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

Interactions of limonene with the water dimer

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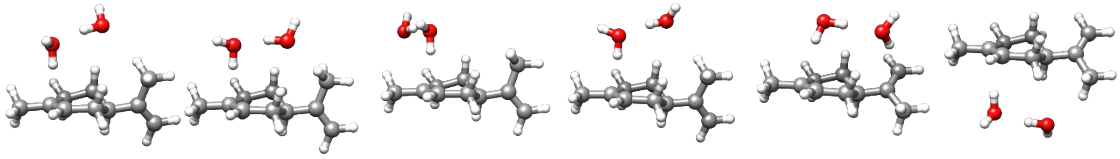
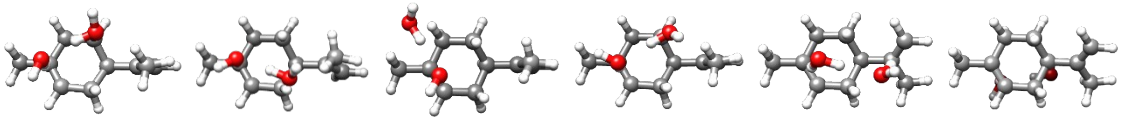
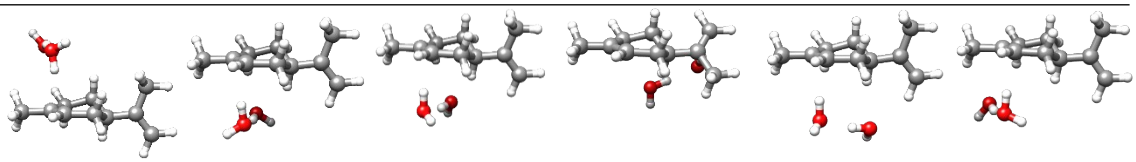
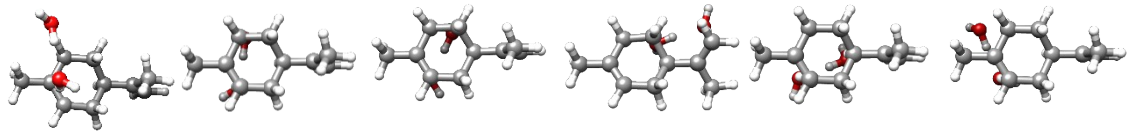
Supplementary Information

TABLE OF CONTENTS

Table S1. Calculated spectroscopic parameters for the isomers of limonene-$(H_2O)_2$ at B3LYP-D3BJ/6-311++G(d,p) and MP2/6-311++G(d,p) levels of theory within 4 kJ mol^{-1}.

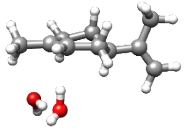
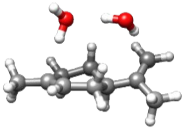
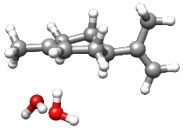
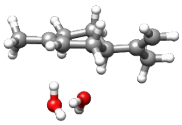
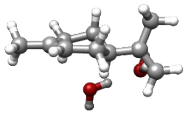
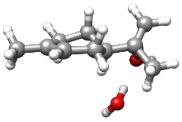
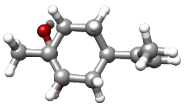
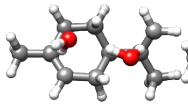
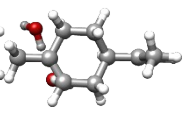
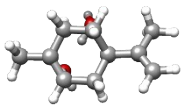
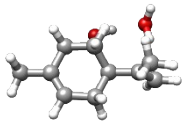
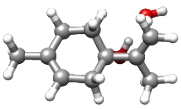
	EQA-3-I		EQA-3-II		EQA-3-III		EQA-3-IV		EQC-1-I		EQC-4-I	
	B3LYP	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**
A[a] (MHz)	971.5	970.2	959.3	966.6	1232.0	1197.0	969.2	956.3	1072.0	1058.6	964.3	962.3
B (MHz)	597.8	597.5	607.0	606.5	472.3	479.8	597.5	599.2	579.3	581.3	605.5	603.9
C (MHz)	447.3	443.7	441.1	444.7	430.0	432.5	446.2	443.2	477.2	475.4	445.6	450.0
κ	-0.43	-0.42	-0.36	-0.36	-0.89	-0.88	-0.42	-0.39	-0.66	-0.64	-0.38	-0.40
μ_a (D)	2.7	-2.7	2.9	-3.0	0.0	0.1	2.7	-2.7	-2.6	2.9	-3.0	-2.9
μ_b (D)	0.4	0.2	0.3	-0.2	-0.2	-0.1	-0.6	0.7	2.5	2.2	-0.1	-0.1
μ_c (D)	0.7	0.9	-0.5	0.0	-1.6	-1.8	-0.5	0.7	0.2	0.1	-0.5	-0.6
ΔE (cm^{-1})	88.7	29.8	45.1	0.0	103.8	67.2	164.4	132.8	0.0	184.1	140.4	106.3
ΔE_{ZPC} (cm^{-1})	0.0	53.8	27.2	0.0	41.3	82.7	59.5	111.5	70.2	304.9	80.5	149.7
ΔE(BSSE)(kJ mol^{-1})	-55.6	-38.5	-55.8	-39.1	-55.3	-39.5	-54.8	-37.9	-54.7	-38.1	-55.0	-39.2
Side view												
Top view												

[a] A, B and C are the rotational constants; μ_a, μ_b and μ_c are the electric dipole moments along the principal inertial axes; ΔE are the relative energies; ΔE_{ZPC} are the relative energies including zero-point corrections; ΔE(BSSE) are the interaction energies including BSSE and fragment relaxation; κ is the calculated Ray's asymmetry parameter

	EQA-3-V		EQA-4-I		EQA-4-II		EQC-2-I		EQA-4-III		EQA-4-IV	
	B3LYP	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**
A[a] (MHz)	1239.4	1148.6	1001.5	980.5	1012.1	1001.5	1075.2	1081.3	946.0	939.2	1172.6	Converged to EQA-4-II
B (MHz)	467.4	484.1	557.6	577.1	570.3	577.9	541.4	538.8	609.1	611.5	479.8	
C (MHz)	428.0	433.5	468.4	476.6	471.7	472.0	431.8	436.6	444.0	444.4	435.5	
κ	-0.90	-0.86	-0.67	-0.60	-0.64	-0.60	-0.66	-0.68	-0.34	-0.32	-0.88	
μ_a (D)	-0.7	-0.2	0.5	-1.0	-0.8	-0.9	1.7	-1.8	2.6	2.6	1.0	
μ_b (D)	-0.4	0.2	1.4	0.9	-0.8	0.5	-0.4	0.0	1.3	1.1	-0.2	
μ_c (D)	1.2	-1.8	-1.4	-1.6	-1.3	-1.5	0.6	-0.9	-0.4	0.5	-1.0	
ΔE (cm^{-1})	187.5	182.5	195.8	104.5	172.7	68.0	188.5	202.9	159.8	7.6	234.4	
ΔE_{ZPC} (cm^{-1})	86.9	141.1	87.6	75.7	88.7	62.1	89.3	161.1	92.2	72.9	101.2	
ΔE(BSSE)(kJ mol^{-1})	-54.7	-38.3	-55.0	-37.9	-55.0	-38.1	-54.5	-39.5	-55.0	-38.5	-54.1	
Side view												
Top view												

[a] A, B and C are the rotational constants; μ_a, μ_b and μ_c are the electric dipole moments along the principal inertial axes; ΔE are the relative energies; ΔE_{ZPC} are the relative energies including zero-point corrections; ΔE(BSSE) are the interaction energies including BSSE and fragment relaxation; κ is the calculated Ray's asymmetry parameter

Table S1 (cont.).

	EQA-4-V		EQC-3-I		EQA-4-VI		EQa-4-I		EQA-2-I		EQC-2-II	
	B3LYP	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**
A[a] (MHz)	1165.5	Converged to EQA-4-I	1072.6	1049.7	1163.5	Converged to EQA-4-II	1010.0	1000.1	1010.3	990.5	1132.9	1102.9
B (MHz)	483.5		581.0	581.2	481.5		578.0	589.5	565.9	566.5	485.6	507.3
C (MHz)	437.5		479.3	475.0	436.8		482.8	479.0	422.5	418.6	439.3	444.0
κ	-0.87		-0.66	-0.63	-0.88		-0.64	-0.58	-0.51	-0.48	-0.87	-0.81
μ_a (D)	-0.2		3.0	-3.1	-0.9		1.4	1.4	-1.7	-2.0	-1.0	1.5
μ_b (D)	0.4		-2.5	-2.4	0.3		0.2	0.1	1.0	1.2	0.1	-0.1
μ_c (D)	-1.5		-0.2	-0.1	-1.0		-1.0	-1.4	1.1	-0.8	-1.1	1.1
ΔE (cm^{-1})	196.0		44.0	212.4	234.9		210.0	157.0	279.6	286.5	207.1	255.6
ΔE_{ZPC} (cm^{-1})	118.7		119.6	345.9	120.7		123.3	156.7	129.5	267.1	133.0	235.7
ΔE(BSSE)(kJ mol^{-1})	-54.5		-56.4	-37.5	-54.1		-54.1	-39.6	-53.6	-37.6	-54.1	-38.8
Side view												
Top view												

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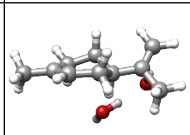
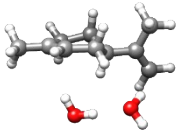
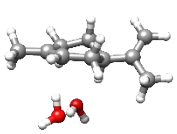
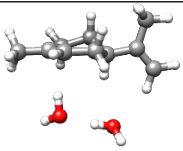
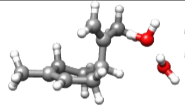
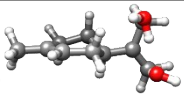
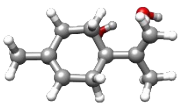
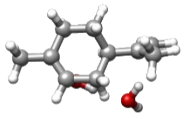
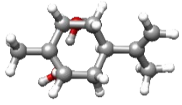
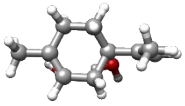
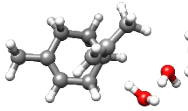
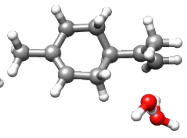
	EQC-2-III		EQA-1-I		EQC-4-II		EQA-4-VII		AXa-1-I		EQA-1-II	
	B3LYP	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**
A[a] (MHz)	1077.6	1064.0	1011.6	1006.4	990.8	982.3	926.1	913.9	1333.5	1322.0	1154.7	1135.1
B (MHz)	540.5	546.2	602.6	604.4	553.1	567.8	615.3	617.7	473.9	472.9	467.3	465.9
C (MHz)	432.2	435.0	458.1	461.5	488.1	494.2	434.5	434.6	454.8	461.5	399.5	397.6
κ	-0.66	-0.65	-0.48	-0.48	-0.91	-0.70	-0.26	-0.24	-0.96	-0.97	-0.82	-0.81
μ_a (D)	2.1	-2.4	-2.0	2.3	1.1	1.8	-2.7	-2.9	-0.1	0.3	0.0	0.0
μ_b (D)	-0.3	0.3	-2.4	2.2	-0.3	-0.2	-1.4	1.1	0.6	0.7	-0.9	0.9
μ_c (D)	-0.1	0.1	1.0	-1.0	1.9	1.7	-0.4	-0.4	-1.1	-1.4	-1.5	1.5
ΔE (cm^{-1})	261.5	235.7	135.7	103.3	260.6	206.4	277.5	164.2	238.5	47.5	255.8	324.6
ΔE_{ZPC} (cm^{-1})	138.0	226.5	139.1	214.9	163.3	158.9	164.2	186.1	168.8	119.0	174.0	355.1
ΔE(BSSE)(kJ mol^{-1})	-53.7	-38.9	-55.0	-37.3	-53.7	-38.2	-53.6	-37.4	-54.1	-39.4	-53.9	-37.5
Side view												
Top view												

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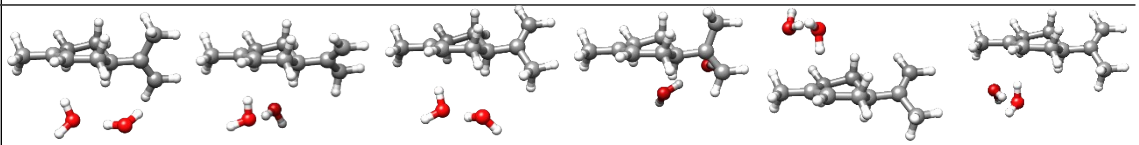
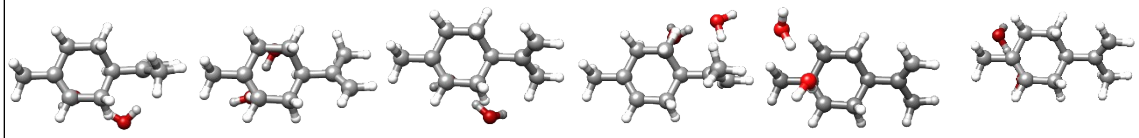
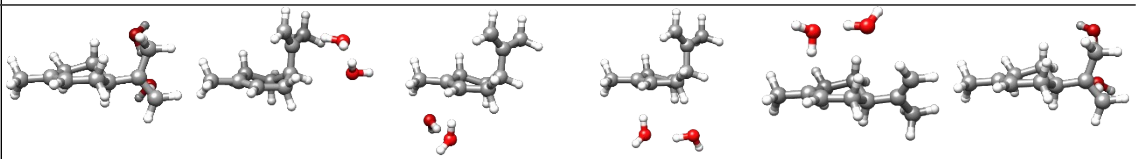
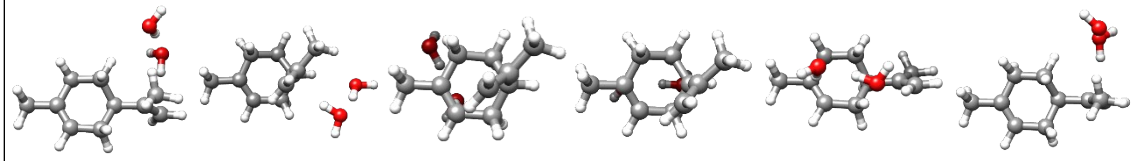
Table S1 (cont.).

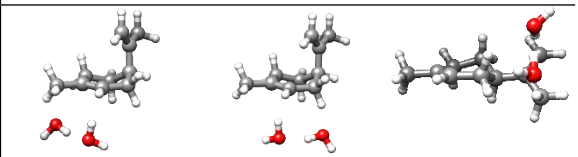
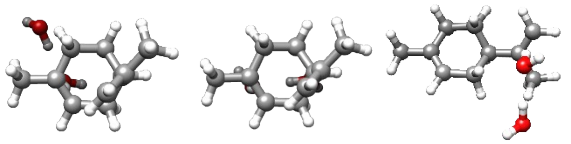
	EQA-1-III		EQa-4-II		EQC-4-III		EQA-2-II		EQC-3-II		EQC-4-IV	
	B3LYP	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**
A[a] (MHz)	985.6	987.2	1011.8	996.7	916.5	910.2	1021.9	1020.8	1273.9	1242.4	1157.1	
B (MHz)	615.2	610.5	576.8	590.0	639.7	641.9	568.3	567.5	455.4	461.5	477.5	
C (MHz)	457.1	458.6	479.2	482.8	432.2	434.9	429.6	431.8	416.4	417.7	443.7	Converged to EQC-4-II
κ	-0.40	-0.43	-0.63	-0.58	-0.14	-0.13	-0.53	-0.54	-0.91	-0.89	-0.91	
μ_a (D)	-3.0	-3.0	2.1	2.4	-2.4	-2.4	-2.5	-2.7	0.4	-0.3	0.2	
μ_b (D)	-2.5	2.5	-0.1	-0.2	-0.5	0.2	0.0	-0.1	0.9	0.8	0.8	
μ_c (D)	0.4	0.4	0.8	1.0	1.1	1.2	-0.5	-0.4	-1.5	-1.7	-1.6	
ΔE (cm^{-1})	159.6	144.0	288.0	209.1	281.2	291.5	306.2	263.9	253.4	286.6	288.3	
ΔE_{ZPC} (cm^{-1})	177.1	227.6	181.5	184.6	182.4	268.9	197.5	294.5	197.7	283.8	215.7	
ΔE(BSSE)(kJ mol^{-1})	-55.0	-36.9	-53.4	-39.1	-53.5	-38.3	-53.3	-37.4	-54.0	-39.0	-53.3	
Side view												
Top view												

[a] A, B and C are the rotational constants; μ_a, μ_b and μ_c are the electric dipole moments along the principal inertial axes; ΔE are the relative energies; ΔE_{ZPC} are the relative energies including zero-point corrections; ΔE(BSSE) are the interaction energies including BSSE and fragment relaxation; κ is the calculated Ray's asymmetry parameter.

	EQA-2-III		AXa-1-II		AXa-4-I		AXa-4-II		EQa-3-I		EQA-2-IV	
	B3LYP	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**B3LYP**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**
A[a] (MHz)	1168.2	1141.3	1349.9	1323.4	1308.9	1264.1	1009.4	1004.6	960.4	949.3	1161.4	1135.1
B (MHz)	459.0	463.7	467.1	463.1	481.9	497.1	609.3	613.6	603.5	606.1	457.3	462.1
C (MHz)	391.8	392.1	451.7	460.9	465.9	476.0	466.2	473.5	435.1	434.6	393.2	394.0
κ	-0.83	-0.81	-0.97	-0.99	-0.96	-0.95	-0.47	-0.47	-0.36	-0.33	-0.83	-0.82
μ_a (D)	0.2	-0.1	0.3	0.0	0.1	-0.2	1.2	1.3	2.2	-2.4	0.5	0.3
μ_b (D)	-0.4	0.4	-1.0	0.5	0.6	-0.9	1.4	-1.6	-1.7	-1.3	-0.4	-0.3
μ_c (D)	1.4	-1.4	0.6	-1.6	1.4	-1.4	-0.3	-0.2	0.7	-0.7	1.8	-2.0
ΔE (cm^{-1})	339.7	429.5	277.7	105.5	258.5	21.0	246.8	80.2	332.2	263.0	319.3	410.4
ΔE_{ZPC} (cm^{-1})	223.2	419.4	232.9	148.8	245.6	104.0	246.9	114.6	248.9	309.7	255.2	443.3
ΔE(BSSE)(kJ mol^{-1})	-53.0	-37.2	-53.6	-39.0	-53.8	-39.4	-53.0	-38.6	-53.2	-37.9	-53.2	-36.8
Side view												
Top view												

[a] A, B and C are the rotational constants; μ_a, μ_b and μ_c are the electric dipole moments along the principal inertial axes; ΔE are the relative energies; ΔE_{ZPC} are the relative energies including zero-point corrections; ΔE(BSSE) are the interaction energies including BSSE and fragment relaxation; κ is the calculated Ray's asymmetry parameter.

Table S1 (cont.).

	AXa-4-III		AXa-4-IV		EQC-1-II	
	B3LYP	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**
A[a] (MHz)	1308.3	1255.0	1012.4	1012.0	1141.2	1123.2
B (MHz)	480.9	498.7	606.7	606.5	469.6	468.4
C (MHz)	464.2	469.7	465.2	470.2	399.8	397.8
κ	-0.96	-0.93	-0.48	-0.50	-0.81	-0.81
μ_a (D)	-0.5	0.3	-0.9	0.9	0.7	-0.8
μ_b (D)	0.2	-1.0	1.5	-1.6	-1.2	1.3
μ_c (D)	1.6	-1.5	0.9	-1.0	1.4	-1.6
ΔE (cm^{-1})	335.7	130.4	368.9	141.3	309.9	525.5
ΔE_{ZPC} (cm^{-1})	256.1	151.7	257.7	155.4	310.8	585.8
ΔE(BSSE)(kJ mol^{-1})	-53.0	-38.6	-52.6	-38.1	-52.1	-34.8
Side view						
Top view						

[a] A, B and C are the rotational constants; μ_a, μ_b and μ_c are the electric dipole moments along the principal inertial axes; ΔE are the relative energies; ΔE_{ZPC} are the relative energies including zero-point corrections; ΔE(BSSE) are the interaction energies including BSSE and fragment relaxation; κ is the calculated Ray's asymmetry parameter.

Table S2. Calculated spectroscopic parameters for the lower-energy isomers of limonene-$(H_2O)_2$ at M062X/6-311++G(d,p) level of theory.

Name	A[a] (MHz)	B (MHz)	C (MHz)	μ_a (D)	μ_b (D)	μ_c (D)	ΔE (cm^{-1})	ΔE_{ZPC} (cm^{-1})
EQC-1-I	1105.9	582.3	486.7	-2.8	2.2	0.2	0.0	0.0
EQC-3-I	1105.1	582.0	488.3	2.9	-2.3	-0.1	35.5	30.5
EQA-3-IV	1002.1	607.3	454.8	-2.3	-0.5	-0.9	292.4	182.2
EQA-1-I	1047.0	605.9	469.9	-2.2	-2.2	1.0	192.8	189.4
EQA-3-II	1012.6	605.3	451.2	2.8	0.1	-0.4	320.2	201.9
EQa-4-I	1047.4	605.2	488.6	2.2	-0.2	-1.1	157.3	205.0
EQA-3-III	1256.5	489.0	438.8	-0.1	-0.7	-1.5	348.6	235.5
EQC-2-I	1101.2	549.6	435.6	1.9	-0.2	0.5	348.9	240.8
EQA-1-III	1040.4	609.7	470.4	-3.1	-2.2	0.4	229.4	246.3
EQA-3-V	1259.6	479.8	434.4	-0.7	-0.5	1.1	445.1	255.7
EQA-4-V	1217.4	481.3	437.3	-0.3	-0.1	-1.3	474.2	297.4
EQa-3-I	1063.1	591.7	475.3	-2.7	2.7	-0.1	317.7	302.2
EQa-4-II	1043.6	614.0	488.6	-2.2	0.3	-1.3	366.5	305.9
EQA-4-II	1025.2	596.3	481.8	1.4	0.5	-1.3	472.0	309.7
EQC-4-I	977.6	611.7	448.7	3.1	0.1	-0.1	333.9	316.7
EQA-2-I	1091.0	557.4	432.3	-1.7	0.7	1.1	465.5	330.7
EQC-2-III	1100.2	551.3	439.9	2.3	-0.2	-0.2	420.3	336.5
EQC-4-III	969.6	638.7	448.4	-2.4	0.0	1.1	422.0	340.0
EQA-4-I	1020.2	612.4	497.0	-1.5	-2.3	-1.6	339.2	344.1
EQC-3-II	1307.9	459.5	419.5	0.4	0.6	-1.6	386.0	354.5
EQC-4-II	998.4	574.5	509.0	1.1	-0.8	2.1	406.1	367.2
EQA-3-I	989.5	604.3	448.1	2.9	0.1	0.5	418.5	369.4
EQA-2-II	1101.9	561.2	440.8	-2.7	0.4	-0.3	502.9	399.2
EQA-4-VI	1203.5	485.0	440.1	-0.9	0.0	-0.8	524.8	399.4
EQA-4-IV	1203.4	485.1	440.1	1.0	0.0	-0.8	524.7	402.3
AXa-4-IV	952.5	659.9	487.5	1.2	1.5	0.9	484.1	407.8
AXa-4-II	951.6	661.7	489.2	-1.5	1.5	-0.7	435.9	408.9
EQC-4-IV	1194.9	475.8	447.5	-0.1	1.1	1.4	477.7	415.0
EQC-2-II	1094.6	494.8	463.8	-0.5	0.4	-1.6	430.5	425.3
AXa-4-I	1297.7	497.5	484.0	-0.2	0.5	1.4	375.7	448.2
EQA-4-VII	989.1	626.8	448.0	-2.4	1.0	-0.4	535.8	452.8
EQA-4-III	947.0	619.7	447.3	2.8	1.1	-0.2	466.8	457.2
AXa-1-I	1383.7	475.5	456.1	-0.2	1.2	0.7	440.7	462.2
AXa-1-II	1380.3	476.2	457.7	0.3	1.1	0.3	453.7	466.6
EQC-1-II	1125.9	492.2	406.3	0.3	-1.2	1.4	526.0	481.3
AXa-4-III	1294.7	498.0	481.7	0.4	0.2	1.6	465.7	489.4
EQA-2-III	1137.8	483.1	402.3	-0.2	-0.5	1.6	622.8	492.1
EQA-1-II	1134.2	486.8	413.5	-0.2	-0.9	-1.5	476.2	509.0
EQA-2-IV	1132.7	480.8	403.0	0.3	-0.5	1.9	628.0	546.1

Table S3. Calculated spectroscopic parameters for the lower-energy isomers of limonene-$(H_2O)_2$ at wB97XD/6-311++G(d,p) level of theory.

Name	A[a] (MHz)	B (MHz)	C (MHz)	μ_a (D)	μ_b (D)	μ_c (D)	ΔE (cm^{-1})	ΔE_{ZPC} (cm^{-1})
EQC-1-I	1082.2	581.4	480.7	-2.5	2.5	0.1	0.0	0.0
EQA-3-II	968.5	610.2	445.2	2.8	0.4	-0.6	176.9	12.5
EQC-3-I	1083.1	582.6	482.7	2.9	-2.5	-0.3	35.4	34.0
EQA-3-V	1248.3	475.7	431.6	-0.8	-0.3	1.1	303.9	75.9
EQA-1-I	1020.5	604.2	461.7	-1.9	-2.4	1.0	159.4	81.9
EQA-3-III	1243.0	476.6	432.1	0.1	-0.3	-1.5	241.9	84.7
EQa-4-I	1012.5	592.1	489.9	1.6	0.2	-1.0	293.0	101.8
EQA-4-IV/VI	1180.8	487.1	440.1	1.0	-0.2	-0.8	370.0	119.8
EQA-3-I	973.1	603.4	449.0	2.8	0.5	0.6	218.2	124.7
EQA-4-I	990.0	587.6	482.9	0.7	-1.9	1.5	292.0	132.1
EQC-4-II	993.3	560.7	496.1	1.0	-0.5	2.0	372.4	143.3
EQA-4-V	1188.6	483.4	437.5	-0.3	0.2	-1.4	351.0	147.7
EQC-2-I	1067.9	550.5	434.8	1.8	-0.5	0.6	330.8	153.2
EQC-4-I	964.2	610.6	444.9	3.1	-0.2	0.2	243.1	155.8
EQA-3-IV	973.5	602.9	448.0	-2.7	0.7	-0.6	290.1	160.2
EQC-2-II	1125.9	492.5	444.3	-0.8	0.1	-1.2	354.3	168.1
AXa-1-II	1324.8	477.4	459.9	0.4	0.8	0.9	476.3	170.3
EQA-4-II	1008.1	579.7	480.1	-0.6	-0.8	-1.2	335.8	178.0
EQA-1-III	1007.9	613.5	463.2	-3.0	-2.4	0.3	171.3	181.7
EQA-4-III	939.8	616.7	444.3	2.7	1.4	-0.3	292.7	185.0
EQA-4-VII	924.4	622.9	435.6	-2.9	-1.5	-0.4	407.3	198.8
AXa-1-I	1322.2	478.6	459.3	0.1	0.5	1.1	434.9	201.5
EQC-2-III	1070.2	549.3	434.6	2.1	-0.4	0.0	405.7	203.0
EQC-4-IV	1169.7	478.0	446.2	-0.1	0.9	1.6	413.5	228.7
EQC-4-III	931.2	642.0	438.1	-2.3	-0.8	1.1	348.9	276.3
EQA-2-I	1027.8	568.7	429.6	-1.7	1.0	1.1	406.0	281.8
EQC-3-II	1284.0	457.5	418.1	0.6	0.9	-1.5	351.1	289.7
EQA-2-IV	1147.4	470.5	399.4	0.4	-0.6	1.7	450.5	290.8
EQa-4-II	1015.7	587.1	485.9	2.4	0.0	0.7	407.5	292.6
AXa-4-II	996.0	619.3	472.0	-1.0	1.6	-0.7	470.4	301.3
AXa-4-III	1302.3	489.1	473.3	0.6	0.2	1.5	475.0	306.6
AXa-4-I	1300.2	490.1	473.4	0.0	-0.6	1.4	403.4	322.8
EQA-1-II	1144.5	477.8	407.3	0.0	-1.0	-1.4	394.9	329.9
EQA-2-III	1154.6	470.2	397.4	0.1	-0.5	1.5	463.1	358.4
EQA-2-II	1037.8	569.2	434.4	2.5	0.1	0.6	472.2	361.9
EQC-1-II	1127.5	482.3	406.8	0.8	-1.4	1.4	511.9	363.7
AXa-4-IV	995.4	621.1	472.9	0.8	1.6	0.9	487.6	363.9
EQa-3-I	1034.8	593.1	466.4	2.6	-2.9	-0.2	369.7	385.6

Table S4. Calculated spectroscopic parameters for the lower-energy isomers of limonene-$(H_2O)_2$ at B2PLYP-D3BJ/def2-TZVP level of theory.

Name	A[a] (MHz)	B (MHz)	C (MHz)	μ_a (D)	μ_b (D)	μ_c (D)	ΔE (cm^{-1})	ΔE_{ZPC} (cm^{-1})
EQA-3-II	974.4	608.3	445.5	2.6	0.6	-0.7	108.1	0.0
EQC-1-I	1082.5	582.3	481.0	-2.5	2.3	0.1	0.0	13.4
EQA-3-III	1233.3	481.3	434.7	0.2	-0.3	-1.5	178.8	29.8
EQA-4-I	990.7	581.1	479.6	0.7	-1.6	1.5	229.9	41.7
EQA-3-I	970.1	603.1	447.2	2.8	0.8	0.4	194.0	45.7
EQC-3-I	1081.1	584.7	482.6	2.7	-2.4	-0.3	20.1	46.5
EQA-1-I	1024.5	606.1	462.8	-2.0	-2.2	0.8	106.3	63.4
EQA-3-IV	980.5	598.4	446.3	-2.5	0.9	-0.7	275.3	72.0
EQA-3-V	1229.6	477.9	433.6	-0.7	-0.1	1.2	242.8	72.4
EQA-4-II	1008.7	582.1	478.4	-0.8	-0.7	-1.2	253.5	78.6
EQA-1-III	1007.4	616.3	463.9	-2.8	-2.3	0.2	98.3	80.1
EQC-2-I	1097.9	539.2	437.2	-1.5	-0.2	-0.8	262.8	84.1
EQa-4-I	1016.9	590.5	488.1	1.6	0.2	-0.9	255.9	88.0
EQA-4-IV/6	1155.3	493.5	443.7	-0.8	0.4	-1.0	298.8	93.5
EQC-4-I	968.0	608.1	447.9	3.0	-0.5	0.2	237.2	101.2
EQA-4-V	1207.0	479.4	431.7	-0.9	0.2	-1.2	272.5	108.4
EQA-4-III	944.5	615.2	444.0	2.7	1.5	-0.2	268.7	112.6
EQC-4-III	932.0	642.4	440.3	-2.1	-0.9	1.0	281.3	134.3
EQa-4-II	1004.6	595.4	482.8	1.4	-0.8	1.1	345.2	140.9
EQA-2-I	1034.8	566.8	430.9	-1.5	0.8	1.2	333.7	150.6
EQC-4-II	986.1	563.7	495.2	0.9	-0.7	2.0	305.7	151.9
EQA-4-VII	935.2	618.1	435.8	-2.6	-1.7	-0.5	384.3	164.2
EQC-3-II	1284.4	460.5	419.3	0.7	0.6	-1.4	339.9	172.9
EQC-2-II	1098.9	491.6	451.5	-0.3	-0.1	-1.6	313.5	176.9
EQa-3-I	1013.5	599.9	458.2	2.2	-2.6	0.1	281.5	195.8
EQC-4-IV	1183.7	475.7	440.8	-0.7	0.7	1.4	359.2	200.6
EQA-1-II	1140.0	477.2	404.8	0.2	-1.1	-1.5	332.4	205.4
EQA-2-II	1031.0	565.1	434.0	2.1	0.3	-0.2	395.8	212.2
AXa-1-II	1341.8	472.4	457.0	0.4	0.7	0.9	357.0	212.9
AXa-1-I	1342.2	476.4	456.3	0.2	0.8	1.0	358.0	213.1
AXa-4-I	1302.7	488.7	474.7	-0.2	-0.3	1.5	325.4	215.3
AXa-4-II	1006.4	614.1	472.0	-0.6	1.8	-0.8	365.2	241.2
AXa-4-III	1295.6	489.7	472.8	0.6	0.5	1.3	379.2	256.6
EQA-2-IV	1142.4	470.8	399.1	0.5	-0.6	1.7	419.7	258.1
EQA-2-III	1152.6	469.3	397.0	0.1	-0.5	1.4	437.3	267.3
AXa-4-IV	1000.0	621.2	473.6	0.7	1.5	0.7	421.7	268.2
EQC-1-II	1126.0	482.0	403.7	0.8	-1.5	1.3	482.8	347.0
EQC-2-III	Not converged at B2PLYP-D3BJ/def2-TZVP level of theory							

Table S5. Experimental spectroscopic parameters for the isotopic species of **isomer 1 / EQA-3-II**.

Parameter	$(H_2{}^{18}O)(H_2{}^{16}O)$	$(H_2{}^{16}O)(H_2{}^{18}O)$	$(H_2{}^{18}O)(H_2{}^{18}O)$
A[a] (MHz)	933.1763(38)	910.2621(12)	897.8046(24)
B (MHz)	589.54146(69)	597.86601(24)	589.52432(57)
C (MHz)	424.99072(45)	424.33470(17)	417.53181(45)
Δ_J[b] (kHz)	0.1173(39)	0.0970(14)	0.1095(29)
Δ_{JK} (kHz)	0.234(42)	0.399(15)	0.248(22)
δ_J (kHz)	0.0440(27)	0.0374(11)	0.0386(25)
σ[d]	5.7	1.9	2.5
N[e]	38	35	36

Table S6. Experimental spectroscopic parameters for the isotopic species of **isomer 2 / EQA-4-II**.

Parameter	$(H_2{}^{18}O)(H_2{}^{16}O)$	$(H_2{}^{16}O)(H_2{}^{18}O)$	$(H_2{}^{18}O)(H_2{}^{18}O)$
A[a] (MHz)	951.0674(13)	934.06420(85)	919.5171(13)
B (MHz)	570.17231(57)	576.56319(40)	567.95688(92)
C (MHz)	454.84926(39)	453.86332(32)	447.66688(62)
Δ_J[b] (kHz)	0.1705(78)	0.1828(46)	0.188(10)
Δ_{JK} (kHz)	0.781(81)	0.985(53)	0.686(65)
δ_J (kHz)	0.0405(38)	0.0579(25)	0.0522(54)
δ_K (kHz)	0.789(72)	0.840(43)	0.900(97)
σ[d]	4.6	4.4	5.7
N[e]	33	41	35

Table S7. Experimental spectroscopic parameters for the isotopic species of **isomer 3 / EQC-4-I**.

Parameter	$(H_2{}^{18}O)(H_2{}^{16}O)$	$(H_2{}^{16}O)(H_2{}^{18}O)$	$(H_2{}^{18}O)(H_2{}^{18}O)$
A[a] (MHz)	903.4523(27)	888.6196(24)	871.1300(20)
B (MHz)	599.20014(23)	602.25182(26)	597.61671(28)
C (MHz)	429.94788(22)	428.69218(21)	422.27315(26)
Δ_J[b] (kHz)	0.0554(30)	0.0565(36)	0.0580(26)
Δ_{JK} (kHz)	0.831(18)	0.8947(18)	0.823(20)
δ_J (kHz)	[-0.006]	[-0.006]	[-0.006]
δ_K (kHz)	0.418(30)	0.485(32)	0.429(38)
σ[d]	3.6	3.2	4.2
N[e]	40	31	37

Table S8. Experimental spectroscopic parameters for the isotopic species of **isomer 4 / EQC-1-I**.

Parameter	$(H_2{}^{18}O)(H_2{}^{16}O)$	$(H_2{}^{16}O)(H_2{}^{18}O)$
A[a] (MHz)	990.092(17)	991.486(18)
B (MHz)	577.2998(22)	576.5887(17)
C (MHz)	455.69130(51)	455.68055(76)
Δ_J[b] (kHz)	[0.0116]	[0.0116]
Δ_{JK} (kHz)	[1.048]	[1.048]
σ[d]	9.1	5.3
N[e]	10	8

Table S9. Experimental spectroscopic parameters for the isotopic species of **isomer 5 / EQC-2-I**.

Parameter	$(H_2{}^{18}O)(H_2{}^{16}O)$	$(H_2{}^{16}O)(H_2{}^{18}O)$	$(H_2{}^{18}O)(H_2{}^{18}O)$
A[a] (MHz)	1035.2487(76)	1010.6869(73)	1001.4047(94)
B (MHz)	524.50158(60)	533.94459(73)	522.5763(11)
C (MHz)	414.96815(56)	417.87349(54)	409.48791(93)
Δ_J[b] (kHz)	0.1099(23)	0.1053(39)	0.1165(52)
δ_J (kHz)	0.0309(26)	0.0305(36)	0.0350(57)
σ[d]	5.4	4.7	7.0
N[e]	35	30	25

Table S10. Experimental spectroscopic parameters for the isotopic species of **isomer 6 / EQa-4-I**.

Parameter	$(H_2{}^{18}O)(H_2{}^{16}O)$	$(H_2{}^{16}O)(H_2{}^{18}O)$	$(H_2{}^{18}O)(H_2{}^{18}O)$
A[a] (MHz)	952.445(12)	937.1582(92)	920.031(15)
B (MHz)	577.61355(77)	585.33491(89)	577.3785(12)
C (MHz)	466.44558(69)	464.10488(58)	458.64240(83)
Δ_J[b] (kHz)	0.084(10)	0.0782(80)	0.060(16)
Δ_{JK} (kHz)	[0.531]	[0.531]	[0.531]
δ_K (kHz)	[0.542]	[0.542]	[0.542]
σ[d]	6.9	7.0	6.6
N[e]	15	14	11

Table S11. Experimental spectroscopic parameters for the isotopic species of **isomer 7 / EQA-2-I**.

Parameter	$(H_2{}^{18}O)(H_2{}^{16}O)$	$(H_2{}^{16}O)(H_2{}^{18}O)$	$(H_2{}^{18}O)(H_2{}^{18}O)$
A[a] (MHz)	983.9449(75)	960.2550(48)	951.2087(59)
B (MHz)	544.6077(11)	555.14250(83)	543.03954(47)
C (MHz)	407.53152(71)	409.51888(65)	401.58818(53)
Δ_J[b] (kHz)	0.1074(52)	0.1154(37)	0.1108(62)
Δ_K (kHz)	[1.40]	[1.40]	[1.40]
δ_J (kHz)	0.0252(45)	0.0253(39)	0.0247(53)
δ_K (kHz)	[0.147]	[0.147]	[0.147]
σ[d]	6.0	5.5	6.9
N[e]	27	28	24

Table S12. Experimental coordinates of the water oxygen atoms for the observed limonene-$(H_2O)_2$ complexes compared with possible equilibrium structures from MP2 and B3LYP-D3BJ calculations using the 6-311++G(d,p) basis set.

	Isomer 1	**EQA-3-II**		**EQA-3-I**		**EQA-3-IV**		**EQC-4-I**		**EQ1-4 W3**	
	r_s	B3LYP[c]	MP2[d]	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
		O1		O1		O1		O1		O1	
$\|a\|$[a]	2.41601(64)	2.155	2.165	2.273	2.373	2.260	2.3023	1.810	1.779	1.949	1.904
$\|b\|$	2.02680(76)	2.113	2.100	2.046	1.994	2.049	2.0379	2.408	2.404	2.342	2.351
$\|c\|$	0.2471(63)	0.421	0.433	0.494	0.394	0.584	0.5464	0.045	0.070	0.245	0.325
		O2		O2		O2		O2		O2	
$\|a\|$	0.00(14)	0.327	0.328	0.094	0.058	0.036	0.0272	0.863	0.881	0.641	0.670
$\|b\|$	3.29759(46)	3.262	3.260	3.157	3.195	3.154	3.2109	3.036	3.037	3.285	3.316
$\|c\|$	0.1559(97)	0.262	0.310	0.549	0.461	0.619	0.5904	0.707	0.733	0.406	0.457

	Isomer 2	**EQA-4-II**		**EQA-4-I**	
	r_s	B3LYP	MP2	B3LYP	MP2
		O1		O1	
$\|a\|$[a]	2.21868(68)	2.206	2.207	1.979	1.876
$\|b\|$	1.75027(87	1.703	1.762	1.591	1.745
$\|c\|$	1.2422(12)	1.328	1.241	1.492	1.428
		O2		O2	
$\|a\|$	0.8278(18)	1.040	0.838	1.696	1.219
$\|b\|$	2.91887(52)	2.718	2.780	2.664	2.773
$\|c\|$	0.9459(16)	1.023	1.026	1.100	1.141

	Isomer 3	**EQC-4-I**	
	r_s	B3LYP	MP2
		O1	
$\|a\|$[a]	1.81352(84)	1.810	1.779
$\|b\|$	2.42823(63	2.408	2.404
$\|c\|$	0.030(51)	0.045	0.070
		O2	
$\|a\|$	0.8932(17)	0.863	0.881
$\|b\|$	3.17782(48)	3.036	3.037
$\|c\|$	0.6607(23)	0.707	0.732

	Isomer 4	**EQC-1-I**		**EQC-3-I**	
	r_s	B3LYP	MP2	B3LYP	MP2
		O1		O1	
$\|a\|$[a]	1.56268(99)	1.693	1.499	1.210	1.123
$\|b\|$	2.64337(59)	2.466	2.546	2.511	2.554
$\|c\|$	0.2860(55)	0.379	0.395	0.315	0.303
		O2		O2	
$\|a\|$	1.4114(11)	1.157	1.413	1.625	1.753
$\|b\|$	2.72564(58)	2.708	2.684	2.663	2.694
$\|c\|$	0.000(19)	0.196	0.112	0.352	0.334

	Isomer 5	**EQC-2-I**		**EQC-2-III**	
	r_s	B3LYP	MP2	B3LYP	MP2
		O1		O1	
$\|a\|$[a]	3.18344(51)	3.114	3.111	2.045	3.029
$\|b\|$	1.5975(10)	1.657	1.639	2.453	1.700
$\|c\|$	0.2966(56)	0.234	0.333	0.465	0.381
		O2		O2	
$\|a\|$	0.8856(18)	0.790	0.822	0.587	0.765
$\|b\|$	2.75224(60)	2.659	2.622	2.757	2.670
$\|c\|$	0.9857(17)	1.032	1.057	0.786	1.071

	Isomer 6	**EQa-4-I**		**EQA-4-II**	
	r_s	B3LYP	MP2	B3LYP	MP2
		O1		O1	
$\|a\|$[a]	1.90799(96)	1.946	1.937	1.939	1.781
$\|b\|$	1.7305(11)	1.632	1.676	1.581	1.661
$\|c\|$	1.5120(12)	1.590	1.541	1.631	1.643
		O2		O2	
$\|a\|$	0.122(14)	0.411	0.374	0.612	0.479
$\|b\|$	3.07631(57)	2.937	2.954	2.924	2.934
$\|c\|$	0.3053(59)	0.383	0.468	0.460	0.544

Table S12 (cont.). Experimental coordinates of the water oxygen atoms for the observed limonene-$(H_2O)_2$ complexes compared with possible equilibrium structures from MP2 and B3LYP-D3BJ calculations using the 6-311++G(d,p) basis set.

	Isomer 7	**EQA-2-I**		**EQA-2-II**		**EQC-2-III**	
	r_s	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
		O1		O1		O1	
$\|a\|$[a]	3.13337(52)	3.057	3.091	2.919	2.917	2.045	3.029
$\|b\|$	1.6332(10)	1.748	1.720	1.717	1.706	2.453	1.700
$\|c\|$	0.4568(36)	0.308	0.264	0.550	0.577	0.465	0.381
		O2		O2		O2	
$\|a\|$	0.8678(18)	0.668	0.698	0.697	0.708	0.587	0.765
$\|b\|$	2.94549(54)	2.943	3.029	2.855	2.862	2.757	2.670
$\|c\|$	0.7069(23)	0.611	0.556	0.806	0.833	0.786	1.071

[a] Absolute co-ordinate values in Å along the principal axis. [b] rs co-ordinate values determined using Kraitchman equations given with costain errors. [c] Co-ordinates determined using B3LYP-D3BJ/6-311++G(d,p) calculation. [d] Co-ordinates determined using MP2/6-311++G(d,p) calculation.

Table S13. Intermolecular stabilising energy contributions (≥0.42 kJ mol^{-1}) for **isomer 1 / EQA-3-II** of limonene-$(H_2O)_2$ from Natural Bond Orbital (NBO) analysis at the B3LYP-D3BJ/6-311++G(d,p) level of theory.

From Limonene to Water1		
Donor	**Acceptor**	**kJ/mol**
BD(1)C3-C4	RY*(1)H30	0.63
BD(1)C3-C4	RY*(2)H30	0.42
BD(1)C3-C4	RY*(4)H30	0.46
BD(2)C3-C4	RY*(4)H30	1.00
BD(2)C3-C4	BD*(1)O11-H30	21.42
BD(1)C6-H19	RY*(1)O11	0.46
From Limonene to Water2		
Donor	**Acceptor**	**kJ/mol**
BD(1)C2-H16	RY*(1)O12	0.71
BD(1)C2-H16	BD*(1)O12-H31	0.50
From Water1 to Limonene		
Donor	**Acceptor**	**kJ/mol**
LP(1)O11	BD*(2)C3-C4	0.54
LP(2)O11	BD*(2)C3-C4	0.59
From Water1 to Water2		
Donor	**Acceptor**	**kJ/mol**
LP(1)O11	BD*(1)O12-H32	0.92
LP(2)O11	RY*(2)O12	0.46
LP(2)O11	RY*(5)H32	0.46
LP(2)O11	BD*(1)O12-H32	45.44
From Water2 to Limonene		
Donor	**Acceptor**	**kJ/mol**
BD(1)O12-H31	RY*(1)H16	2.97
BD(1)O12-H31	RY*(3)H16	0.63
BD(1)O12-H32	RY*(1)H16	0.46
BD(1)O12-H32	BD*(1)C2-H16	0.50
LP(1)O12	BD*(1)C2-H16	1.05
LP(2)O12	RY*(1)H22	0.46
LP(2)O12	BD*(1)C2-H16	2.76
LP(2)O12	BD*(1)C10-H22	7.36

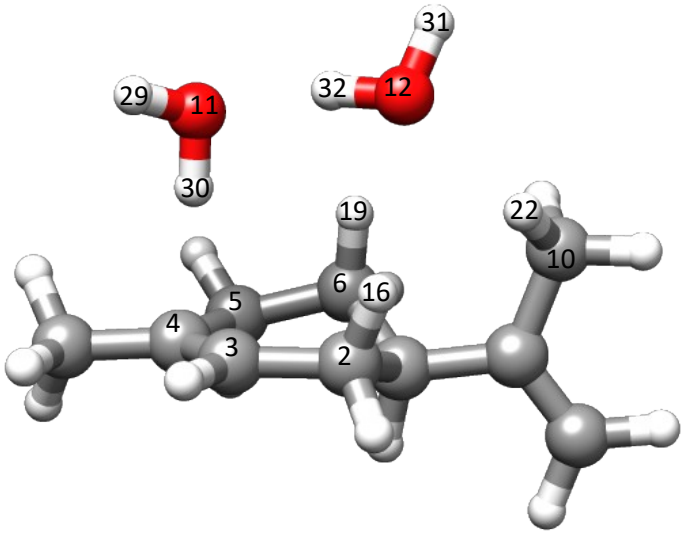


Table S14. Intermolecular stabilising energy contributions (≥0.42 kJ mol^{-1}) for **isomer 2 / EQA-4-II** of limonene-$(H_2O)_2$ from Natural Bond Orbital (NBO) analysis at the B3LYP-D3BJ/6-311++G(d,p) level of theory.

From Limonene to Water1		
Donor	**Acceptor**	**kJ/mol**
BD(1)C4-C5	RY*(1)H30	0.50
BD(1)C4-C5	RY*(2)H30	0.50
BD(1)C4-C5	RY*(4)H30	0.50
BD(2)C4-C5	RY*(4)H30	0.88
BD(2)C4-C5	BD*(1)O11-H30	20.33
From Limonene to Water2		
Donor	**Acceptor**	**kJ/mol**
BD(1)C2-H17	BD*(1)O12-H31	0.59
From Water1 to Water2		
Donor	**Acceptor**	**kJ/mol**
LP(1)O11	BD*(1)O12-H32	0.59
LP(2)O11	RY*(5)H32	0.42
LP(2)O11	BD*(1)O12-H32	44.10
From Water2 to Limonene		
Donor	**Acceptor**	**kJ/mol**
BD(1)O12-H31	RY*(1)H13	0.42
LP(1)O12	BD*(1)C2-H17	2.51
BD(1)O12-H31	RY*(1)H17	2.64
BD(1)O12-H32	RY*(1)H17	0.46
BD(1)O12-H32	BD*(1)C2-H17	0.63
LP(2)O12	BD*(1)C6-H13	5.52
From Water2 to Water1		
Donor	**Acceptor**	**kJ/mol**
BD(1)O12-H32	BD*(1)O11-H29	0.42

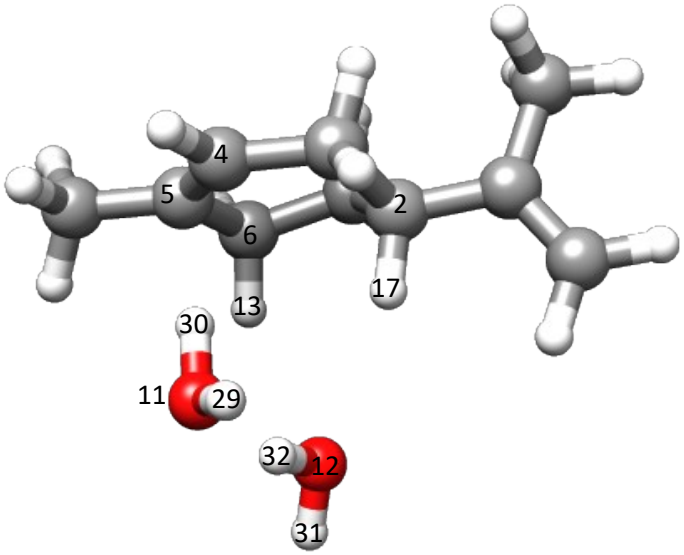


Table S15. Intermolecular stabilising energy contributions (≥0.42 kJ mol^{-1}) for **isomer 3 / EQC-4-I** of limonene-$(H_2O)_2$ from Natural Bond Orbital (NBO) analysis at the B3LYP-D3BJ/6-311++G(d,p) level of theory.

From Limonene to Water1		
Donor	**Acceptor**	**kJ/mol**
BD(1)C1-C6	RY*(1)H30	0.75
BD(1)C1-C6	RY*(4)H30	0.50
BD(2)C1-C6	RY*(4)H30	0.96
BD(2)C1-C6	BD*(1)O11-H30	20.50
From Water1 to Limonene		
Donor	**Acceptor**	**kJ/mol**
LP(1)O11	BD*(2)C1-C6	0.84
From Water1 to Water2		
Donor	**Acceptor**	**kJ/mol**
LP(2)O11	BD*(1)O12-H31	44.81
LP(1)O11	BD*(1)O12-H31	0.88
LP(2)O11	RY*(2)O12	0.63
From Water2 to Limonene		
Donor	**Acceptor**	**kJ/mol**
BD(1)O12-H31	RY*(1)H17	0.84
BD(1)O12-H31	RY*(1)H22	0.88
BD(1)O12-H31	BD*(1)C4-H17	0.79
BD(1)O12-H32	RY*(1)H22	0.50
LP(1)O12	BD*(1)C8-H22	2.09
LP(2)O12	RY*(1)H17	0.46
LP(2)O12	BD*(1)C4-H17	5.56
LP(2)O12	BD*(1)C8-H22	2.68

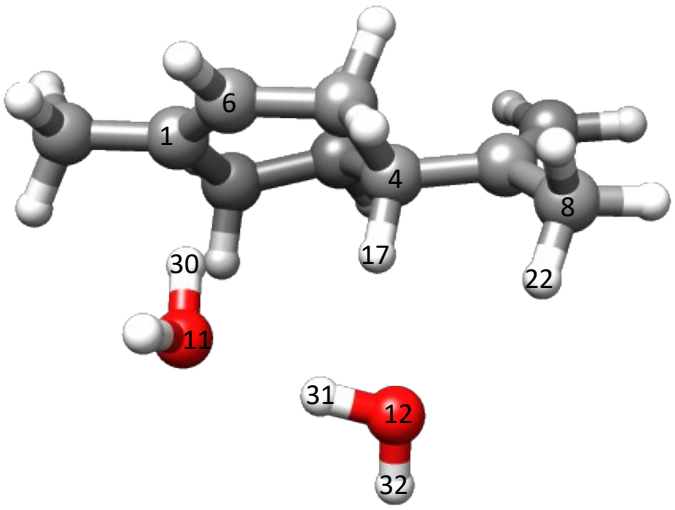


Table S16. Intermolecular stabilising energy contributions (≥0.42 kJ mol^{-1}) for **isomer 4 / EQC-1-I** of limonene-$(H_2O)_2$ from Natural Bond Orbital (NBO) analysis at the B3LYP-D3BJ/6-311++G(d,p) level of theory.

From Limonene to Water1		
Donor	**Acceptor**	**kJ/mol**
BD(1)C3-H16	RY*(1)O11	0.79
BD(1)C3-H16	BD*(1)O11-H29	0.71
BD(1)C7-C10	RY*(1)H30	0.79
BD(2)C7-C10	BD*(1)O11-H30	15.82
BD(1)C7-C10	RY*(4)H30	0.42
BD(2)C7-C10	RY*(4)H30	0.50
From Limonene to Water2		
Donor	**Acceptor**	**kJ/mol**
BD(1)C4-C5	RY*(3)H31	0.50
BD(2)C4-C5	BD*(1)O12-H31	5.69
From Water1 to Limonene		
Donor	**Acceptor**	**kJ/mol**
BD(1)O11-H29	RY*(1)H16	2.80
BD(1)O11-H29	RY*(4)H16	0.59
BD(1)O11-H30	BD*(1)C3-H16	0.42
LP(1)O11	BD*(1)C3-H16	2.55
LP(1)O11	BD*(2)C7-C10	0.67
LP(2)O11	BD*(1)C3-H16	0.96
From Water1 to Water2		
Donor	**Acceptor**	**kJ/mol**
LP(2)O11	RY*(3)O12	0.46
LP(2)O11	BD*(1)O12-H32	30.08
From Water2 to Limonene		
Donor	**Acceptor**	**kJ/mol**
BD(1)O12-H31	RY*(1)H19	0.50
BD(1)O12-H32	RY*(1)H19	0.54
BD(1)O12-H32	BD*(1)C1-H19	0.46
LP(2)O12	BD*(1)C1-H19	2.89

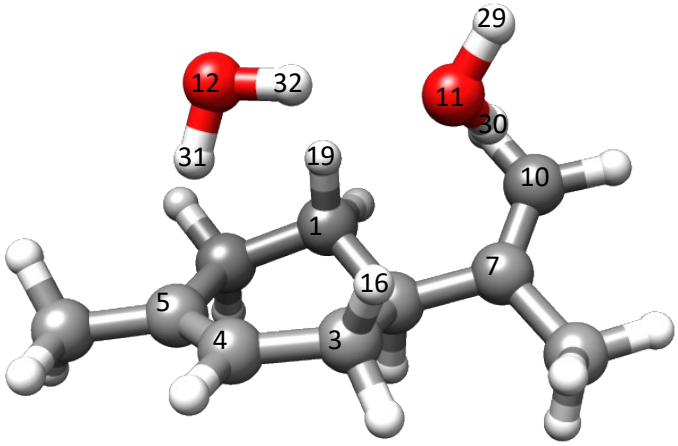


Table S17. Intermolecular stabilising energy contributions (≥0.42 kJ mol^{-1}) for **isomer 5 / EQC-2-I** of limonene-$(H_2O)_2$ from Natural Bond Orbital (NBO) analysis at the B3LYP-D3BJ/6-311++G(d,p) level of theory.

From Limonene to Water1		
Donor	**Acceptor**	**kJ/mol**
BD(1)C8-C9	RY*(1)H30	0.96
BD(1)C8-C9	RY*(4)H30	0.59
BD(2)C8-C9	RY*(4)H30	0.71
BD(2)C8-C9	BD*(1)O11-H30	20.59
From Water1 to Limonene		
Donor	**Acceptor**	**kJ/mol**
LP(2)O11	BD*(2)C8-C9	0.63
From Water1 to Water2		
Donor	**Acceptor**	**kJ/mol**
LP(1)O11	BD*(1)O12-H31	0.54
LP(2)O11	RY*(2)O12	0.46
LP(2)O11	RY*(3)O12	0.46
LP(2)O11	BD*(1)O12-H31	43.51
From Water2 to Limonene		
Donor	**Acceptor**	**kJ/mol**
BD(1)O12-H31	RY*(1)H13	0.42
BD(1)O12-H32	RY*(1)H13	0.79
LP(1)O12	BD*(1)C5-H13	2.18
LP(2)O12	RY*(2)H17	0.42
LP(2)O12	BD*(1)C1-H17	3.93
LP(2)O12	BD*(1)C5-H13	0.79
From Water2 to Water1		
Donor	**Acceptor**	**kJ/mol**
BD(1)O12-H31	BD*(1)O11-H29	0.46

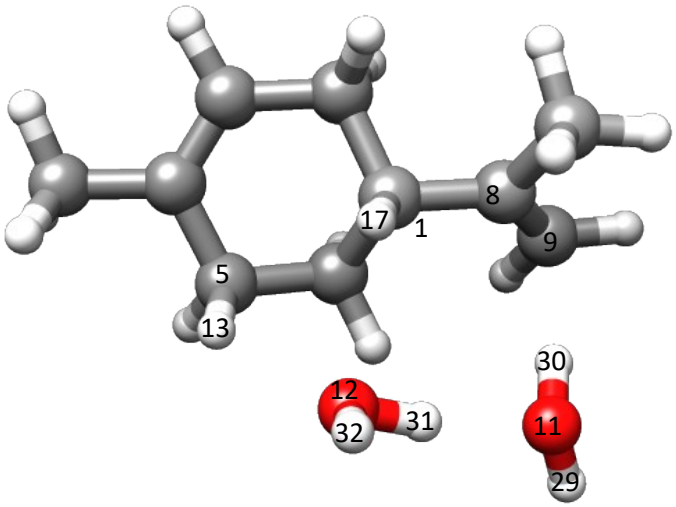


Table S18. Intermolecular stabilising energy contributions (≥0.42 kJ mol^{-1}) for **isomer 6 / EQa-4-I** of limonene-$(H_2O)_2$ from Natural Bond Orbital (NBO) analysis at the B3LYP-D3BJ/6-311++G(d,p) level of theory.

From Limonene to Water1		
Donor	**Acceptor**	**kJ/mol**
BD(1)C4-C5	RY*(1)H32	0.67
BD(1)C4-C5	RY*(4)H32	0.50
BD(2)C4-C5	RY*(4)H32	0.88
BD(2)C4-C5	BD*(1)O11-H32	20.08
From Limonene to Water2		
Donor	**Acceptor**	**kJ/mol**
BD(1)C1-H18	BD*(1)O12-H30	0.75
From Water1 to Limonene		
Donor	**Acceptor**	**kJ/mol**
LP(2)O11	BD*(1)C1-H18	0.46
From Water1 to Water2		
Donor	**Acceptor**	**kJ/mol**
LP(1)O11	BD*(1)O12-H29	0.67
LP(2)O11	RY*(5)H29	0.50
LP(2)O11	BD*(1)O12-H29	43.56
From Water2 to Limonene		
Donor	**Acceptor**	**kJ/mol**
BD(1)O12-H29	RY*(1)H18	0.67
BD(1)O12-H29	BD*(1)C1-H18	0.84
LP(1)O12	BD*(1)C1-H18	2.59
LP(2)O12	BD*(1)C3-H26	3.81
BD(1)O12-H30	RY*(1)H18	2.85
From Water2 to Water1		
Donor	**Acceptor**	**kJ/mol**
BD(1)O12-H29	BD*(1)O11-H31	0.46

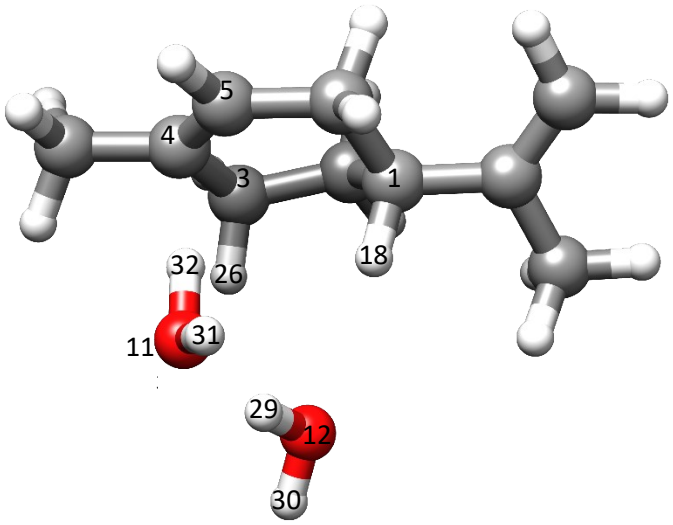


Table S19. Intermolecular stabilising energy contributions (≥0.42 kJ mol^{-1}) for **isomer 7 / EQA-2-I** of limonene-$(H_2O)_2$ from Natural Bond Orbital (NBO) analysis at the B3LYP-D3BJ/6-311++G(d,p) level of theory.

From Limonene to Water1		
Donor	**Acceptor**	**kJ/mol**
BD(1)C8-C9	RY*(1)H30	1.05
BD(1)C8-C9	RY*(4)H30	0.50
BD(2)C8-C9	RY*(4)H30	0.67
BD(2)C8-C9	BD*(1)O11-H30	20.17
From Water1 to Water2		
Donor	**Acceptor**	**kJ/mol**
BD(1)O11-H29	RY*(2)H31	0.46
LP(1)O11	BD*(1)O12-H31	1.17
LP(2)O11	RY*(2)O12	0.50
LP(2)O11	RY*(4)O12	0.42
LP(2)O11	BD*(1)O12-H31	42.59
From Water2 to Limonene		
Donor	**Acceptor**	**kJ/mol**
BD(1)O12-H31	RY*(1)H13	0.54
BD(1)O12-H32	RY*(1)H13	1.09
LP(1)O12	BD*(1)C3-H13	1.38
LP(2)O12	BD*(1)C3-H13	3.60
LP(2)O12	BD*(1)C5-H17	1.26
From Water2 to Water1		
Donor	**Acceptor**	**kJ/mol**
BD(1)O12-H31	BD*(1)O11-H29	0.46
LP(1)O12	RY*(1)O11	0.46

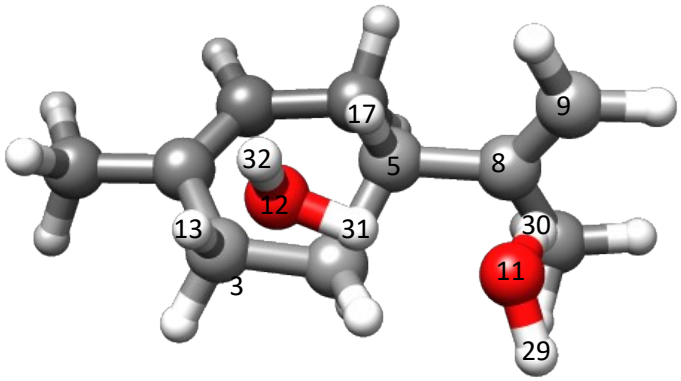
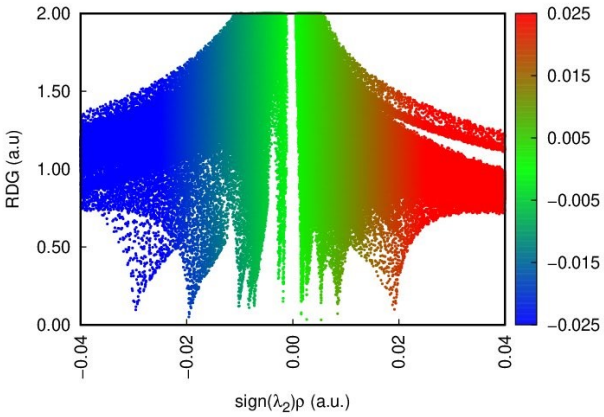
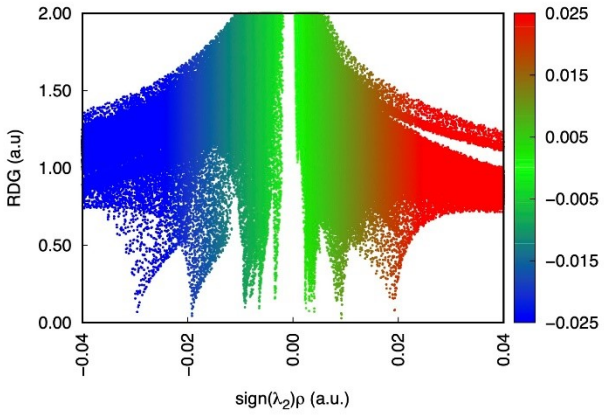


Figure S1. Plots of the reduced density gradient (RDG) versus sign(λ2)ρ for the observed isomers of limonene-$(H_2O)_2$.

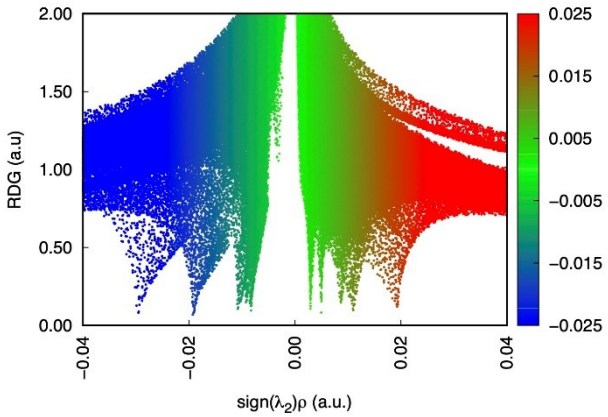
EQA-3-II



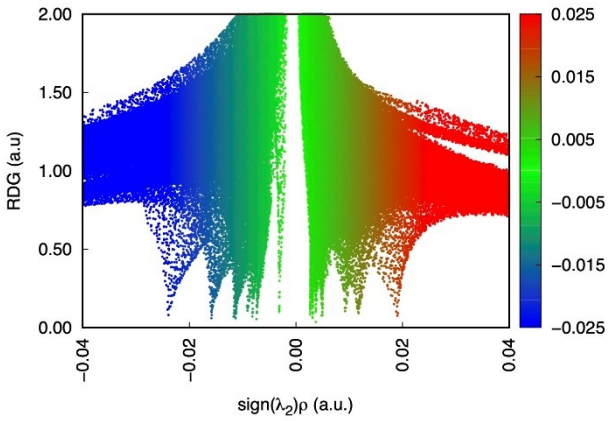
EQA-4-II



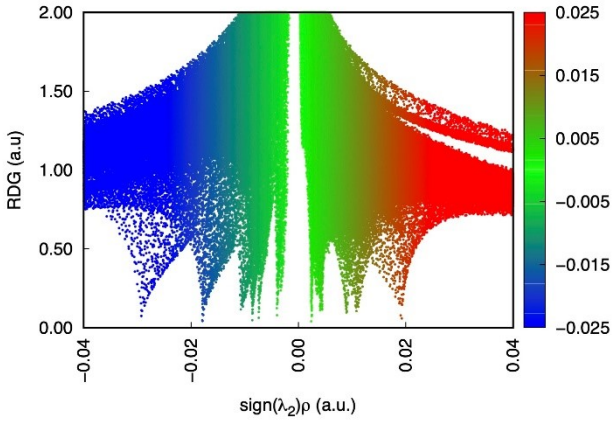
EQC-4-I



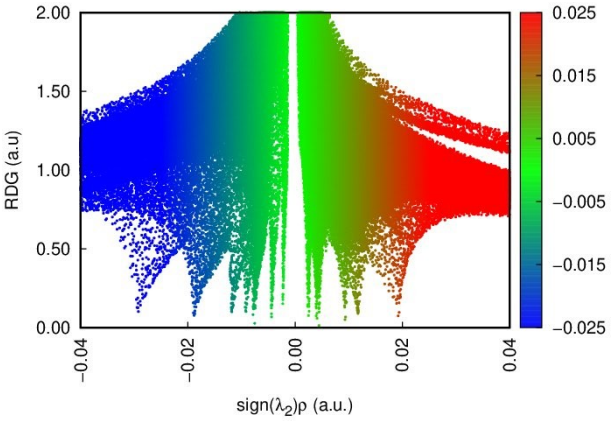
EQC-1-I



EQC-2-I



EQa-4-I



EQA-2-I

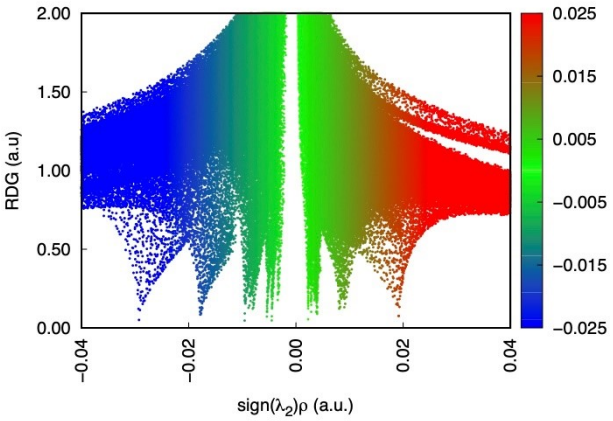

2.00
1.50
1.00
0.50
0.00
RDG (a.u)
−0.04
−0.02
0.00
0.02
0.04
sign(λ2)ρ (a.u.)
0.025
0.015
0.005
−0.005
−0.015
−0.025

Table S20. Cartesian coordinates of **isomer 1 / EQA-3-II** from B3LYP-D3BJ/6-311++G(d,p) calculations.

	X	Y	Z
C	-1.00074	-0.96339	-0.09599
C	-0.26148	-0.21792	-1.22471
C	1.22332	-0.46932	-1.19283
C	1.88246	-1.00457	-0.15521
C	1.16881	-1.36556	1.12726
C	-0.23584	-0.76346	1.22258
C	3.35595	-1.30624	-0.20206
C	-2.45802	-0.56016	-0.01618
C	-3.41578	-1.39165	-0.43293
C	-2.77449	0.80391	0.53967
O	2.10483	2.15273	0.41460
O	-0.39628	3.25291	-0.27911
H	1.11760	-2.46087	1.19947
H	1.77960	-0.22439	-2.09603
H	-0.66042	-0.54015	-2.19219
H	-0.46044	0.85837	-1.16417
H	-0.96673	-2.03296	-0.33589
H	-0.78401	-1.21980	2.05173
H	-0.15761	0.30661	1.44028
H	-4.46383	-1.11321	-0.40236
H	-3.18109	-2.37773	-0.82059
H	-2.17395	1.58705	0.06908
H	-3.83163	1.04229	0.40914
H	-2.55131	0.84410	1.61170
H	3.79675	-1.03142	-1.16276
H	3.53334	-2.37548	-0.04020
H	3.89365	-0.77758	0.59333
H	1.77680	-1.04220	1.98031
H	2.91146	2.49881	0.02036
H	1.99741	1.25830	0.04332
H	-0.64149	3.99850	0.27552
H	0.49242	2.98684	0.01852

Table S21. Cartesian coordinates of **isomer 2 / EQA-4-II** from B3LYP-D3BJ/6-311++G(d,p) calculations.

	X	Y	Z
C	-0.56347	-0.70956	-1.27506
C	-1.01418	-0.03146	0.02970
C	-0.46498	-0.82848	1.22886
C	0.98411	-1.20598	1.05509
C	1.64464	-1.14825	-0.11045
C	0.96346	-0.70018	-1.38213
C	-2.51267	0.17197	0.10948
C	-3.40009	-1.04073	-0.01185
C	3.09635	-1.52167	-0.23062
C	-3.02253	1.39554	0.26609
O	2.20077	1.72760	1.32282
O	1.04157	2.72081	-1.04155
H	1.30711	0.31028	-1.63510
H	1.50610	-1.57099	1.93826
H	-0.59175	-0.24041	2.14537
H	-1.05340	-1.74169	1.38349
H	-0.55267	0.96037	0.04608
H	-1.00105	-0.19192	-2.13253
H	-0.92460	-1.74409	-1.29747
H	-4.09314	1.56293	0.32232
H	-2.38177	2.26847	0.32835
H	-3.16854	-1.79081	0.75098
H	-4.45188	-0.76880	0.09102
H	-3.26978	-1.52861	-0.98311
H	3.53271	-1.78313	0.73558
H	3.67479	-0.69514	-0.65813
H	3.21911	-2.37454	-0.90726
H	1.28994	-1.34831	-2.20394
H	1.83242	1.96797	2.17858
H	1.95357	0.79500	1.18706
H	1.45723	3.50776	-1.40393
H	1.51309	2.53116	-0.21048

Table S22. Cartesian coordinates of **isomer 3 / EQC-4-I** from B3LYP-D3BJ/6-311++G(d,p) calculations.

	X	Y	Z
C	2.02380	-0.81330	0.14463
C	1.31319	-1.20557	-1.13000
C	-0.16829	-1.52592	-0.91414
C	-0.84294	-0.43795	-0.07582
C	-0.16670	-0.37259	1.31072
C	1.33517	-0.45248	1.23632
C	-2.34747	-0.56119	0.06192
C	-3.03121	0.62514	0.69399
C	3.52647	-0.86200	0.11393
C	-3.03723	-1.62897	-0.34568
O	1.78630	2.42036	-0.07867
O	-0.88818	3.01845	-0.76114
H	1.42349	-0.39380	-1.86228
H	1.88220	-0.21828	2.14841
H	-0.45310	0.55117	1.82252
H	-0.54348	-1.19200	1.93823
H	-0.66172	0.52582	-0.56877
H	-0.67003	-1.62618	-1.87972
H	-0.25636	-2.49178	-0.40366
H	-4.11522	-1.67194	-0.23280
H	-2.56519	-2.48889	-0.80421
H	-2.70899	1.55410	0.21445
H	-4.11709	0.53903	0.62358
H	-2.77227	0.71092	1.75517
H	3.96484	-0.52613	1.05618
H	3.91991	-0.23426	-0.69359
H	3.87532	-1.88183	-0.08219
H	1.82622	-2.06840	-1.57040
H	2.22938	2.92094	0.61329
H	1.78787	1.49514	0.22594
H	0.05781	2.90549	-0.55845
H	-0.91733	3.48934	-1.59846

Table S23. Cartesian coordinates of **isomer 4 / EQC-1-I** from B3LYP-D3BJ/6-311++G(d,p) calculations.

	X	Y	Z
C	0.17441	-0.48401	1.31642
C	-0.60938	-1.02817	0.11907
C	-0.03905	-0.45403	-1.20026
C	1.46361	-0.37422	-1.21170
C	2.24714	-0.55451	-0.14333
C	1.65959	-0.83733	1.21847
C	-2.11031	-0.82290	0.19504
C	-2.91149	-1.41032	-0.93858
C	3.74691	-0.49596	-0.22176
C	-2.71523	-0.16914	1.19503
O	-1.70351	2.46160	-0.39705
O	1.14812	2.72586	0.16176
H	1.81787	-1.89833	1.45777
H	1.92412	-0.16123	-2.17386
H	-0.36399	-1.07351	-2.04243
H	-0.46272	0.54023	-1.38783
H	-0.44813	-2.11604	0.08505
H	-0.23654	-0.88326	2.24755
H	0.07735	0.60463	1.35832
H	-3.79530	-0.06797	1.21987
H	-2.16857	0.24479	2.03302
H	-2.65695	-2.46538	-1.08470
H	-3.98338	-1.33666	-0.74934
H	-2.69660	-0.89914	-1.88176
H	4.09373	-0.32852	-1.24328
H	4.19077	-1.42976	0.14243
H	4.13851	0.30710	0.41248
H	2.21992	-0.27629	1.97432
H	-2.26960	3.21058	-0.18623
H	-2.10561	1.69107	0.03616
H	1.52653	1.93724	-0.24535
H	0.20442	2.68428	-0.06019

Table S24. Cartesian coordinates of **isomer 5 / EQC-2-I** from B3LYP-D3BJ/6-311++G(d,p) calculations.

	X	Y	Z
C	0.22682	-0.57047	-0.06392
C	-0.79313	-1.66363	-0.45391
C	-2.20752	-1.14731	-0.47185
C	-2.59228	0.01854	0.05422
C	-1.61399	0.92253	0.76469
C	-0.31118	0.21157	1.13734
C	-4.00870	0.51424	-0.03433
C	1.60981	-1.16073	0.10912
C	2.24943	-1.21488	1.28495
C	2.24997	-1.69895	-1.14501
O	3.08280	1.71483	0.19692
O	0.74242	2.64918	-1.09097
H	-1.38474	1.78405	0.12570
H	-2.94599	-1.77672	-0.96336
H	-0.54955	-2.06790	-1.44172
H	-0.70702	-2.50716	0.24571
H	0.28149	0.13516	-0.90256
H	0.42169	0.94964	1.47352
H	-0.49156	-0.47492	1.97314
H	3.23250	-1.66717	1.36609
H	1.80142	-0.85236	2.20202
H	2.26105	-0.93502	-1.92915
H	3.27420	-2.02941	-0.96498
H	1.68331	-2.54830	-1.53807
H	-4.64564	-0.17373	-0.59425
H	-4.04585	1.49347	-0.52572
H	-4.43995	0.64782	0.96460
H	-2.08891	1.32802	1.66619
H	3.44717	2.15840	0.96894
H	2.86889	0.81108	0.48822
H	1.58617	2.41359	-0.66503
H	0.98412	3.13410	-1.88460

Table S25. Cartesian coordinates of **isomer 6 / EQa-4-I** from B3LYP-D3BJ/6-311++G(d,p) calculations.

	X	Y	Z
C	-0.96074	-0.28005	0.05580
C	-0.45462	-0.50738	-1.38279
C	1.05740	-0.28330	-1.47185
C	1.82393	-0.93044	-0.34350
C	1.20077	-1.38290	0.75389
C	-0.28788	-1.30124	0.97920
C	3.31313	-1.03459	-0.52556
C	-2.47391	-0.24454	0.13238
C	-3.11251	0.97059	-0.49310
C	-3.21489	-1.19007	0.71517
O	1.91953	1.62314	1.63090
O	0.37184	2.94594	-0.32041
H	-4.29631	-1.11109	0.74328
H	-2.78471	-2.06666	1.18280
H	-4.19251	0.97739	-0.33648
H	-2.68713	1.88766	-0.07338
H	-2.92647	1.00990	-1.57083
H	-0.61768	0.71934	0.34956
H	-0.49564	-1.05278	2.02603
H	-0.71970	-2.29742	0.81981
H	1.78900	-1.87469	1.52680
H	3.80217	-1.46731	0.34960
H	3.75188	-0.04840	-0.71391
H	3.55104	-1.65613	-1.39588
H	1.44049	-0.66786	-2.42458
H	1.26690	0.79365	-1.47502
H	-0.70378	-1.53267	-1.68032
H	-0.95882	0.16317	-2.08023
H	0.94597	2.62991	0.40047
H	0.67236	3.83675	-0.51971
H	1.65263	1.60291	2.55507
H	1.83527	0.70526	1.31505

Table S26. Cartesian coordinates of **isomer 7 / EQA-2-I** from B3LYP-D3BJ/6-311++G(d,p) calculations.

	X	Y	Z
C	-2.19183	-1.09483	-0.64682
C	-2.54717	-0.00158	0.03440
C	-1.54118	0.80212	0.82328
C	-0.22997	0.04845	1.05475
C	0.25618	-0.58861	-0.25702
C	-0.78395	-1.62288	-0.73366
C	-3.95943	0.51357	0.04753
C	1.63530	-1.20587	-0.16212
C	2.55630	-0.98301	-1.10881
C	1.92816	-2.09914	1.01527
O	3.01822	1.81493	0.29672
O	0.60212	2.96464	-0.61048
H	-1.32934	1.74062	0.29782
H	-2.95153	-1.64845	-1.19408
H	-0.55752	-1.90840	-1.76669
H	-0.69836	-2.54630	-0.14479
H	0.29457	0.20785	-1.00679
H	0.52557	0.73465	1.44790
H	-0.38522	-0.73414	1.80610
H	3.53338	-1.45424	-1.07695
H	2.34187	-0.35034	-1.96431
H	1.18717	-2.90015	1.09651
H	2.91626	-2.55475	0.93314
H	1.88310	-1.53917	1.95454
H	-4.61889	-0.09421	-0.57559
H	-3.99737	1.54636	-0.31783
H	-4.36302	0.52647	1.06668
H	-1.98259	1.08468	1.78678
H	3.32353	1.81018	1.20886
H	2.91602	0.88130	0.04260
H	1.46426	2.66885	-0.26817
H	0.80102	3.68339	-1.21645

Table S27. Measured frequencies and residuals (in MHz) of the rotational transitions of the parent species of **isomer 1 / EQA-3-II.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	1	1	1	0	2225.8395		-0.0008		
3	1	3	2	1	2	2815.6395		-0.0001		
3	0	3	2	0	2	2924.2405		-0.0006		
3	2	2	2	2	1	3090.1294		-0.0018		
3	2	1	2	2	0	3256.0312		-0.0006		
3	1	2	2	1	1	3304.3425		0.0006		
4	0	4	3	0	3	3783.4761		-0.0005		
4	2	3	3	2	2	4083.3389		0.0012		
4	3	2	3	3	1	4192.9554		0.0009		
4	3	1	3	3	0	4241.1819		-0.0070		
4	1	3	3	1	2	4330.6149		0.0007		
4	2	2	3	2	1	4418.7507		-0.0002		
5	1	5	4	1	4	4599.5010		0.0015		
5	0	5	4	0	4	4631.9765		-0.0010		
5	2	4	4	2	3	5047.7071		0.0024		
5	3	3	4	3	2	5241.4692		0.0003		
5	4	2	4	4	1	5252.6209		0.0001		
5	1	4	4	1	3	5279.8477		-0.0013		
5	3	2	4	3	1	5389.6398		0.0063		
6	1	6	5	1	5	5472.7525		0.0003		
6	0	6	5	0	5	5486.1607		-0.0006		
5	2	3	4	2	2	5555.9945		0.0010		
6	2	5	5	2	4	5981.7957		0.0013		
6	1	5	5	1	4	6152.8771		-0.0020		
6	3	4	5	3	3	6270.7061		0.0013		
6	4	3	5	4	2	6325.6023		0.0022		
7	1	7	6	1	6	6340.6926		0.0009		
7	0	7	6	0	6	6345.7582		-0.0014		
6	4	2	5	4	1	6367.2918		-0.0016		
6	3	3	5	3	2	6583.2769		-0.0008		
6	2	4	5	2	3	6634.1425		0.0018		
7	2	6	6	2	5	6889.0557		0.0063		
7	1	6	6	1	5	6988.6949		-0.0041		
8	1	8	7	1	7	7206.2905		0.0008		
8	0	8	7	0	7	7208.0950		-0.0057		
7	3	5	6	3	4	7271.1175		-0.0002		
7	4	4	6	4	3	7396.4819		-0.0023		
7	4	3	6	4	2	7518.7954		-0.0027		
7	2	5	6	2	4	7630.9362		-0.0029		
8	2	7	7	2	6	7776.4352		0.0055		
8	1	7	7	1	6	7825.0100		0.0014		

Table S28. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{18}O$)($H_2{}^{16}O$) isotopologue of **isomer 1/ EQA-3-II.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	1	3	2	1	2	2770.9011		-0.0026		
3	0	3	2	0	2	2877.9819		-0.0035		
3	2	2	2	2	1	3043.5840		0.0057		
3	2	1	2	2	0	3209.1768		0.0000		
3	1	2	2	1	1	3255.9846		0.0224		
4	1	4	3	1	3	3656.3610		0.0169		
4	0	4	3	0	3	3722.6041		-0.0030		
4	2	3	3	2	2	4021.2693		-0.0033		
4	3	2	3	3	1	4130.7407		-0.0037		
4	3	1	3	3	0	4179.2646		-0.0042		
4	1	3	3	1	2	4265.9986		-0.0015		
4	2	2	3	2	1	4355.4537		-0.0033		
5	1	5	4	1	4	4525.2840		-0.0027		
5	0	5	4	0	4	4556.9383		-0.0006		
5	2	4	4	2	3	4970.1683		-0.0014		
5	3	3	4	3	2	5163.4848		-0.0004		
5	1	4	4	1	3	5199.0531		-0.0025		
5	3	2	4	3	1	5312.2457		-0.0008		
6	1	6	5	1	5	5384.0049		-0.0017		
6	0	6	5	0	5	5396.9981		-0.0037		
5	2	3	4	2	2	5475.7540		-0.0025		
6	2	5	5	2	4	5888.9044		-0.0009		
6	1	5	5	1	4	6056.5984		-0.0024		
6	3	4	5	3	3	6176.8168		-0.0011		
7	1	7	6	1	6	6237.5150		0.0012		
7	0	7	6	0	6	6242.3963		-0.0028		
6	3	3	5	3	2	6489.7070		0.0006		
6	2	4	5	2	3	6536.7532		-0.0028		
7	2	6	6	2	5	6781.0129		0.0023		
7	1	6	6	1	5	6878.0257		-0.0022		
8	1	8	7	1	7	7088.7417		0.0046		
8	0	8	7	0	7	7090.4747		0.0009		
7	3	5	6	3	4	7161.2728		0.0042		
7	2	5	6	2	4	7516.3269		-0.0011		
7	3	4	6	3	3	7663.3319		0.0008		
8	1	7	7	1	6	7700.4919		0.0060		
9	1	9	8	1	8	7939.0769		0.0074		
9	0	9	8	0	8	7939.6519		-0.0117		

Table S29. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{16}O$) ($H_2{}^{18}O$) isotopologue of **isomer 1 / EQA-3-II.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	1	3	2	1	2	2776.1333		-0.0024		
3	0	3	2	0	2	2876.0654		0.0019		
3	2	2	2	2	1	3066.5797		-0.0024		
3	2	1	2	2	0	3257.1088		-0.0014		
3	1	2	2	1	1	3285.2796		0.0004		
4	1	4	3	1	3	3658.2739		0.0020		
4	0	4	3	0	3	3714.2245		-0.0032		
4	2	3	3	2	2	4045.1542		-0.0015		
4	3	2	3	3	1	4172.1989		-0.0002		
4	3	1	3	3	0	4235.7816		0.0023		
4	1	3	3	1	2	4288.7986		0.0008		
4	2	2	3	2	1	4417.7397		0.0016		
5	1	5	4	1	4	4523.4643		0.0000		
5	0	5	4	0	4	4547.6089		0.0015		
5	2	4	4	2	3	4990.4369		0.0035		
5	1	4	4	1	3	5202.8647		0.0002		
5	3	3	4	3	2	5211.0280		-0.0043		
6	1	6	5	1	5	5379.0674		-0.0002		
6	0	6	5	0	5	5388.0707		-0.0008		
5	3	2	4	3	1	5398.9455		-0.0006		
5	2	3	4	2	2	5538.7716		0.0004		
6	2	5	5	2	4	5902.3233		0.0022		
6	1	5	5	1	4	6042.3881		-0.0004		
6	3	4	5	3	3	6224.4732		0.0004		
7	1	7	6	1	6	6230.2525		0.0002		
7	0	7	6	0	6	6233.3379		-0.0012		
6	2	4	5	2	3	6585.8034		-0.0013		
6	3	3	5	3	2	6599.3333		0.0015		
7	2	6	6	2	5	6786.7020		0.0025		
7	1	6	6	1	5	6858.8025		0.0008		
8	1	8	7	1	7	7079.6991		0.0032		
8	0	8	7	0	7	7080.6948		-0.0039		
7	3	5	6	3	4	7202.7999		-0.0003		
7	2	5	6	2	4	7535.4108		-0.0012		
7	3	4	6	3	3	7773.6385		-0.0007		

Table S30. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{18}O$) ($H_2{}^{18}O$) isotopologue of **isomer 1 / EQA-3-II.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	1	3	2	1	2	2733.1916		0.0005		
3	0	3	2	0	2	2831.8659		0.0078		
3	2	2	2	2	1	3021.1502		-0.0004		
3	2	1	2	2	0	3210.4457		-0.0033		
3	1	2	2	1	1	3237.7466		0.0039		
4	1	4	3	1	3	3601.3096		-0.0009		
4	2	3	3	2	2	3984.8223		0.0010		
4	3	2	3	3	1	4111.0861		-0.0014		
4	3	1	3	3	0	4174.4930		-0.0010		
4	1	3	3	1	2	4225.8581		0.0039		
4	2	2	3	2	1	4354.6560		0.0027		
5	1	5	4	1	4	4452.6499		-0.0033		
5	0	5	4	0	4	4476.3478		-0.0003		
5	2	4	4	2	3	4915.4066		0.0005		
5	1	4	4	1	3	5125.0937		0.0026		
5	3	3	4	3	2	5134.5379		-0.0014		
5	4	2	4	4	1	5154.9817		-0.0144		
5	4	1	4	4	0	5170.0237		0.0029		
6	1	6	5	1	5	5294.5269		0.0000		
6	0	6	5	0	5	5303.3358		-0.0028		
5	3	2	4	3	1	5321.7157		-0.0030		
5	2	3	4	2	2	5459.2595		0.0003		
6	2	5	5	2	4	5812.8594		0.0014		
6	1	5	5	1	4	5950.6690		0.0023		
7	1	7	6	1	6	6132.0496		-0.0003		
6	3	4	5	3	3	6132.6743		-0.0005		
7	0	7	6	0	6	6135.0609		-0.0017		
6	4	3	5	4	2	6208.9166		-0.0025		
6	4	2	5	4	1	6270.4702		0.0154		
6	2	4	5	2	3	6490.1770		-0.0042		
6	3	3	5	3	2	6505.4673		0.0008		
7	2	6	6	2	5	6683.0753		0.0035		
7	1	6	6	1	5	6753.7670		0.0004		
8	1	8	7	1	7	6967.8720		0.0090		
8	0	8	7	0	7	6968.8276		-0.0115		
7	3	5	6	3	4	7095.8743		-0.0019		
7	2	5	6	2	4	7424.2212		-0.0066		
7	4	3	6	4	2	7428.3894		0.0011		
8	1	7	7	1	6	7565.6426		0.0063		
7	3	4	6	3	3	7662.7087		-0.0021		

Table S31. Measured frequencies and residuals (in MHz) of the rotational transitions of the parent species of **isomer 2 / EQA-4-II.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	1	1	0	1	2703.0340		-0.0032		
3	0	3	2	1	2	2740.1899		0.0000		
3	1	3	2	1	2	2931.4708		0.0023		
3	0	3	2	0	2	3034.4714		-0.0005		
3	2	2	2	2	1	3120.1613		0.0011		
3	2	1	2	2	0	3205.8666		-0.0047		
3	1	3	2	0	2	3225.7533		0.0028		
3	1	2	2	1	1	3279.9859		0.0017		
2	2	1	1	1	0	3363.2767		-0.0121		
2	2	0	1	1	0	3385.9992		0.0002		
2	2	0	1	1	1	3503.1115		-0.0005		
4	0	4	3	1	3	3779.7695		0.0077		
4	1	4	3	1	3	3887.8062		0.0014		
3	1	2	2	0	2	3925.6012		-0.0020		
4	0	4	3	0	3	3971.0415		0.0011		
4	2	3	3	2	2	4142.3709		-0.0042		
4	3	2	3	3	1	4198.3602		0.0057		
4	3	1	3	3	0	4214.7937		-0.0157		
3	2	2	2	1	1	4286.2096		-0.0027		
4	2	2	3	2	1	4331.2706		-0.0012		
4	1	3	3	1	2	4339.7843		0.0022		
3	2	1	2	1	1	4394.6349		0.0013		
3	2	2	2	1	2	4637.5496		0.0003		
3	2	1	2	1	2	4745.9682		-0.0024		
5	0	5	4	1	4	4777.9024		0.0036		
5	0	5	4	0	4	4885.9434		0.0017		
5	1	5	4	0	4	4940.7228		-0.0008		
4	2	3	3	1	2	5148.6118		0.0087		
5	2	4	4	2	3	5149.9379		0.0018		
4	1	3	3	0	3	5230.9089		-0.0046		
5	3	3	4	3	2	5253.3456		0.0052		
5	3	2	4	3	1	5307.6981		0.0019		
5	1	4	4	1	3	5363.8261		0.0025		
4	2	2	3	1	2	5445.9164		-0.0047		
5	2	3	4	2	2	5461.9769		-0.0007		
6	0	6	5	1	5	5742.7638		0.0001		
6	1	6	5	1	5	5768.5563		0.0013		
6	0	6	5	0	5	5797.5447		-0.0009		
6	1	6	5	0	5	5823.3377		0.0008		
4	2	3	3	1	3	5848.4524		-0.0035		
5	2	4	4	1	3	5958.7458		-0.0114		
6	2	5	5	2	4	6140.6611		0.0034		
6	3	4	5	3	3	6302.9278		-0.0004		
6	1	5	5	1	4	6341.1212		0.0030		
6	3	3	5	3	2	6432.7072		-0.0031		
4	3	2	3	2	2	6447.5784		0.0081		
5	2	3	4	1	3	6568.1108		-0.0059		
6	2	4	5	2	3	6573.4634		-0.0034		
5	1	4	4	0	4	6623.7016		0.0049		
7	0	7	6	1	6	6686.8444		0.0006		
7	1	7	6	1	6	6698.3926		0.0014		
7	0	7	6	0	6	6712.6375		0.0024		
7	1	7	6	0	6	6724.1765		-0.0061		
6	2	5	5	1	4	6735.5845		-0.0068		

7	2	6	6	2	5	7114.0155	-0.0012
7	1	6	6	1	5	7273.2443	0.0006
5	3	2	4	2	2	7334.8492	0.0056
7	3	5	6	3	4	7341.4765	-0.0026
5	3	3	4	2	3	7558.5397	0.0040
7	3	4	6	3	3	7584.8817	-0.0065
8	1	8	7	1	7	7624.6677	-0.0091
8	0	8	7	0	7	7631.2364	0.0019
8	1	8	7	0	7	7636.2326	0.0084
7	2	5	6	2	4	7650.2993	0.0033
6	2	4	5	1	4	7777.7692	0.0094

The $5_{1,5} \leftarrow 4_{1,4}$ transition appeared as a shoulder of a water heptamer transition and cold not be measured adequately.

Table S32. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{18}O$)($H_2{}^{16}O$) isotopologue of **isomer 2 / EQA-4-II.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	1	1	0	1	2661.5586		-0.0094		
3	1	3	2	1	2	2889.1735		-0.0003		
3	0	3	2	0	2	2990.3403		0.0002		
3	1	2	2	1	1	3232.3296		0.0003		
2	2	0	1	1	0	3330.4967		0.0121		
4	0	4	3	1	3	3726.3591		-0.0015		
4	1	4	3	1	3	3831.6673		0.0014		
4	0	4	3	0	3	3913.2201		-0.0018		
4	2	3	3	2	2	4082.3952		-0.0016		
4	2	2	3	2	1	4268.9323		0.0022		
4	1	3	3	1	2	4276.5948		0.0051		
3	2	1	2	1	1	4324.8633		-0.0018		
3	2	2	2	1	2	4563.6554		-0.0064		
5	1	5	4	1	4	4762.8611		0.0004		
5	0	5	4	0	4	4814.9045		0.0030		
5	1	5	4	0	4	4868.1657		-0.0003		
5	2	4	4	2	3	5075.2833		0.0025		
5	1	4	4	1	3	5285.4629		0.0013		
5	2	3	4	2	2	5383.1454		0.0057		
6	0	6	5	1	5	5660.1882		0.0045		
6	1	6	5	1	5	5685.2037		0.0033		
6	0	6	5	0	5	5713.4469		-0.0012		
6	1	6	5	0	5	5738.4530		-0.0119		
4	2	3	3	1	3	5756.8875		0.0028		
6	2	5	5	2	4	6051.5317		0.0011		
6	1	5	5	1	4	6248.1328		-0.0105		
5	2	3	4	1	3	6468.0151		-0.0007		
6	2	4	5	2	3	6478.1898		-0.0022		
5	1	4	4	0	4	6524.8011		-0.0019		
7	0	7	6	1	6	6590.4408		0.0006		
7	1	7	6	1	6	6601.6121		-0.0024		
7	1	7	6	0	6	6626.6352		0.0039		
7	1	6	6	1	5	7166.3966		0.0043		

Table S33. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{16}O$) ($H_2{}^{18}O$) isotopologue of **isomer 2 / EQA-4-II.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	1	1	0	1	2663.7346		-0.0003		
3	0	3	2	1	2	2731.0696		0.0013		
3	1	3	2	1	2	2892.1055		0.0055		
3	0	3	2	0	2	2992.4009		-0.0045		
3	1	3	2	0	2	3153.4392		0.0020		
3	1	2	2	1	1	3256.4868		-0.0016		
2	2	0	1	1	0	3282.5632		-0.0018		
2	2	1	1	1	1	3378.7226		-0.0038		
4	0	4	3	1	3	3747.1906		-0.0071		
4	1	4	3	1	3	3832.4687		0.0004		
3	1	2	2	0	2	3885.9133		0.0026		
4	0	4	3	0	3	3908.2318		0.0024		
4	1	4	3	0	3	3993.5120		0.0119		
4	2	3	3	2	2	4100.7629		0.0039		
3	2	1	2	1	1	4289.1132		-0.0045		
4	1	3	3	1	2	4301.8154		0.0015		
4	2	2	3	2	1	4313.7667		0.0013		
3	2	2	2	1	2	4531.8157		0.0018		
5	1	5	4	1	4	4760.5544		-0.0050		
5	0	5	4	0	4	4805.4135		-0.0033		
5	1	5	4	0	4	4845.8299		-0.0002		
5	1	4	4	1	3	5304.3152		-0.0001		
4	2	2	3	1	2	5346.3984		0.0036		
5	2	3	4	2	2	5436.6041		-0.0069		
6	0	6	5	1	5	5661.7692		-0.0009		
6	1	6	5	1	5	5679.5638		-0.0005		
6	0	6	5	0	5	5702.1846		0.0014		
6	1	6	5	0	5	5719.9677		-0.0098		
6	2	5	5	2	4	6066.7359		0.0059		
6	3	4	5	3	3	6249.5173		-0.0021		
6	1	5	5	1	4	6253.7030		0.0034		
6	3	3	5	3	2	6411.0296		-0.0018		
5	2	3	4	1	3	6481.1905		-0.0015		
6	2	4	5	2	3	6532.5872		-0.0008		
7	0	7	6	1	6	6585.4432		0.0131		
5	1	4	4	0	4	6591.4056		0.0007		
7	0	7	6	0	6	6603.2203		-0.0041		
7	1	7	6	0	6	6610.6807		-0.0014		
7	1	6	6	1	5	7158.3444		-0.0042		
7	3	4	6	3	3	7564.4422		0.0006		
6	2	4	5	1	4	7709.4680		0.0032		

Table S34. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{18}O$) ($H_2{}^{18}O$) isotopologue of **isomer 2 / EQA-4-II.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	1	3	2	1	2	2851.6427		0.0030		
3	0	3	2	0	2	2950.1544		0.0004		
3	1	2	2	1	1	3208.8950		0.0047		
2	2	0	1	1	0	3232.1474		0.0013		
4	0	4	3	1	3	3694.8576		0.0021		
4	1	4	3	1	3	3779.0345		0.0060		
4	0	4	3	0	3	3853.5641		0.0026		
4	2	3	3	2	2	4042.0193		-0.0012		
3	2	1	2	1	1	4224.1500		-0.0040		
4	1	3	3	1	2	4239.2630		-0.0008		
4	2	2	3	2	1	4250.4951		0.0010		
3	2	2	2	1	2	4462.3662		0.0008		
5	0	5	4	1	4	4654.4274		0.0013		
5	1	5	4	1	4	4694.3897		0.0045		
5	1	5	4	0	4	4778.5568		-0.0015		
5	2	4	4	2	3	5020.6093		0.0087		
3	3	0	2	2	0	5097.7595		0.0067		
5	1	4	4	1	3	5227.7856		0.0009		
4	2	2	3	1	2	5265.7607		0.0028		
5	2	3	4	2	2	5356.7967		-0.0033		
6	0	6	5	1	5	5583.1817		-0.0184		
6	1	6	5	1	5	5600.8172		-0.0062		
6	0	6	5	0	5	5623.1510		-0.0082		
6	1	6	5	0	5	5640.7764		-0.0062		
4	2	3	3	1	3	5652.7406		-0.0057		
6	2	5	5	2	4	5980.4693		-0.0032		
6	1	5	5	1	4	6164.3179		-0.0001		
4	3	2	3	2	2	6178.5155		-0.0034		
5	2	3	4	1	3	6383.2919		-0.0021		
6	2	4	5	2	3	6436.9266		0.0034		
7	0	7	6	1	6	6494.2816		0.0053		
7	1	7	6	1	6	6501.6733		-0.0012		
7	0	7	6	0	6	6511.8977		-0.0019		
7	1	7	6	0	6	6519.3152		0.0174		
5	3	3	4	2	3	7272.6008		0.0005		

Table S35. Measured frequencies and residuals (in MHz) of the rotational transitions of the parent species of **isomer 3 / EQC-4-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	0	2	1	0	1	2030.8677		-0.0011		
2	1	1	1	1	0	2248.8860		0.0039		
3	1	3	2	1	2	2843.2301		0.0003		
3	0	3	2	0	2	2944.1993		-0.0005		
3	2	2	2	2	1	3122.2836		0.0042		
3	2	1	2	2	0	3300.3804		0.0006		
3	1	2	2	1	1	3335.1483		-0.0008		
4	1	4	3	1	3	3750.3127		-0.0003		
4	0	4	3	0	3	3809.0137		-0.0004		
4	2	3	3	2	2	4122.7232		-0.0020		
4	3	1	3	3	0	4297.7147		-0.0015		
4	1	3	3	1	2	4363.0346		-0.0014		
4	2	2	3	2	1	4475.1057		0.0009		
5	1	5	4	1	4	4640.8586		0.0001		
5	0	5	4	0	4	4667.1606		-0.0012		
5	2	4	4	2	3	5092.1024		-0.0004		
5	3	3	4	3	2	5298.8775		0.0008		
5	1	4	4	1	3	5307.4300		-0.0005		
5	4	2	4	4	1	5315.3579		0.0040		
5	4	1	4	4	0	5328.1143		-0.0046		
5	3	2	4	3	1	5468.8100		-0.0015		
6	1	6	5	1	5	5521.7176		0.0013		
6	0	6	5	0	5	5531.8816		0.0002		
5	2	3	4	2	2	5615.9902		-0.0004		
6	2	5	5	2	4	6029.7883		-0.0007		
6	1	5	5	1	4	6177.5775		0.0000		
6	3	4	5	3	3	6334.0256		-0.0003		
7	1	7	6	1	6	6397.9376		0.0040		
6	4	3	5	4	2	6401.0229		-0.0008		
7	0	7	6	0	6	6401.5386		-0.0010		
6	4	2	5	4	1	6453.8082		-0.0011		
6	3	3	5	3	2	6679.8814		0.0008		
6	2	4	5	2	3	6689.6498		0.0005		
7	2	6	6	2	5	6940.6550		-0.0001		
7	1	6	6	1	5	7020.1008		-0.0021		
8	1	8	7	1	7	7272.2512		0.0070		
8	0	8	7	0	7	7273.4481		-0.0073		
7	3	5	6	3	4	7336.9540		0.0023		
7	5	3	6	5	2	7468.1063		0.0023		
7	5	2	6	5	1	7480.5446		-0.0013		
7	4	4	6	4	3	7481.7872		0.0029		
7	4	3	6	4	2	7632.4673		-0.0024		
7	2	5	6	2	4	7673.3308		0.0019		
8	2	7	7	2	6	7832.8585		0.0003		
8	1	7	7	1	6	7868.7577		-0.0028		
7	3	4	6	3	3	7873.7992		-0.0003		

Table S36. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{18}O$)($H_2{}^{16}O$) isotopologue of **isomer 3 / EQC-4-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	1	3	2	1	2	2804.1150		0.0018		
3	0	3	2	0	2	2901.4570		-0.0001		
3	2	2	2	2	1	3087.4074		-0.0107		
3	2	1	2	2	0	3273.4011		0.0020		
3	1	2	2	1	1	3300.6819		0.0004		
4	1	4	3	1	3	3696.6190		0.0049		
4	0	4	3	0	3	3751.0648		-0.0022		
4	2	3	3	2	2	4073.9769		0.0014		
4	3	2	3	3	1	4197.9772		0.0046		
4	3	1	3	3	0	4260.1181		0.0047		
4	2	2	3	2	1	4437.5626		0.0020		
5	1	5	4	1	4	4572.5920		0.0008		
5	0	5	4	0	4	4596.0584		-0.0022		
5	2	4	4	2	3	5028.0360		0.0029		
5	1	4	4	1	3	5234.9518		-0.0018		
5	3	3	4	3	2	5243.3295		-0.0006		
5	4	2	4	4	1	5263.2209		-0.0046		
5	4	1	4	4	0	5277.9111		-0.0028		
5	3	2	4	3	1	5426.9247		-0.0030		
6	1	6	5	1	5	5439.2224		-0.0009		
6	0	6	5	0	5	5447.9650		-0.0014		
5	2	3	4	2	2	5562.9971		0.0007		
6	2	5	5	2	4	5949.5106		0.0003		
6	1	5	5	1	4	6085.7864		-0.0010		
6	3	4	5	3	3	6263.8793		-0.0022		
7	1	7	6	1	6	6301.5535		0.0033		
7	0	7	6	0	6	6304.5404		-0.0040		
6	4	3	5	4	2	6338.4900		0.0030		
6	4	2	5	4	1	6398.6891		0.0071		
6	2	4	5	2	3	6616.1459		0.0004		
6	3	3	5	3	2	6629.9452		-0.0022		
7	2	6	6	2	5	6844.1630		0.0019		
7	1	6	6	1	5	6914.2212		-0.0003		
8	1	8	7	1	7	7162.1875		0.0087		
8	0	8	7	0	7	7163.1432		-0.0071		
7	3	5	6	3	4	7250.1418		-0.0034		
7	2	5	6	2	4	7574.1536		0.0024		
7	4	3	6	4	2	7575.9317		-0.0035		
8	1	7	7	1	6	7751.1851		0.0000		
7	3	4	6	3	3	7807.3251		0.0008		

Table S37. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{16}O$) ($H_2{}^{18}O$) isotopologue of **isomer 3 / EQC-4-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	1	3	2	1	2	2800.5570		0.0010		
3	0	3	2	0	2	2893.0013		-0.0013		
3	1	2	2	1	1	3308.1454		-0.0026		
4	1	4	3	1	3	3689.1411		0.0014		
4	0	4	3	0	3	3737.8229		0.0017		
4	2	3	3	2	2	4077.1364		0.0011		
4	3	1	3	3	0	4283.0269		0.0023		
4	2	2	3	2	1	4460.6594		-0.0027		
5	1	5	4	1	4	4561.1750		0.0033		
5	2	4	4	2	3	5026.4674		-0.0003		
5	1	4	4	1	3	5221.4269		-0.0025		
5	3	3	4	3	2	5256.8571		0.0034		
5	4	1	4	4	0	5301.0060		-0.0023		
6	1	6	5	1	5	5424.3493		0.0013		
6	0	6	5	0	5	5431.2987		-0.0030		
5	3	2	4	3	1	5463.9929		0.0035		
6	2	5	5	2	4	5941.7048		-0.0035		
6	1	5	5	1	4	6061.9311		0.0009		
6	3	4	5	3	3	6274.0897		-0.0001		
7	1	7	6	1	6	6283.6914		0.0053		
7	0	7	6	0	6	6285.9373		-0.0031		
6	4	3	5	4	2	6361.8139		-0.0042		
6	2	4	5	2	3	6622.2342		-0.0002		
6	3	3	5	3	2	6674.0141		-0.0008		
7	2	6	6	2	5	6830.0957		-0.0098		
7	1	6	6	1	5	6887.7957		0.0004		
7	3	5	6	3	4	7253.5938		0.0070		
7	4	4	6	4	3	7430.9402		0.0012		
7	2	5	6	2	4	7559.0396		0.0040		
7	4	3	6	4	2	7631.8739		-0.0001		
7	3	4	6	3	3	7844.6749		-0.0012		

Table S38. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{18}O$) ($H_2{}^{18}O$) isotopologue of **isomer 3 / EQC-4-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	1	3	2	1	2	2763.2203		0.0016		
3	0	3	2	0	2	2851.8209		0.0018		
3	2	2	2	2	1	3059.6489		0.0042		
3	2	1	2	2	0	3267.4990		0.0096		
3	1	2	2	1	1	3274.8585		-0.0022		
4	1	4	3	1	3	3637.8239		-0.0010		
4	0	4	3	0	3	3682.6258		-0.0015		
4	2	3	3	2	2	4030.4229		-0.0045		
4	3	2	3	3	1	4170.5218		0.0062		
4	3	1	3	3	0	4248.8178		-0.0051		
4	1	3	3	1	2	4260.8859		-0.0026		
4	2	2	3	2	1	4424.5730		0.0031		
5	1	5	4	1	4	4496.0172		0.0000		
5	0	5	4	0	4	4513.4864		-0.0023		
5	2	4	4	2	3	4964.7609		-0.0026		
5	1	4	4	1	3	5150.2658		0.0001		
5	3	3	4	3	2	5203.8326		-0.0029		
5	4	2	4	4	1	5233.9120		-0.0050		
5	4	1	4	4	0	5254.8239		0.0122		
6	1	6	5	1	5	5345.7510		0.0003		
6	0	6	5	0	5	5351.6707		-0.0017		
5	3	2	4	3	1	5425.8267		0.0060		
5	2	3	4	2	2	5529.8006		0.0005		
6	2	5	5	2	4	5864.3086		-0.0028		
6	1	5	5	1	4	5973.6909		-0.0027		
7	1	7	6	1	6	6191.9720		0.0071		
7	0	7	6	0	6	6193.8142		-0.0018		
6	3	4	5	3	3	6206.4228		-0.0003		
6	4	3	5	4	2	6302.8177		0.0010		
6	4	2	5	4	1	6386.1534		-0.0098		
6	2	4	5	2	3	6548.4982		-0.0035		
6	3	3	5	3	2	6625.9377		0.0032		
7	2	6	6	2	5	6737.3016		-0.0063		
7	1	6	6	1	5	6787.4644		0.0012		
7	3	5	6	3	4	7169.2498		0.0029		
7	4	4	6	4	3	7359.4372		-0.0028		
7	2	5	6	2	4	7459.3382		0.0056		
7	4	3	6	4	2	7581.8361		-0.0020		
8	1	7	7	1	6	7613.7385		0.0045		
7	3	4	6	3	3	7777.7163		-0.0028		

Table S39. Measured frequencies and residuals (in MHz) of the rotational transitions of the parent species of **isomer 4 / EQC-1-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	0	3	2	0	2	3053.1971		0.0023		
3	2	1	2	2	0	3207.8016		0.0051		
2	2	1	1	1	0	3520.8559		-0.0137		
4	1	4	3	1	3	3906.2871		0.0028		
4	0	4	3	0	3	3999.9870		-0.0018		
4	2	3	3	2	2	4158.0892		-0.0053		
4	3	1	3	3	0	4221.7885		-0.0077		
4	2	2	3	2	1	4331.9141		0.0043		
4	1	3	3	1	2	4359.1786		-0.0014		
3	2	2	2	1	1	4447.8280		-0.0025		
5	0	5	4	1	4	4782.0062		0.0067		
5	1	5	4	1	4	4857.5413		-0.0035		
5	0	5	4	0	4	4921.9540		0.0012		
5	1	5	4	0	4	4997.4930		-0.0052		
5	2	4	4	2	3	5172.5561		0.0089		
5	3	3	4	3	2	5266.8095		-0.0045		
5	3	2	4	3	1	5310.9018		-0.0069		
5	1	4	4	1	3	5396.0393		0.0043		
5	2	3	4	2	2	5466.4717		-0.0105		
3	3	0	2	2	1	5631.3105		0.0044		
6	0	6	5	1	5	5761.8131		0.0030		
6	1	6	5	1	5	5799.6696		-0.0031		
6	1	6	5	0	5	5875.2097		-0.0084		
6	2	5	5	2	4	6171.6410		0.0127		
6	3	4	5	3	3	6321.3471		0.0080		
6	1	5	5	1	4	6390.8759		0.0017		
6	3	3	5	3	2	6429.0891		-0.0027		
6	2	4	5	2	3	6588.1571		0.0015		
4	3	2	3	2	1	6609.6149		0.0052		
7	0	7	6	1	6	6717.2507		0.0028		
4	3	1	3	2	2	6722.6166		-0.0026		
7	1	7	6	1	6	6735.2776		-0.0013		
7	0	7	6	0	6	6755.1058		-0.0047		
7	2	6	6	2	5	7154.4087		0.0076		
7	1	6	6	1	5	7340.7560		0.0108		
7	3	4	6	3	3	7576.3855		-0.0159		
8	0	8	7	1	7	7658.4996		0.0030		
8	1	8	7	1	7	7666.7743		-0.0040		
8	0	8	7	0	7	7676.5256		-0.0019		
7	2	5	6	2	4	7681.0088		0.0111		
8	1	8	7	0	7	7684.8027		-0.0066		

Table S40. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{18}O$)($H_2{}^{16}O$) isotopologue of **isomer 4 / EQC-1-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	ν_{obs}-ν_{calc}
4	0	4	3	0	3	3938.1033		-0.0129		
5	1	5	4	1	4	4784.3129		0.0050		
5	0	5	4	0	4	4841.6301		0.0074		
5	1	4	4	1	3	5337.8347		-0.0036		
6	1	6	5	1	5	5709.5291		-0.0071		
6	0	6	5	0	5	5741.1251		-0.0132		
6	1	5	5	1	4	6308.2553		0.0063		
7	1	7	6	1	6	6628.4061		0.0048		
7	0	7	6	0	6	6644.1279		0.0083		
7	1	6	6	1	5	7231.6087		0.0255		

Table S41. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{16}O$)($H_2{}^{18}O$) isotopologue of **isomer 4 / EQC-1-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	ν_{obs}-ν_{calc}
4	1	3	3	1	2	4316.3003		-0.0018		
5	1	5	4	1	4	4783.4077		0.0025		
5	0	5	4	0	4	4841.3752		-0.0059		
5	1	4	4	1	3	5334.6828		0.0033		
6	0	6	5	0	5	5740.8908		-0.0079		
6	1	5	5	1	4	6305.9705		-0.0052		
7	0	7	6	0	6	6643.7831		0.0072		
7	1	6	6	1	5	7230.4154		0.0051		

Table S42. Measured frequencies and residuals (in MHz) of the rotational transitions of the parent species of **isomer 5 / EQC-2-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	1	3	2	1	2	2700.8586		0.0016		
3	0	3	2	0	2	2814.8541		-0.0031		
3	2	2	2	2	1	2878.7850		0.0044		
3	2	1	2	2	0	2942.7043		0.0000		
3	1	2	2	1	1	3035.8060		-0.0002		
4	1	4	3	1	3	3585.0797		0.0016		
4	0	4	3	0	3	3690.8433		-0.0038		
4	3	1	3	3	0	3876.4603		0.0045		
4	2	2	3	2	1	3972.8233		0.0028		
4	1	3	3	1	2	4024.5935		-0.0021		
5	1	5	4	1	4	4459.3497		0.0011		
5	0	5	4	0	4	4539.4748		-0.0042		
5	2	4	4	2	3	4761.2456		0.0075		
5	3	3	4	3	2	4840.4548		0.0011		
5	3	2	4	3	1	4871.4155		-0.0095		
5	1	4	4	1	3	4989.1743		-0.0038		
5	2	3	4	2	2	5018.7494		0.0040		
6	1	6	5	1	5	5324.7968		0.0031		
6	0	6	5	0	5	5376.6934		-0.0041		
6	2	5	5	2	4	5684.1648		0.0064		
6	3	4	5	3	3	5811.9626		-0.0018		
6	3	3	5	3	2	5889.6567		-0.0037		
6	1	5	5	1	4	5919.9663		-0.0069		
6	2	4	5	2	3	6060.7696		0.0060		
7	0	7	6	0	6	6213.5129		-0.0015		
7	2	6	6	2	5	6592.9433		0.0098		
7	3	5	6	3	4	6777.8432		-0.0051		
7	1	6	6	1	5	6810.6216		0.0008		
7	3	4	6	3	3	6935.2549		-0.0056		
8	0	8	7	0	7	7053.4803		-0.0060		
8	2	7	7	2	6	7487.4374		0.0091		
8	1	7	7	1	6	7664.5048		-0.0006		
8	3	6	7	3	5	7734.1044		-0.0007		

Table S43. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{18}O$)($H_2{}^{16}O$) isotopologue of **isomer 5 / EQC-2-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	1	3	2	1	2	2644.8512		0.0041		
3	0	3	2	0	2	2757.2656		0.0059		
3	2	1	2	2	0	2879.5342		-0.0006		
3	1	2	2	1	1	2971.9999		0.0018		
4	1	4	3	1	3	3511.0590		-0.0001		
4	0	4	3	0	3	3616.3423		-0.0045		
4	2	3	3	2	2	3745.5021		0.0039		
4	2	2	3	2	1	3886.8906		-0.0025		
4	1	3	3	1	2	3940.6416		-0.0008		
5	1	5	4	1	4	4367.6551		0.0018		
5	0	5	4	0	4	4448.3894		-0.0027		
5	2	4	4	2	3	4662.2483		0.0023		
5	3	3	4	3	2	4738.1774		0.0106		
5	3	2	4	3	1	4767.1335		-0.0063		
5	1	4	4	1	3	4886.3023		-0.0068		
5	2	3	4	2	2	4910.2838		0.0006		
6	1	6	5	1	5	5215.6459		-0.0002		
6	0	6	5	0	5	5268.6237		-0.0059		
6	2	5	5	2	4	5566.6531		0.0089		
6	3	4	5	3	3	5689.3808		0.0059		
6	3	3	5	3	2	5762.2690		0.0017		
6	1	5	5	1	4	5799.8229		-0.0040		
6	2	4	5	2	3	5930.9055		-0.0059		
7	1	7	6	1	6	6056.8855		-0.0025		
7	0	7	6	0	6	6088.0300		-0.0100		
7	2	6	6	2	5	6457.4469		0.0048		
7	3	5	6	3	4	6635.4141		0.0023		
7	3	4	6	3	3	6783.7980		-0.0043		
8	1	8	7	1	7	6893.3985		-0.0007		
8	0	8	7	0	7	6910.4142		-0.0041		
7	2	5	6	2	4	6933.1282		-0.0004		
8	2	7	7	2	6	7334.4401		0.0113		
8	3	6	7	3	5	7572.4486		0.0117		
8	3	5	7	3	4	7826.9159		-0.0042		
8	2	6	7	2	5	7906.8696		-0.0075		

Table S44. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{16}O$) ($H_2{}^{18}O$) isotopologue of **isomer 5 / EQC-2-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	1	3	2	1	2	2670.4388		-0.0065		
3	0	3	2	0	2	2783.5470		0.0043		
3	2	2	2	2	1	2855.4542		0.0111		
3	2	1	2	2	0	2927.3400		-0.0032		
3	1	2	2	1	1	3016.7308		-0.0022		
4	1	4	3	1	3	3542.7239		0.0048		
4	0	4	3	0	3	3643.4554		-0.0012		
4	2	3	3	2	2	3792.5826		-0.0015		
4	3	1	3	3	0	3850.9535		0.0048		
4	2	2	3	2	1	3956.2140		0.0038		
4	1	3	3	1	2	3995.6749		-0.0024		
5	1	5	4	1	4	4404.2981		-0.0004		
5	0	5	4	0	4	4476.7928		-0.0008		
5	2	4	4	2	3	4717.5204		0.0086		
5	3	3	4	3	2	4805.8534		-0.0009		
5	3	2	4	3	1	4843.9245		-0.0101		
5	2	3	4	2	2	4998.4653		-0.0040		
6	1	6	5	1	5	5256.7249		-0.0040		
6	0	6	5	0	5	5301.2049		0.0000		
6	2	5	5	2	4	5628.0436		0.0037		
6	3	4	5	3	3	5769.3797		0.0003		
6	1	5	5	1	4	5858.7010		-0.0005		
6	3	3	5	3	2	5863.6622		0.0050		
6	2	4	5	2	3	6031.9772		-0.0042		
7	1	7	6	1	6	6102.3596		0.0003		
7	0	7	6	0	6	6126.8470		-0.0098		
7	2	6	6	2	5	6523.0390		0.0016		
7	3	5	6	3	4	6725.5856		0.0003		
7	1	6	6	1	5	6727.1760		0.0005		
8	1	8	7	1	7	6943.5149		0.0052		

Table S45. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{18}O$) ($H_2{}^{18}O$) isotopologue of **isomer 5 / EQC-2-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	1	3	2	1	2	2616.1961		-0.0030		
3	0	3	2	0	2	2727.8264		-0.0074		
3	2	2	2	2	1	2796.1933		0.0135		
3	2	1	2	2	0	2864.5282		0.0022		
3	1	2	2	1	1	2953.6811		-0.0044		
4	1	4	3	1	3	3471.2186		0.0002		
4	0	4	3	0	3	3571.9088		-0.0005		
4	2	2	3	2	1	3870.4958		0.0013		
4	1	3	3	1	2	3913.1017		-0.0036		
5	1	5	4	1	4	4315.9263		-0.0027		
5	0	5	4	0	4	4389.5311		-0.0044		
5	2	4	4	2	3	4620.8736		0.0090		
5	1	4	4	1	3	4846.0671		-0.0036		
6	0	6	5	0	5	5197.6256		-0.0021		
6	2	5	5	2	4	5513.6933		0.0061		
6	3	4	5	3	3	5648.7382		0.0110		
6	3	3	5	3	2	5736.3801		0.0060		
6	1	5	5	1	4	5742.4415		0.0046		
6	2	4	5	2	3	5903.2224		-0.0201		
7	1	7	6	1	6	5980.7898		-0.0076		
7	0	7	6	0	6	6006.4830		-0.0027		
7	2	6	6	2	5	6391.6431		0.0100		
7	1	6	6	1	5	6596.7743		0.0023		
7	3	4	6	3	3	6760.6819		0.0010		
7	2	5	6	2	4	6892.9780		-0.0055		

Table S46. Measured frequencies and residuals (in MHz) of the rotational transitions of the parent species of **isomer 6 / EQa-4-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	1	1	0	1	2727.6721		0.0054		
3	1	3	2	1	2	2990.9915		-0.0060		
3	0	3	2	0	2	3091.9507		-0.0040		
3	2	2	2	2	1	3173.1695		0.0120		
3	2	1	2	2	0	3254.3661		-0.0069		
3	1	2	2	1	1	3328.0363		0.0004		
2	2	0	1	1	0	3407.5197		0.0189		
2	2	1	1	1	1	3499.2241		-0.0218		
4	1	4	3	1	3	3968.2099		-0.0022		
4	0	4	3	0	3	4050.8537		-0.0042		
4	2	3	3	2	2	4214.0201		-0.0048		
4	3	2	3	3	1	4267.0890		0.0027		
4	3	1	3	3	0	4282.2967		-0.0043		
4	2	2	3	2	1	4393.7928		0.0028		
4	1	3	3	1	2	4405.8475		-0.0011		
3	2	1	2	1	1	4433.2197		0.0070		
5	1	5	4	1	4	4934.4143		0.0015		
5	0	5	4	0	4	4988.1042		-0.0037		
5	2	4	4	2	3	5241.0217		-0.0002		
5	3	3	4	3	2	5339.2514		0.0100		
5	3	2	4	3	1	5389.6398		-0.0013		
5	1	4	4	1	3	5450.0423		-0.0111		
4	2	2	3	1	2	5498.9730		0.0064		
5	2	3	4	2	2	5539.4542		0.0021		
6	1	6	5	1	5	5891.8774		0.0142		
6	0	6	5	0	5	5921.5332		-0.0048		
6	2	5	5	2	4	6252.0184		-0.0020		
6	3	4	5	3	3	6406.5449		0.0002		
6	1	5	5	1	4	6449.9445		0.0040		
5	2	3	4	1	3	6632.5648		-0.0053		
6	2	4	5	2	3	6667.8121		0.0076		
7	1	7	6	1	6	6843.3645		0.0010		
7	0	7	6	0	6	6858.1491		-0.0066		
7	2	6	6	2	5	7246.4203		0.0028		
5	3	2	4	2	2	7402.4012		0.0129		
7	1	6	6	1	5	7405.9775		-0.0020		
7	3	5	6	3	4	7463.6503		-0.0029		
5	3	3	4	2	3	7616.6061		-0.0164		
7	3	4	6	3	3	7692.2714		-0.0022		
7	2	5	6	2	4	7763.8153		0.0027		

Table S47. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{18}O$) ($H_2{}^{16}O$) isotopologue of **isomer 6 / EQa-4-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	ν_{obs}-ν_{calc}
3	1	3	2	1	2	2953.1925		0.0045		
3	0	3	2	0	2	3051.7747		-0.0022		
3	1	2	2	1	1	3284.0897		0.0048		
4	1	4	3	1	3	3918.0307		0.0065		
4	0	4	3	0	3	3998.3125		-0.0039		
4	2	3	3	2	2	4159.5009		-0.0088		
4	2	2	3	2	1	4337.1597		0.0136		
4	1	3	3	1	2	4347.4765		-0.0013		
5	1	5	4	1	4	4872.0116		-0.0090		
5	0	5	4	0	4	4923.8648		-0.0059		
5	2	3	4	2	2	5467.4423		-0.0042		
6	1	6	5	1	5	5817.4530		0.0086		
6	2	5	5	2	4	6170.9319		-0.0016		
6	1	5	5	1	4	6363.6669		0.0086		
6	2	4	5	2	3	6580.2498		-0.0071		

Table S48. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{16}O$) ($H_2{}^{18}O$) isotopologue of **isomer 6 / EQa-4-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	ν_{obs}-ν_{calc}
3	1	3	2	1	2	2951.4920		0.0069		
3	0	3	2	0	2	3050.3536		-0.0025		
3	1	2	2	1	1	3311.5033		0.0049		
4	1	4	3	1	3	3911.8739		-0.0033		
4	0	4	3	0	3	3986.3911		-0.0040		
4	2	3	3	2	2	4177.0318		0.0020		
5	1	5	4	1	4	4860.1261		-0.0077		
6	1	6	5	1	5	5799.4417		0.0158		
6	2	5	5	2	4	6181.9112		-0.0112		
6	1	5	5	1	4	6365.9453		-0.0005		
6	2	4	5	2	3	6642.5991		0.0027		
7	2	6	6	2	5	7156.0732		-0.0070		
7	1	6	6	1	5	7290.8042		0.0053		
7	2	5	6	2	4	7714.2000		0.0006		

Table S49. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{18}O$) ($H_2{}^{18}O$) isotopologue of **isomer 6 E/ Qa-4-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	ν_{obs}-ν_{calc}
3	1	3	2	1	2	2915.2068		-0.0099		
3	0	3	2	0	2	3011.7325		0.0038		
3	1	2	2	1	1	3267.7930		0.0038		
4	1	4	3	1	3	3863.9239		-0.0012		
4	0	4	3	0	3	3936.4427		0.0002		
4	2	3	3	2	2	4123.7025		0.0142		
4	1	3	3	1	2	4317.7972		-0.0120		
4	2	2	3	2	1	4330.8945		-0.0001		
5	2	4	4	2	3	5122.7891		-0.0004		
5	1	4	4	1	3	5326.0005		0.0022		
6	2	4	5	2	3	6554.9380		-0.0011		

Table S50. Measured frequencies and residuals (in MHz) of the rotational transitions of the parent species of **isomer 7 / EQA-2-I**.

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	1	1	0	1	2664.4870		0.0056		
3	1	3	2	1	2	2689.7257		-0.0006		
3	0	3	2	0	2	2809.2456		-0.0004		
3	2	2	2	2	1	2917.4929		0.0003		
3	2	1	2	2	0	3025.7391		-0.0002		
3	1	2	2	1	1	3108.4437		-0.0011		
2	2	0	1	1	0	3428.0896		-0.0122		
4	0	4	3	1	3	3447.3140		-0.0065		
2	2	1	1	1	1	3540.0743		-0.0040		
4	1	4	3	1	3	3560.2037		0.0015		
2	2	0	1	1	1	3568.9364		-0.0034		
4	0	4	3	0	3	3653.6341		0.0025		
4	1	4	3	0	3	3766.5226		0.0094		
4	2	3	3	2	2	3867.2938		-0.0032		
4	3	2	3	3	1	3938.0904		0.0069		
4	3	1	3	3	0	3960.1730		0.0028		
4	1	3	3	1	2	4101.4544		-0.0027		
4	2	2	3	2	1	4103.2298		-0.0025		
5	0	5	4	1	4	4361.3692		0.0001		
3	2	1	2	1	1	4367.9952		-0.0090		
5	1	5	4	1	4	4416.7249		0.0013		
5	0	5	4	0	4	4474.2493		-0.0015		
5	1	5	4	0	4	4529.6119		0.0066		
3	2	1	2	1	2	4790.5170		-0.0002		
5	2	4	4	2	3	4798.5555		0.0007		
5	3	3	4	3	2	4928.5414		0.0013		
5	3	2	4	3	1	5000.9558		0.0001		
5	1	4	4	1	3	5048.4358		-0.0012		
5	2	3	4	2	2	5183.5247		-0.0025		
6	0	6	5	1	5	5237.3872		-0.0032		
6	1	6	5	1	5	5262.5961		-0.0059		
6	0	6	5	0	5	5292.7428		-0.0020		
6	1	6	5	0	5	5317.9540		-0.0024		
4	2	2	3	1	2	5362.8103		0.0185		
3	3	1	2	2	1	5475.0398		-0.0079		
6	2	5	5	2	4	5708.7046		-0.0035		
4	2	3	3	1	3	5830.9701		-0.0095		
6	3	4	5	3	3	5911.3285		0.0010		
6	4	3	5	4	2	5928.7734		0.0020		
6	1	5	5	1	4	5936.6738		0.0005		
6	4	2	5	4	1	5942.8097		-0.0047		
6	3	3	5	3	2	6081.8386		-0.0119		
7	0	7	6	1	6	6090.6806		0.0203		
7	1	7	6	1	6	6101.5869		0.0007		
7	0	7	6	0	6	6115.8702		-0.0017		
4	2	2	3	1	3	6204.0452		0.0221		
6	2	4	5	2	3	6236.8222		-0.0109		
4	3	1	3	2	1	6384.3985		-0.0100		
5	2	3	4	1	3	6444.8551		-0.0067		
4	3	2	3	2	2	6495.6367		-0.0019		
5	1	4	4	0	4	6543.8011		-0.0039		
7	2	6	6	2	5	6597.4697		0.0029		

7	1	6	6	1	5	6771.7009	0.0018
7	3	5	6	3	4	6879.3607	0.0103
8	1	8	7	1	7	6936.6725	0.0035
8	0	8	7	0	7	6943.0046	-0.0187
5	3	2	4	2	2	7282.1441	0.0122
5	3	3	4	2	3	7556.8899	0.0080
8	1	7	7	1	6	7579.3905	0.0038

Table S51. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{18}O$) ($H_2{}^{16}O$) isotopologue of **isomer 7 / EQA-2-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	0	3	2	0	2	2753.4052		-0.0097		
3	1	2	2	1	1	3042.8153		-0.0086		
4	1	4	3	1	3	3488.5501		-0.0016		
4	0	4	3	0	3	3582.5004		-0.0005		
4	2	3	3	2	2	3787.0306		0.0056		
4	3	1	3	3	0	3874.7949		0.0065		
4	2	2	3	2	1	4012.6872		0.0034		
4	1	3	3	1	2	4016.4181		0.0013		
5	1	5	4	1	4	4328.4958		-0.0001		
5	0	5	4	0	4	4387.3972		-0.0034		
5	2	4	4	2	3	4700.0244		0.0079		
5	3	3	4	3	2	4823.9963		0.0036		
5	2	3	4	2	2	5070.3444		-0.0069		
6	1	6	5	1	5	5157.9998		0.0039		
6	0	6	5	0	5	5189.4207		0.0031		
6	2	5	5	2	4	5592.8653		0.0097		
6	3	4	5	3	3	5786.7020		-0.0029		
6	1	5	5	1	4	5820.7278		-0.0076		
6	3	3	5	3	2	5946.0365		0.0053		
7	1	7	6	1	6	5980.6090		-0.0106		
7	0	7	6	0	6	5995.7616		-0.0045		
6	2	4	5	2	3	6103.5155		-0.0010		
7	2	6	6	2	5	6465.1062		0.0055		
7	1	6	6	1	5	6642.4894		0.0036		
8	0	8	7	0	7	6806.1277		-0.0026		
7	2	5	6	2	4	7094.2436		-0.0110		
8	1	7	7	1	6	7435.4480		0.0084		

Table S52. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{16}O$) ($H_2{}^{18}O$) isotopologue of **isomer 7 / EQA-2-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	1	3	2	1	2	2656.9559		0.0016		
3	0	3	2	0	2	2772.7014		-0.0025		
3	1	2	2	1	1	3089.0904		0.0068		
4	1	4	3	1	3	3513.7324		0.0049		
4	0	4	3	0	3	3598.9514		-0.0058		
4	2	3	3	2	2	3832.8547		0.0048		
4	3	1	3	3	0	3939.6731		-0.0038		
4	1	3	3	1	2	4068.8022		0.0056		
4	2	2	3	2	1	4091.9396		-0.0035		
5	1	5	4	1	4	4355.8547		-0.0011		
5	0	5	4	0	4	4404.9011		-0.0008		
5	2	4	4	2	3	4750.8717		0.0056		
5	3	2	4	3	1	4983.8150		0.0108		
5	1	4	4	1	3	4995.3148		-0.0080		
5	2	3	4	2	2	5164.7846		-0.0029		
6	1	6	5	1	5	5187.3879		0.0001		
6	2	5	5	2	4	5645.5881		0.0032		
6	1	5	5	1	4	5857.3998		-0.0024		
6	3	4	5	3	3	5868.0014		-0.0118		
7	1	7	6	1	6	6012.4646		-0.0022		
7	0	7	6	0	6	6023.1706		-0.0064		
6	2	4	5	2	3	6202.9052		-0.0076		
7	2	6	6	2	5	6517.4440		0.0116		
7	1	6	6	1	5	6668.2691		0.0012		
7	3	5	6	3	4	6822.7795		0.0057		
7	3	4	6	3	3	7183.0594		-0.0028		
7	2	5	6	2	4	7187.6068		0.0027		
8	1	7	7	1	6	7459.7191		-0.0001		

Table S53. Measured frequencies and residuals (in MHz) of the rotational transitions of the ($H_2{}^{18}O$) ($H_2{}^{18}O$) isotopologue of **isomer 7 / EQA-2-I.**

			J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	1	3	2	1	2	2604.1390		0.0025		
3	1	2	2	1	1	3024.1563		-0.0106		
4	1	4	3	1	3	3444.7291		-0.0100		
4	0	4	3	0	3	3531.1300		0.0113		
4	1	3	3	1	2	3985.4531		-0.0016		
5	1	5	4	1	4	4271.1717		-0.0009		
5	0	5	4	0	4	4322.0183		0.0019		
5	2	4	4	2	3	4654.8509		0.0087		
5	3	3	4	3	2	4791.8707		0.0109		
5	3	2	4	3	1	4873.3122		-0.0111		
5	1	4	4	1	3	4896.8981		-0.0007		
5	2	3	4	2	2	5051.9994		0.0085		
6	1	6	5	1	5	5087.1632		-0.0067		
6	2	5	5	2	4	5533.3117		0.0064		
6	1	5	5	1	4	5746.8043		-0.0037		
7	1	7	6	1	6	5896.6708		-0.0077		
7	0	7	6	0	6	5908.2599		-0.0059		
6	2	4	5	2	3	6071.3533		-0.0016		
7	2	6	6	2	5	6389.7795		0.0114		
7	1	6	6	1	5	6545.4971		-0.0017		
7	3	5	6	3	4	6682.0073		-0.0003		
8	1	8	7	1	7	6702.6812		0.0064		
7	2	5	6	2	4	7040.9602		-0.0059		
8	1	7	7	1	6	7322.4620		-0.0011		