6	6	1	8	3	6	6	
$[[0, 0_{00}]_0, 2]_2$	1	1	1	1	1	1	1	1	1	1	A_1^+
$[[0, 1_{11}]_1, 1]_2$	1	1	1	1	1	1	1	1	1	1	A_1^+
$[[0, 1_{11}]_1, 2]_2$	1	1	1	−1	−1	1	1	1	−1	−1	A_2^+
$[[0, 1_{11}]_1, 3]_2$	1	1	1	1	1	1	1	1	1	1	A_1^+
$[[1, 0_{00}]_1, 1]_2$	3	0	−1	−1	1	3	0	−1	−1	1	F_2^+
$[[1, 0_{00}]_1, 2]_2$	3	0	−1	1	−1	3	0	−1	1	−1	F_1^+
$[[1, 0_{00}]_1, 3]_2$	3	0	−1	−1	1	3	0	−1	−1	1	F_2^+
$[[1, 1_{11}]_0, 2]_2$	3	0	−1	−1	1	3	0	−1	−1	1	F_2^+
$[[1, 1_{11}]_1, 1]_2$	3	0	−1	1	−1	3	0	−1	1	−1	F_1^+
$[[1, 1_{11}]_1, 2]_2$	3	0	−1	−1	1	3	0	−1	−1	1	F_2^+
$[[1, 1_{11}]_1, 3]_2$	3	0	−1	1	−1	3	0	−1	1	−1	F_1^+
$[[2, 0_{00}]_2, 0]_2$	5	−1	1	−1	1	5	−1	1	−1	1	$\mathrm{E}^+ \oplus \mathrm{F}_2^+$
$[[2, 0_{00}]_2, 1]_2$	5	−1	1	1	−1	5	−1	1	1	−1	$\mathrm{E}^+ \oplus \mathrm{F}_1^+$
$[[2, 0_{00}]_2, 2]_2$	5	−1	1	−1	1	5	−1	1	−1	1	$\mathrm{E}^+ \oplus \mathrm{F}_2^+$
$[[2, 0_{00}]_2, 3]_2$	5	−1	1	1	−1	5	−1	1	1	−1	$\mathrm{E}^+ \oplus \mathrm{F}_1^+$
$[[2, 0_{00}]_2, 4]_2$	5	−1	1	−1	1	5	−1	1	−1	1	$\mathrm{E}^+ \oplus \mathrm{F}_2^+$
$[[2, 1_{11}]_1, 1]_2$	5	−1	1	−1	1	5	−1	1	−1	1	$\mathrm{E}^+ \oplus \mathrm{F}_2^+$
$[[2, 1_{11}]_1, 2]_2$	5	−1	1	1	−1	5	−1	1	1	−1	$\mathrm{E}^+ \oplus \mathrm{F}_1^+$
$[[2, 1_{11}]_1, 3]_2$	5	−1	1	−1	1	5	−1	1	−1	1	$\mathrm{E}^+ \oplus \mathrm{F}_2^+$
$[[2, 1_{11}]_2, 0]_2$	5	−1	1	1	−1	5	−1	1	1	−1	$\mathrm{E}^+ \oplus \mathrm{F}_1^+$
$[[2, 1_{11}]_2, 1]_2$	5	−1	1	−1	1	5	−1	1	−1	1	$\mathrm{E}^+ \oplus \mathrm{F}_2^+$
$[[2, 1_{11}]_2, 2]_2$	5	−1	1	1	−1	5	−1	1	1	−1	$\mathrm{E}^+ \oplus \mathrm{F}_1^+$
$[[2, 1_{11}]_2, 3]_2$	5	−1	1	−1	1	5	−1	1	−1	1	$\mathrm{E}^+ \oplus \mathrm{F}_2^+$
$[[2, 1_{11}]_2, 4]_2$	5	−1	1	1	−1	5	−1	1	1	−1	$\mathrm{E}^+ \oplus \mathrm{F}_1^+$
$[[2, 1_{11}]_3, 1]_2$	5	−1	1	−1	1	5	−1	1	−1	1	$\mathrm{E}^+ \oplus \mathrm{F}_2^+$
$[[2, 1_{11}]_3, 2]_2$	5	−1	1	1	−1	5	−1	1	1	−1	$\mathrm{E}^+ \oplus \mathrm{F}_1^+$
$[[2, 1_{11}]_3, 3]_2$	5	−1	1	−1	1	5	−1	1	−1	1	$\mathrm{E}^+ \oplus \mathrm{F}_2^+$
$[[2, 1_{11}]_3, 4]_2$	5	−1	1	1	−1	5	−1	1	1	−1	$\mathrm{E}^+ \oplus \mathrm{F}_1^+$
$[[2, 1_{11}]_3, 5]_2$	5	−1	1	−1	1	5	−1	1	−1	1	$\mathrm{E}^+ \oplus \mathrm{F}_2^+$

TABLE S26: Characters and irrep decomposition of the $[[j^{\mathrm{M}}, j^{\mathrm{W}}_{k_\mathrm{a}k_\mathrm{c}}]_j, \Lambda]_J$ coupled-rotor functions which dominate the ZPV(GM) splitting manifold with $J = 2$ and Γ^- symmetry in the G_{48} group (see also Figure 4).

Γ	E	(123)	(14)(23)	[(1423)(ab)]*	[(23)(ab)]*	(ab)	(123)(ab)	(14)(23)(ab)	[(1423)]*	[(23)]*	Irreps
	1	8	3	6	6	1	8	3	6	6	
$[[0, 1_{01}]_1, 1]_2$	1	1	1	−1	−1	−1	−1	−1	1	1	A_2^-
$[[0, 1_{01}]_1, 2]_2$	1	1	1	1	1	−1	−1	−1	−1	−1	A_1^-
$[[0, 1_{01}]_1, 3]_2$	1	1	1	−1	−1	−1	−1	−1	1	1	A_2^-
$[[0, 1_{10}]_1, 1]_2$	1	1	1	1	1	−1	−1	−1	−1	−1	A_1^-
$[[0, 1_{10}]_1, 2]_2$	1	1	1	−1	−1	−1	−1	−1	1	1	A_2^-
$[[0, 1_{10}]_1, 3]_2$	1	1	1	1	1	−1	−1	−1	−1	−1	A_1^-
$[[1, 1_{01}]_0, 2]_2$	3	0	−1	1	−1	−3	0	1	−1	1	F_1^-
$[[1, 1_{01}]_1, 1]_2$	3	0	−1	−1	1	−3	0	1	1	−1	F_2^-
$[[1, 1_{01}]_1, 2]_2$	3	0	−1	1	−1	−3	0	1	−1	1	F_1^-
$[[1, 1_{01}]_1, 3]_2$	3	0	−1	−1	1	−3	0	1	1	−1	F_2^-
$[[1, 1_{01}]_2, 0]_2$	3	0	−1	1	−1	−3	0	1	−1	1	F_1^-
$[[1, 1_{01}]_2, 1]_2$	3	0	−1	−1	1	−3	0	1	1	−1	F_2^-
$[[1, 1_{01}]_2, 2]_2$	3	0	−1	1	−1	−3	0	1	−1	1	F_1^-
$[[1, 1_{01}]_2, 3]_2$	3	0	−1	−1	1	−3	0	1	1	−1	F_2^-
$[[1, 1_{01}]_2, 4]_2$	3	0	−1	1	−1	−3	0	1	−1	1	F_1^-
$[[1, 1_{10}]_0, 2]_2$	3	0	−1	−1	1	−3	0	1	1	−1	F_2^-
$[[1, 1_{10}]_1, 1]_2$	3	0	−1	1	−1	−3	0	1	−1	1	F_1^-
$[[1, 1_{10}]_1, 2]_2$	3	0	−1	−1	1	−3	0	1	1	−1	F_2^-
$[[1, 1_{10}]_1, 3]_2$	3	0	−1	1	−1	−3	0	1	−1	1	F_1^-
$[[1, 1_{10}]_2, 0]_2$	3	0	−1	−1	1	−3	0	1	1	−1	F_2^-
$[[1, 1_{10}]_2, 1]_2$	3	0	−1	1	−1	−3	0	1	−1	1	F_1^-
$[[1, 1_{10}]_2, 2]_2$	3	0	−1	−1	1	−3	0	1	1	−1	F_2^-
$[[1, 1_{10}]_2, 3]_2$	3	0	−1	1	−1	−3	0	1	−1	1	F_1^-
$[[1, 1_{10}]_2, 4]_2$	3	0	−1	−1	1	−3	0	1	1	−1	F_2^-
$[[2, 1_{01}]_1, 1]_2$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2, 1_{01}]_1, 2]_2$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2, 1_{01}]_1, 3]_2$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2, 1_{01}]_2, 0]_2$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2, 1_{01}]_2, 1]_2$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2, 1_{01}]_2, 2]_2$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2, 1_{01}]_2, 3]_2$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2, 1_{01}]_2, 4]_2$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2, 1_{01}]_3, 1]_2$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2, 1_{01}]_3, 2]_2$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2, 1_{01}]_3, 3]_2$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2, 1_{01}]_3, 4]_2$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2, 1_{01}]_3, 5]_2$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2, 1_{10}]_1, 1]_2$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2, 1_{10}]_1, 2]_2$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2, 1_{10}]_1, 3]_2$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2, 1_{10}]_2, 0]_2$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2, 1_{10}]_2, 1]_2$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2, 1_{10}]_2, 2]_2$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2, 1_{10}]_2, 3]_2$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2, 1_{10}]_2, 4]_2$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2, 1_{10}]_3, 1]_2$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2, 1_{10}]_3, 2]_2$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2, 1_{10}]_3, 3]_2$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$
$[[2, 1_{10}]_3, 4]_2$	5	−1	1	1	−1	−5	1	−1	−1	1	$E^- \oplus F_1^-$
$[[2, 1_{10}]_3, 5]_2$	5	−1	1	−1	1	−5	1	−1	1	−1	$E^- \oplus F_2^-$

[1] L. Dore, R. C. Cohen, C. A. Schmuttenmaer, K. L. Busarow, M. J. Elrod, J. G. Loeser, and R. J. Saykally, J. Chem. Phys. **100**, 863 (1994).