

Electronic Supplementary Material (ESI)

Probing the Microsolvation of a Quaternary Ion: Gas Phase

Vibrational Spectroscopy of $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_{n=0-6, 8}$

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Table S1. Experimental absorption frequencies (cm^{-1}) for bare and microhydrated $(\text{NaSO}_4^-)_2$ dianions (denoted as $[2,n]$)

complex	water bend	sulfate stretching					sulfate bend	libration
	band A	band B	band C	band D	band E	band F	band H	band G
[2,0]	–	–	1167	1083	1050	920	619	–
[2,1]	1706	–	1185	1095	1047	943	626	–
[2,2]	1700	1196	1166	1100	1055	951	627	–
[2,3]	1700	1202	1168	1102	1056	952	631	–
[2,4]	1688	–	1165	1111, 1094	1055	– ^b	627, 611	–
[2,5]	1695	1181 ^a	1172	1114	1058	959	622, 614	810
[2,6]	1683	1188	1174	1116, 1099	1071, 1055	– ^b	617	–
[2,8]	1689	1164	1143	1110	1074	– ^b	616	808

^a Peak resolved as a shoulder.

^b Band not observed with a laser pulse energy of 3 mJ. For higher pulse energies band F is superposed by monomer contributions (band c).

Table S2. Experimental absorption frequencies (cm^{-1}) for microhydrated NaSO_4^- anions (denoted $[1,k]$)

complex	sulfate stretching			water libration
	band a	band b	band c	band d
[1,1]	1234	–	–	–
[1,2]	1236	1038	941	–
[1,3]	1247	1038	943	–
[1,4]	1246	1024	945	865

Table S3. Calculated sulfate stretching frequencies (in cm^{-1}) of representative low-lying isomers for bare and microhydrated $(\text{NaSO}_4^-)_2$ dianions. Harmonic vibrational frequencies are calculated using B3LYP/def2-TZVP. Relative energies (in kJ/mol) include zero-point vibrational energies (ZPE)

complex	Isomers	Relative energies	Bands of sulfate stretching				
			band B	band C	band D	band E	band F
[2,0]	exp		—	1167	1083	1067, 1050	920
	0-a	0.0	—	1186	1081	1033	930
	0-b	10.6	—	1187	1083	1047, 1010	932
[2,1]	exp		—	1185	1095	1047	943
	1-1a	0.0	—	1196	1090	1031	926
	1-0b	0.9	—	1190	1077	1024	927
	1-0c	3.3	1197	1162	1088	1041	928
[2,2]	exp		1196	1166	1100	1055	951
	2-1a	0.0	1207	1161	1090	1045, 1015	928
	2-1b	1.1	1208	1167	1095, 1079	1034, 1014	933
	2-2c	1.3		1207	1093	1027	932
	2-1d	2.4	1206	1173	1095, 1073	1035	935
	2-1e	3.6	1205	1171	1094, 1071	1038	935
[2,3]	exp		1202	1168	1102	1056	952
	3-1a	0.0	—	1172	1096	1037	940
	3-1b	0.1	1180	1165	1093	1044	935
	3-1c	0.2	1179 ^a	1166	1092	1043	939
	3-1d	0.7	—	1168	1094	1034	945
	3-3e	1.4	—	1214	1096	1029	925
	3-2f	2.3	1215	1178	1099	1035	931
[2,4]	exp		—	1165	1111, 1094	1055	— ^b
	4-1a	0.0	—	1176	1110, 1095	1035	942
	4-1b	5.5	—	1173	1108, 1089	1035	939
	4-2c	8.8	—	1180	1103	1038	939
[2,5]	exp		1181 ^a	1172	1114	1058	959
	5-2a	0.0	—	1189	1113, 1097	1033	938
	5-1b	0.1	1182	1164	1107, 1097 ^b	1042, 1017	943
	5-1c	1.3	1183	1157	1109, 1096	1046, 1023	953
	5-3f	8.0	—	1185	1105	1041	937

^a Peak resolved as a shoulder. ^b Band not observed with a laser pulse energy of 3 mJ. For higher pulse energies band F is superposed by monomer contribution (band c).

Table S4. B3LYP/def2-TZVP and MP2/def2-TZVP relative energies of several low-lying isomers for the $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_n$ complexes with $n = 0-5$

Isomers	"class" of isomer	B3LYP	MP2
0-a	C_{2h}	0.0	0.0
0-b	C_{2v}	10.6	9.9
1-1a	1-bridge	0.0	0.0
1-0b		0.9	4.6
1-0c		3.3	7.1
2-1a	1-bridge	0.0	9.1
2-1b	1-bridge	1.1	9.8
2-2c	2-bridge	1.3	0.0
2-1d	1-bridge	2.4	6.7
2-1e	1-bridge	3.6	7.8
3-1a	1-bridge	0.0	14.4
3-1b	1-bridge	0.1	13.9
3-1c	1-bridge	0.2	13.6
3-1d	1-bridge	0.7	14.5
3-3e	3-bridge	1.4	0.0
3-2f	2-bridge	2.3	5.6
4-1a	1-bridge	0.0	—
4-1b	1-bridge	5.5	—
4-2c	2-bridge	8.8	—
5-2a	2-bridge	0.0	—
5-1b	1-bridge	0.1	—
5-1c	1-bridge	1.3	—
5-3f	3-bridge	8.0	—

Table S5. Na–Na, S–S, Na–S, and S–O distances (in Å) of low-lying isomers of NaSO_4^- and $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_n$ complexes with $n = 0-5$ calculated at the B3LYP/def2-TZVP level of theory

Isomers	Na–Na	S–S	Na–S1 Na–S2	S1–O S2–O
$\text{NaSO}_4^- (C_{3v})$	–	–	2.422	1.514, 1.514, 1.514, 1.457
0-a	2.910	4.922	2.859, 2.859 2.859, 2.859	1.520, 1.502, 1.502, 1.467 1.520, 1.502, 1.502, 1.467
1-1a	3.023	4.933	2.962, 2.849 2.916, 2.851	1.519, 1.505, 1.500, 1.464 1.529, 1.500, 1.498, 1.463
1-0b	3.001	5.136	2.853, 2.849 3.334, 2.882	1.524, 1.502, 1.501, 1.465 1.517, 1.506, 1.497, 1.465
2-1a	3.072	5.123	3.404, 2.876 2.860, 2.848	1.513, 1.500, 1.495, 1.474 1.527, 1.502, 1.500, 1.462
2-2c	3.160	4.903	2.929, 2.904 2.929, 2.904	1.526, 1.504, 1.495, 1.461 1.526, 1.504, 1.495, 1.461
3-1a	3.093	5.117	3.388, 2.877 2.869, 2.861	1.514, 1.509, 1.487, 1.471 1.516, 1.509, 1.492, 1.469
3-3e	3.293	4.877	2.914, 2.981 2.988, 2.896	1.523, 1.501, 1.500, 1.459 1.533, 1.502, 1.493, 1.458
4-1a	3.167	5.139	2.888, 2.882 3.322, 2.998	1.519, 1.505, 1.489, 1.469 1.520, 1.509, 1.479, 1.474
5-2a	3.306	5.112	2.966, 2.879 3.388, 2.968	1.516, 1.509, 1.488, 1.467 1.521, 1.514, 1.476, 1.469
5-1b	3.202	5.121	2.902, 2.875 3.315, 3.006	1.521, 1.506, 1.487, 1.469 1.516, 1.501, 1.475, 1.486

Kinetic Energy Release

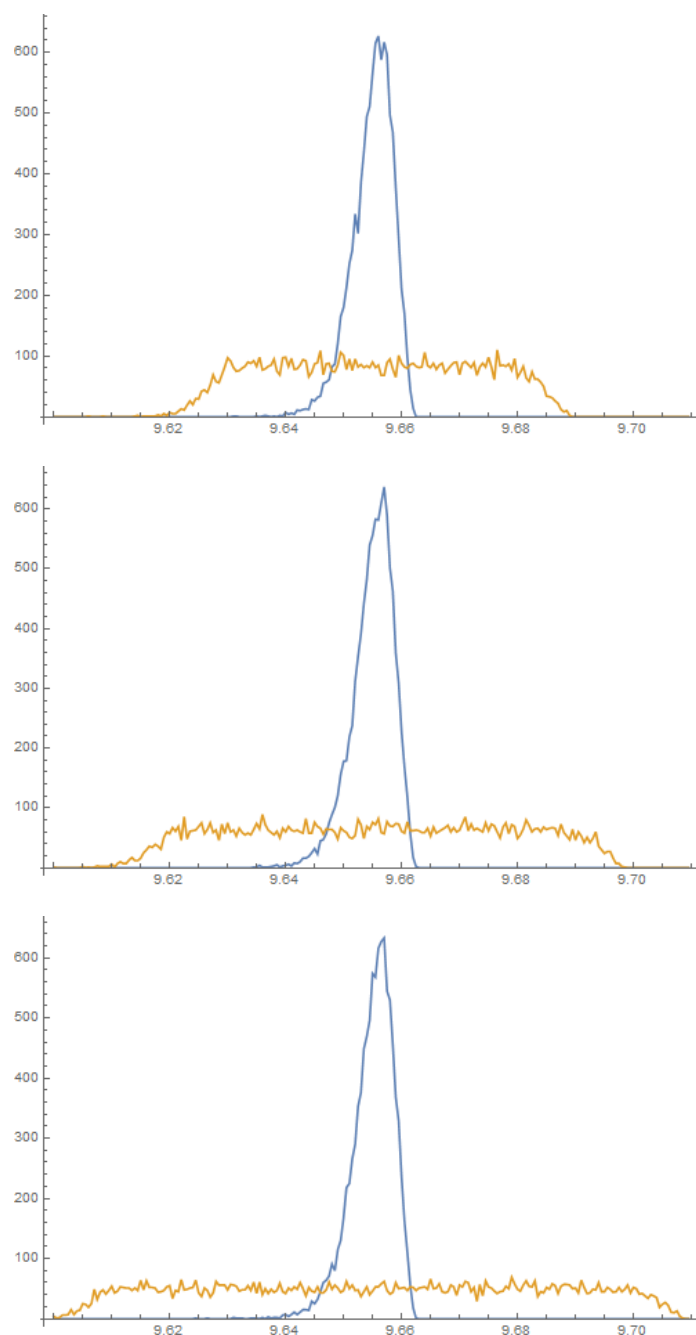


Fig. S1 Simulated arrival time distributions (x-axis: arrival times in μs , y-axis: counts in arb. units) of NaSO_4^- ions produced without (blue trace) and with (orange trace) kinetic energy release prior to acceleration. The simulations were performed for a Wiley-McLaren time-of-flight mass spectrometer with a field-free flight path of 700 mm, acceleration voltages of $U_{\text{ext}} = -3993 \text{ V}$ and $U_{\text{acc}} = -3413 \text{ V}$, a translational temperature of 50 K, an ion cloud diameter of 4 mm and kinetic energy releases of 0.5 eV (top), 0.9 eV (center) and 1.5 eV (bottom).

Dependence of Fragment Ion Yield on the Pulse Energy

IRMPD of the complexes [2,2] and [1,1], corresponding to $m/z = 137$ amu/e, serve as an example to illustrate how the fragmentation yield depends on the applied laser pulse energy. Fig. S1 displays the fragmentation yield in the IR range from $980 - 1380$ cm^{-1} as a function of the laser pulse energy. Two fragmentation channels are observed which correspond to $m/z = 128$ amu/e ($\Delta m = -9$ amu/e) and $m/z = 119$ amu/e ($\Delta m = -18$ amu/e). The former channel is exclusively attributed to loss of a single water molecule from the [2,2] complex leading to [2,1]. The latter channel originates from two processes, i.e. loss of two water molecules from [2,2] and loss of one water molecule from [1,1], resulting in the formation of [2,0] and [1,0], respectively. When pulse energies of ≥ 8 mJ are applied, the mass channel 119 amu/e is predominantly populated (top, Fig. S2), making the assignment of IR bands to [2,2] and [1,1] complexes ambiguous. In contrast, when lower pulse energies of ≤ 3 mJ are used, photofragment ions with $m/z = 128$ amu/e are predominantly formed while contributions to mass channel 119 amu/e are significantly reduced (bottom, Fig. S2). These conditions allow for unambiguously identifying the characteristic IR absorption bands of the dimer dianion complexes: bands B-E are attributed to fragmentation of the [2,2] complex; band a arises exclusively from dissociation of [1,1]. In this manner, IRMPD spectra of the [2, n] complexes with even $n = 2-8$ are measured.

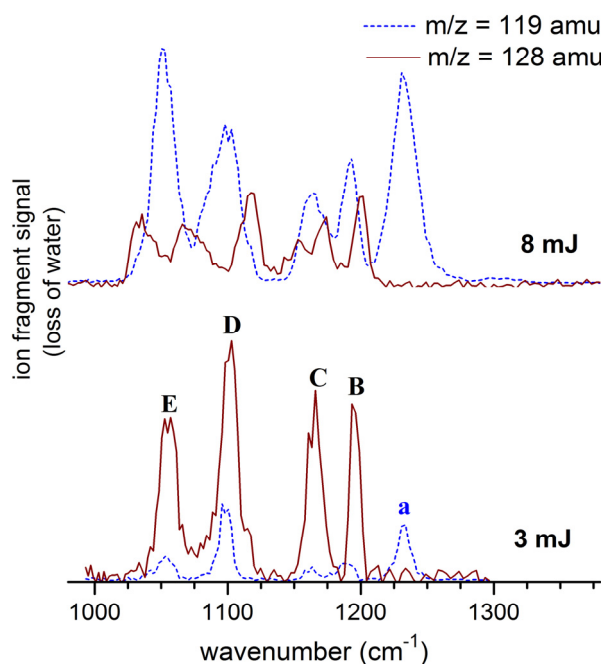


Fig. S2 Photofragment ion yield for $m/z = 137$ amu/e corresponding to [2,2] and [1,1] as a function of the wavenumber for two laser pulse energies. Two fragmentation channels are observed at $m/z = 128$ amu/e (solid trace) and $m/z = 119$ amu/e (dashed trace), corresponding to the formation of [2,1] and [2,0] as well as [1,0], respectively. See text for peak labeling.

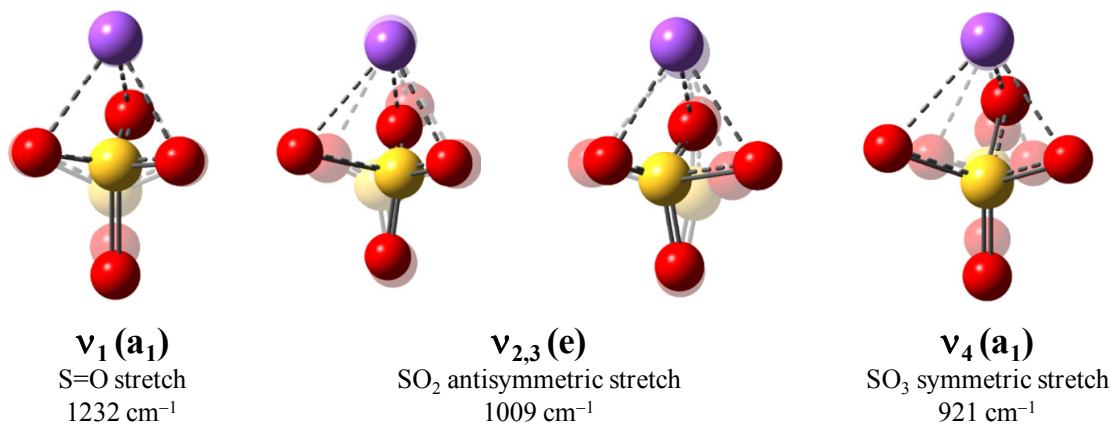


Fig. S3 Fundamental sulfate stretching modes of the C_{3v} isomer of NaSO_4^- (O, red; S, yellow; Na, purple). Given IR frequencies are calculated at the B3LYP/def2-TZVP level of theory.

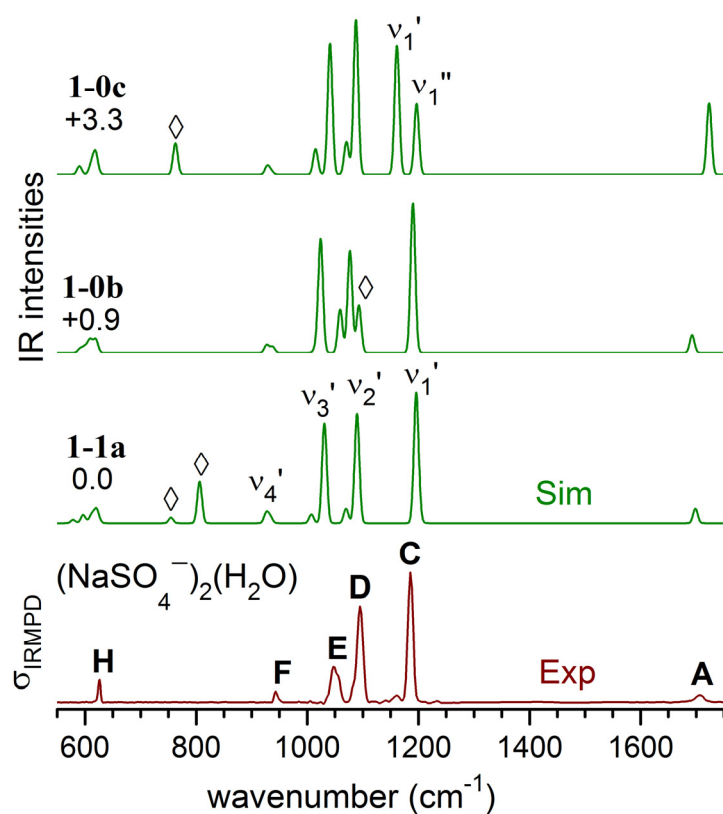


Fig. S4 Comparison between experimental IRMPD spectrum (bottom row) of $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})$ and simulated B3LYP/def2-TZVP vibrational spectra (upper rows) of three energetically low-lying isomers. Calculated water libration modes are denoted with a diamond. Relative energies include ZPE and are given in kJ/mol.

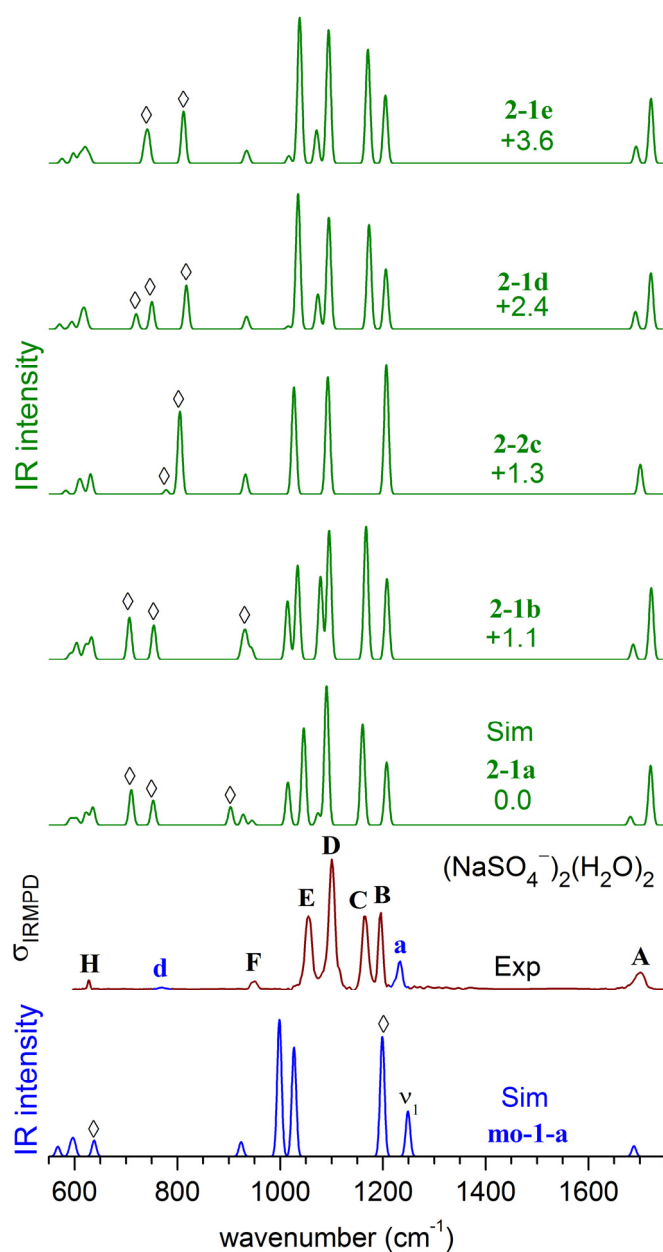


Fig. S5 Comparison between experimental IRMPD spectrum (red trace) of $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_2$ and simulated B3LYP/def2-TZVP vibrational spectra (green trace) of five energetically low-lying isomers. The bottom panel shows the simulated IR spectrum (blue trace) of the most stable isomer of the monomer anion $(\text{NaSO}_4^-)(\text{H}_2\text{O})$. Calculated water libration modes are denoted with a diamond. Relative energies include ZPE and are given in kJ/mol.

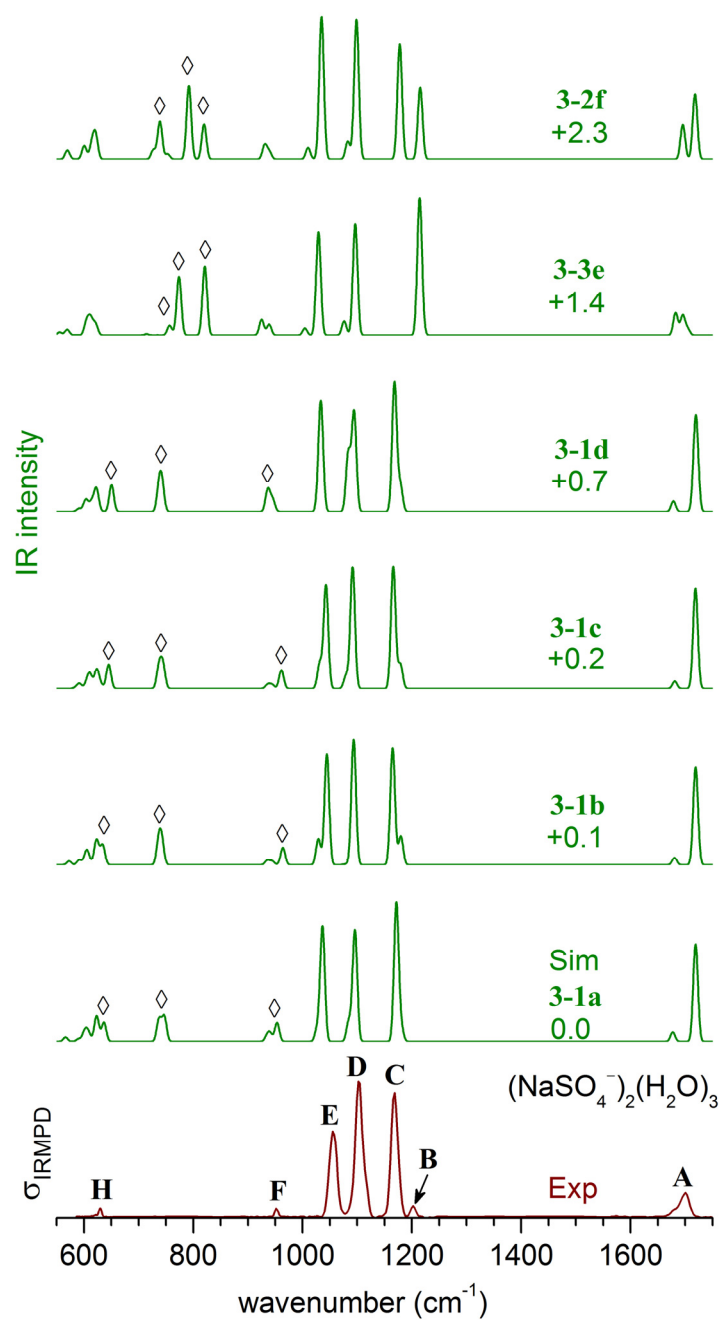


Fig. S6 Comparison between experimental IRMPD spectrum (bottom row) of $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_3$ and simulated B3LYP/def2-TZVP vibrational spectra (upper rows) of six energetically low-lying isomers. Calculated water libration modes are denoted with a diamond. Relative energies include ZPE and are given in kJ/mol.

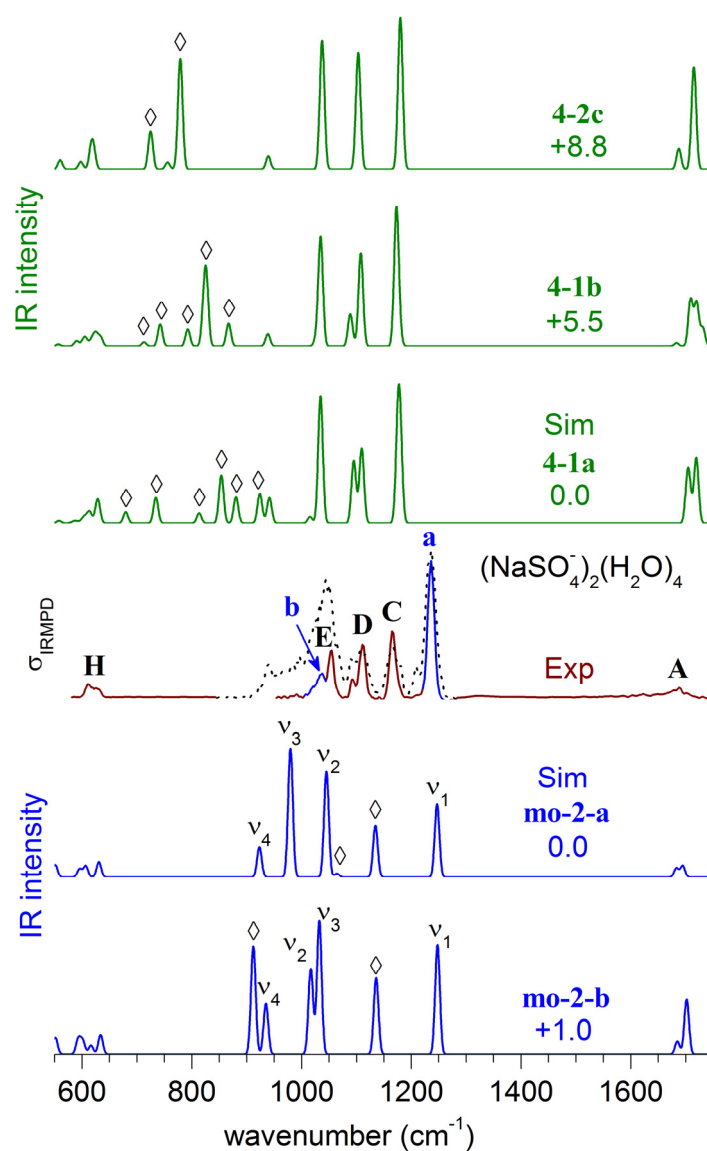


Fig. S7 Comparison between experimental IRMPD spectrum (red trace) of $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_4$ and simulated B3LYP/def2-TZVP vibrational spectra (green trace) of three energetically low-lying isomers. The dashed trace in the experimental plot is recorded with higher laser pulse energies (8 mJ). The bottom panel shows simulated IR spectra (blue trace) of the two most stable isomers of the monomer anion $(\text{NaSO}_4^-)(\text{H}_2\text{O})_2$. Calculated water libration modes are denoted with a diamond. Relative energies include ZPE and are given in kJ/mol.

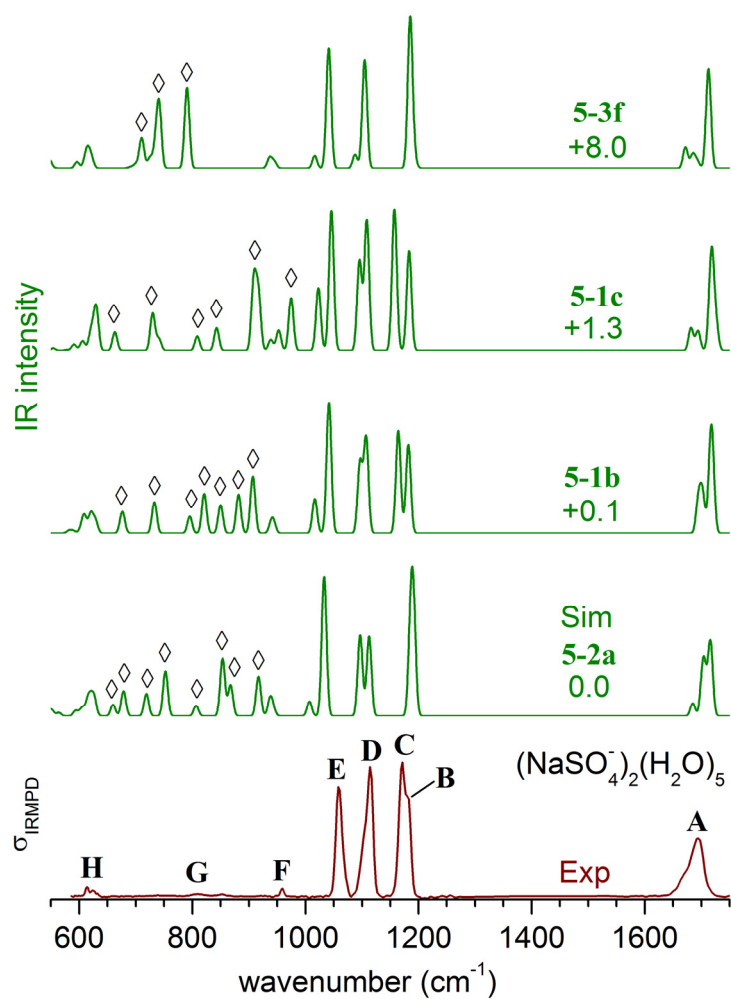


Fig. S8 Comparison between experimental IRMPD spectrum (bottom row) of (NaSO₄)₂(H₂O)₅ and simulated B3LYP/def2-TZVP vibrational spectra (upper rows) of four energetically low-lying isomers. Calculated water libration modes are denoted with a diamond. Relative energies include ZPE and are given in kJ/mol.

Cartesian coordinates for all isomers calculated at the B3LYP/def2-TZVP level of theory:

Cluster: NaSO_4^-

Isomer: C_{3v} structure

Na	0.0000000	0.0000000	-1.9112537
S	0.0000000	0.0000000	0.5108464
O	-0.6967894	1.2068746	-0.0819001
O	-0.6967894	-1.2068746	-0.0819001
O	0.0000000	0.0000000	1.9682373
O	1.3935787	0.0000000	-0.0819001

Cluster: $(\text{NaSO}_4^-)(\text{H}_2\text{O})$

Isomer: mo-1-a

Na	-1.4973350	-1.1046994	0.0017305
S	0.8373661	0.0690257	0.0030210
O	2.2818400	0.2288988	0.0641011
O	0.1471915	1.4052924	-0.1963332
O	0.3974483	-0.8295484	-1.1287585
O	0.2640550	-0.5416287	1.2602757
H	-1.3491180	1.2545395	-0.1505046
O	-2.3681658	1.0176823	-0.0484176
H	-2.6027308	1.4173694	0.7948127

Cluster: $(\text{NaSO}_4^-)_2$

Isomer: 0-a

Na	0.0000000	0.0000000	1.4550487
Na	0.0000000	0.0000000	-1.4550487
S	-0.0036911	2.4612249	0.0000000
S	0.0036911	-2.4612249	0.0000000
O	-0.8170056	2.1744606	1.2302767
O	1.1244498	1.4419205	0.0000000
O	-0.8170056	2.1744606	-1.2302767
O	0.5084004	3.8354264	0.0000000
O	-1.1244498	-1.4419205	0.0000000
O	0.8170056	-2.1744606	-1.2302767
O	0.8170056	-2.1744606	1.2302767
O	-0.5084004	-3.8354264	0.0000000

Cluster: $(\text{NaSO}_4^-)_2$

Isomer: 0-b

Na	0.0000000	-1.4369721	0.1899674
Na	0.0000000	1.4369721	0.1899674
S	-2.4760737	0.0000000	-0.0502396
S	2.4760737	0.0000000	-0.0502396
O	-2.0871718	-1.2279378	-0.8246285

O	-1.6051953	0.0000000	1.1923175
O	-2.0871718	1.2279378	-0.8246285
O	-3.9038327	0.0000000	0.2846561
O	1.6051953	0.0000000	1.1923175
O	2.0871718	1.2279378	-0.8246285
O	2.0871718	-1.2279378	-0.8246285
O	3.9038327	0.0000000	0.2846561

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})$

Isomer: 1-1a

Na	-0.0266570	1.0964181	0.9669242
Na	-0.0036794	-1.4647913	-0.6384013
S	2.4636977	-0.2168976	0.0475271
S	-2.4687993	-0.2095836	0.0530884
O	2.2241799	1.2608835	-0.1098682
O	1.4268160	-0.7018930	1.0464639
O	2.1614511	-0.9199392	-1.2424676
O	3.8256395	-0.4875987	0.5106619
O	-1.4154329	0.3682039	-0.8925063
O	-2.1848969	-1.6811372	0.1107538
O	-2.2096441	0.4143833	1.3902187
O	-3.8234556	0.0666843	-0.4266334
H	-0.6171677	2.0856662	-1.1457624
O	0.0319172	2.7872891	-0.9313352
H	0.8908272	2.3134433	-0.9016614

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})$

Isomer: 1-0b

Na	0.2169845	-1.5263418	-0.1134303
Na	0.2661178	1.4649407	0.1191140
S	2.6656473	-0.0746488	0.0073641
S	-2.4557338	-0.4575974	0.0260820
O	2.3829488	-1.3760765	0.7016608
O	1.6232978	0.0447542	-1.0974175
O	2.4036835	1.0694916	0.9435725
O	4.0272846	-0.0341729	-0.5321586
O	-1.2904038	-0.0258372	0.8960512
O	-2.7088284	0.6584236	-0.9536604
O	-2.0051457	-1.6787826	-0.7131113
O	-3.6469046	-0.7215394	0.8373565
H	-1.9487178	2.9136921	0.7437869
O	-1.6455619	2.9049745	-0.1709986
H	-2.1025254	2.0649082	-0.5293474

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})$

Isomer: 1-0c

Na	0.1714406	-1.3365756	0.2127091
Na	0.5731536	1.5574905	-0.1671788
S	2.7853453	-0.2258963	-0.0290552
S	-2.0674817	0.4731054	0.0752864
O	2.3812919	-1.2992825	0.9408010
O	1.7157564	-0.2229863	-1.1129266
O	2.7002396	1.1205049	0.6323378
O	4.1173982	-0.4711718	-0.5868088
O	-1.0149497	0.4416308	1.1588439
O	-1.6666937	1.5488903	-0.8800786
O	-2.0091771	-1.6787826	-0.7131113
O	-3.4109880	-0.7215394	0.8373565
H	-4.6657065	2.9136921	0.7437869
O	-4.7838855	2.9049745	-0.1709986
H	-3.8669922	2.0649082	-0.5293474

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_2$

Isomer: 2-1a

Na	-0.5880247	1.2688598	0.9539754
Na	-0.5221587	-1.4704790	-0.4353546
S	2.1535162	-0.5368406	0.0547834
S	-2.9447133	-0.0367549	-0.0047579
O	2.4454390	0.7516623	-0.6559552
O	0.9992890	-0.3013638	1.0042823
O	1.6903452	-1.5657153	-0.9255175
O	3.3444387	-0.9937340	0.7925104
O	-1.8018069	0.4150178	-0.9104211
O	-2.7221154	-1.5021325	0.2261422
O	-2.7673554	0.7078000	1.2875204
O	-4.2468184	0.2304826	-0.6128349
H	-0.4000662	1.9150824	-1.3036790
O	0.3061724	2.4525118	-0.9045127
H	1.1083615	1.8665349	-0.9050519
H	4.4922030	1.2324822	-0.4535093
O	5.2971222	0.9198764	-0.0060642
H	4.8970277	0.1419431	0.4302016

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_2$

Isomer: 2-1b

Na	-0.5880247	1.2688598	0.9539754
Na	-0.5221587	-1.4704790	-0.4353546
S	2.1535162	-0.5368406	0.0547834

S	-2.9447133	-0.0367549	-0.0047579
O	2.4454390	0.7516623	-0.6559552
O	0.9992890	-0.3013638	1.0042823
O	1.6903452	-1.5657153	-0.9255175
O	3.3444387	-0.9937340	0.7925104
O	-1.8018069	0.4150178	-0.9104211
O	-2.7221154	-1.5021325	0.2261422
O	-2.7673554	0.7078000	1.2875204
O	-4.2468184	0.2304826	-0.6128349
H	-0.4000662	1.9150824	-1.3036790
O	0.3061724	2.4525118	-0.9045127
H	1.1083615	1.8665349	-0.9050519
H	4.4922030	1.2324822	-0.4535093
O	5.2971222	0.9198764	-0.0060642
H	4.8970277	0.1419431	0.4302016

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_2$

Isomer: 2-2c

Na	-0.0043859	1.1292559	1.1047143
Na	0.0043460	-1.1293378	-1.1048158
S	-2.4516207	0.0163686	0.0052180
S	2.4516353	-0.0163486	-0.0051833
O	-2.1660661	0.4103303	1.4191090
O	-1.3958620	0.7038622	-0.8562700
O	-2.2062832	-1.4572236	-0.1699571
O	-3.8014112	0.3886625	-0.4111220
O	1.3958945	-0.7038123	0.8563542
O	2.1660990	-0.4104631	-1.4190383
O	2.2062445	1.4572388	0.1698823
O	3.8014362	-0.3885697	0.4111807
O	-0.0517457	-3.1116931	0.5269664
H	0.5911671	-2.4463422	0.8459826
H	-0.9099590	-2.6386666	0.5422387
O	0.0517250	3.1117351	-0.5270151
H	0.9099453	2.6387500	-0.5423543
H	-0.5911990	2.4464221	-0.8460865

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_2$

Isomer: 2-1d

Na	0.5566520	1.3004761	0.8818101
Na	0.0672242	-1.4004211	-0.4843315
S	2.7181242	-0.5162290	0.0277957
S	-2.1148998	0.3441772	0.1547049
O	2.7349897	0.9591157	-0.2717641

O	1.6422256	-0.7118546	1.0845436
O	2.2572923	-1.2737343	-1.1811117
O	4.0234326	-0.9773937	0.4981950
O	-1.0324256	0.6235350	-0.8714792
O	-2.1090618	-1.1493682	0.3522903
O	-1.7031919	1.0316490	1.4111426
O	-3.4308015	0.8024712	-0.3162093
H	0.0580526	2.1888091	-1.3163201
O	0.8213829	2.7728563	-1.1429424
H	1.5864185	2.1575663	-1.1021126
H	-3.9659091	-1.8970625	0.0004300
O	-4.8649130	-1.6965229	-0.3185581
H	-4.7307957	-0.7403776	-0.4549169

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_2$

Isomer: 2-1e

Na	-0.1378903	1.2081709	-0.6530141
Na	-0.5204383	-1.6271139	0.4316043
S	-2.7804786	-0.0509305	-0.2470463
S	2.0905707	-0.4925924	0.2385729
O	-2.4735211	1.3507968	0.2077781
O	-1.6596511	-0.4296380	-1.2026289
O	-2.6749427	-0.9942744	0.9143985
O	-4.0890102	-0.1263504	-0.8953315
O	0.9965312	0.0135598	1.1602859
O	1.7289616	-1.8999483	-0.0999143
O	2.0351436	0.3682804	-0.9934588
O	3.4127691	-0.4057738	0.8778315
H	0.2628246	1.7465945	1.6751433
O	-0.3066308	2.5187556	1.4930889
H	-1.1865344	2.1276204	1.2974148
H	3.9457260	0.9368213	-1.5024239
O	4.8706131	0.9611273	-1.1975653
H	4.7291566	0.5018108	-0.3487974

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_2$

Isomer: 3-1a

Na	0.6483233	1.4176084	-0.6499327
Na	-0.3417029	-1.3569741	0.2936981
S	-2.5551151	0.4167282	-0.1901460
S	2.4314907	-0.6601441	0.2079877
O	-2.5209505	1.6421490	0.6521821
O	-1.2893022	0.3669601	-1.0190102
O	-2.5196226	-0.8111580	0.6871046

O	-3.7440774	0.3983007	-1.0554477
O	1.4023315	-0.0018587	1.1053625
O	1.8317587	-1.9482035	-0.2464507
O	2.6105752	0.2640895	-0.9714558
O	3.7075427	-0.8633175	0.9071960
H	0.3884028	1.9077536	1.6844884
O	-0.0759563	2.6338558	1.2396291
H	-1.0062339	2.2994355	1.1053511
H	-4.2793658	-1.8495736	0.4870213
O	-5.0961730	-1.9291909	-0.0369646
H	-4.9470928	-1.1523425	-0.6074619
H	4.6070273	0.6356978	-1.2438230
O	5.5004813	0.5326759	-0.8701409
H	5.2461098	0.0065492	-0.0903628

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_2$

Isomer:3-1b

Na	0.3868508	1.2788905	-0.5987784
Na	0.0268472	-1.6750669	0.2504689
S	-2.5227482	-0.4305498	-0.1658706
S	2.5814105	-0.4099221	0.1782265
O	-2.7719618	0.7498906	0.7261882
O	-1.2924422	-0.1385473	-0.9988275
O	-2.1954856	-1.6326200	0.6598008
O	-3.6882241	-0.6732324	-1.0313067
O	1.4444467	-0.0102627	1.0970464
O	2.2667807	-1.7850207	-0.3091697
O	2.5470239	0.5599592	-0.9770639
O	3.8776928	-0.3533693	0.8672956
H	0.0365922	1.5837483	1.7630577
O	-0.5740266	2.2119304	1.3469563
H	-1.4146238	1.6955130	1.2020474
H	-4.7262205	1.4945406	0.4136312
O	-5.5065692	1.3450504	-0.1465217
H	-5.1497841	0.5914266	-0.6555578
H	4.3920187	1.3957039	-1.2190678
O	5.2871937	1.4972229	-0.8479577
H	5.1724837	0.8999613	-0.0868376

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_3$

Isomer:3-1c

Na	-0.0325562	1.5058643	0.8432351
Na	-0.3599937	-1.3428844	-0.3325078
S	2.4113023	-0.6922435	0.0310725

S	-2.5761422	0.4256473	0.0796854
O	2.8486665	0.5185254	-0.7409006
O	1.3056517	-0.2715733	0.9764561
O	1.8100886	-1.6981859	-0.8958637
O	3.5451317	-1.2574742	0.7797510
O	-1.4448047	0.6516664	-0.9027696
O	-2.5422807	-1.0427905	0.4160212
O	-2.2544304	1.2303499	1.2965889
O	-3.8747130	0.8023109	-0.4951075
H	0.2137963	1.9903157	-1.4957217
O	0.9670948	2.4409098	-1.0822003
H	1.6902019	1.7554002	-1.0481913
H	4.9132429	0.8714921	-0.4194062
O	5.6676820	0.5200904	0.0828158
H	5.1966985	-0.2224779	0.5082424
H	-4.3922760	-1.8541449	0.1371277
O	-5.2882774	-1.7051939	-0.2152434
H	-5.1676548	-0.7714688	-0.4659579

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_3$

Isomer: 3-1d

Na	0.3065786	-1.7727503	0.7885334
Na	0.0066180	1.1432889	-0.2172259
S	-2.5538912	-0.1260534	0.1219176
S	2.5499226	-0.1574449	0.0422162
O	-2.7054262	-1.3435852	-0.7194694
O	-1.3695367	-0.3220940	1.0450347
O	-2.2061772	1.0585832	-0.7444622
O	-3.7759149	0.1414007	0.8961708
O	1.4553649	-0.5564882	-0.9276378
O	2.2249079	1.2496322	0.4714257
O	2.4453094	-1.0791655	1.2132229
O	3.8769945	-0.2228255	-0.5851859
H	0.1499044	-2.2038328	-1.5596990
O	-0.4888596	-2.8226418	-1.1709079
H	-1.3366156	-2.3019139	-1.0977116
H	-3.7794982	2.4184284	-0.7048715
O	-4.6073755	2.6363788	-0.2422739
H	-4.6325472	1.8515953	0.3375211
H	3.8709135	2.4533371	0.2027652
O	4.7661742	2.4948656	-0.1777892
H	4.8144368	1.5692617	-0.4793349

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_3$

Isomer: 3-3e

Na	0.0022938	1.3190915	0.9200073
Na	0.0032485	-1.1009445	-1.3130421
S	-2.4399521	0.0037743	-0.1722137
S	2.4370036	-0.0327858	-0.1624361
O	-2.1635075	0.3708665	1.2558721
O	-1.3890116	0.7231993	-1.0070966
O	-2.1833457	-1.4613791	-0.3728503
O	-3.7903244	0.3782036	-0.5768508
O	1.3592039	-0.7276175	0.6773686
O	2.1732865	-0.4267118	-1.5783561
O	2.1885798	1.4390310	0.0058765
O	3.7735448	-0.4105011	0.2828211
O	-0.0257492	-3.1771562	0.1568137
H	0.6141763	-2.5406087	0.5312195
H	-0.8861935	-2.7153780	0.2273810
O	0.1101240	3.1198423	-0.9048869
H	0.9558604	2.6277884	-0.8695541
H	-0.5464630	2.4463099	-1.1709059
H	0.6024767	-0.4539041	2.4597578
O	-0.0448287	-0.0340818	3.0591283
H	-0.8990085	-0.1421858	2.5932112

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_3$

Isomer: 3-2f

Na	0.5806418	1.2946425	1.0448157
Na	0.0818943	-1.1370212	-0.9764507
S	-2.0904906	0.5008813	0.1750404
S	2.7304100	-0.3280294	-0.0866305
O	-1.6525958	0.9658320	1.5195593
O	-1.0106082	0.9059322	-0.8095079
O	-2.1318461	-1.0059544	0.1378459
O	-3.3944397	1.0615940	-0.2049812
O	1.6284852	-0.7613512	0.8788075
O	2.2942534	-0.7695359	-1.4467642
O	2.7420637	1.1745314	-0.0205151
O	4.0216844	-0.8916857	0.2938817
O	-0.1416855	-2.9274248	0.7893391
H	0.6098818	-2.3460942	1.0309681
H	-0.9248206	-2.3488540	0.8672905
O	0.8380951	3.0824392	-0.7432906
H	1.6113503	2.4796899	-0.7677728
H	0.0856128	2.5180367	-1.0052271
H	-4.0951718	-1.6530296	-0.3485919

O	-4.9591268	-1.2999907	-0.6193167
H	-4.7270350	-0.3526386	-0.5778146

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_4$

Isomer: 4-1a

Na	0.3044158	-1.6046867	0.1050097
Na	-0.4329927	1.3832324	-0.6440560
S	-2.3972401	-0.5852021	0.1135591
S	2.6545380	0.1740672	-0.4429292
O	-1.9404715	-1.8958998	-0.4260390
O	-1.2790479	-0.0852519	1.0126208
O	-2.5117536	0.4220501	-0.9994577
O	-3.6643526	-0.6989529	0.8479352
O	1.3407088	0.0507547	-1.1740330
O	3.1114887	1.5801434	-0.4799063
O	2.3743186	-0.2379847	0.9929066
O	3.6387018	-0.7556688	-1.0253987
O	2.4245261	-2.9256639	0.4542155
H	2.5395801	-2.1183784	1.0024455
H	2.9025037	-2.6075332	-0.3347666
O	0.6432535	1.3795477	2.5002237
H	1.3441801	0.8360847	2.0721746
H	-0.1749207	0.9244067	2.2259061
O	0.9187990	3.1186167	0.2443001
H	0.8182239	2.7538376	1.1478736
H	1.7624375	2.7014698	-0.0597538
H	-4.4728919	0.9963513	-1.2096462
O	-5.3610379	0.9480166	-0.8135490
H	-5.1321692	0.3621338	-0.0692138

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_4$

Isomer: 4-1b

Na	0.2051586	-1.6536639	-0.2554299
Na	-0.5748396	1.5489692	-0.0254110
S	2.2545283	1.1303792	0.0559423
S	-2.5663947	-0.4776827	0.0716987
O	2.5857632	0.2608411	1.2316060
O	1.2824655	0.3608295	-0.8296800
O	1.5319512	2.3507292	0.4993037
O	3.4783646	1.4383230	-0.7020712
O	-1.5784788	-0.1605847	1.1765096
O	-2.5835061	0.7404517	-0.8165600
O	-2.0291857	-1.6446509	-0.6847643
O	-3.9054792	-0.7480332	0.6130493

H	-0.2030930	-1.1078646	2.0427312
O	0.6498858	-1.5876475	2.0829559
H	1.3331275	-0.8966392	1.9318106
H	3.9793555	-0.9381736	0.6068235
O	4.5823936	-1.1948002	-0.1219716
H	4.5532946	-0.3529782	-0.6139925
H	-4.4887323	1.4591523	-0.9692420
O	-5.4008584	1.3801927	-0.6365554
H	-5.2523584	0.6088339	-0.0593713
H	2.0114458	-1.1151145	-1.6561036
O	2.2277213	-2.0747142	-1.6706827
H	3.0695808	-2.0786404	-1.1778406

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_4$

Isomer: 4-2c

Na	0.3955615	1.2599366	0.9413816
Na	-0.3955615	-1.2599366	-0.9413816
S	2.3586284	-0.6186785	-0.2063470
S	-2.3586284	0.6186785	0.2063470
O	2.5341023	0.8779204	-0.2543372
O	1.2840396	-0.8703840	0.8359678
O	1.8278605	-1.1104681	-1.5065302
O	3.6185650	-1.2763690	0.1607539
O	-1.2840396	0.8703840	-0.8359678
O	-2.5341023	-0.8779204	0.2543372
O	-1.8278605	1.1104681	1.5065302
O	-3.6185650	1.2763690	-0.1607539
H	-0.1153177	2.3826028	-1.1350697
O	0.6853502	2.8999421	-0.9178585
H	1.4179538	2.2573314	-0.9993527
H	4.5520651	1.3768864	0.2093215
O	5.3812440	0.9609980	0.4973449
H	5.0706114	0.0360055	0.4919448
H	-4.5520651	-1.3768864	-0.2093215
O	-5.3812440	-0.9609980	-0.4973449
H	-5.0706114	-0.0360055	-0.4919448
H	0.1153177	-2.3826028	1.1350697
O	-0.6853502	-2.8999421	0.9178585
H	-1.4179538	-2.2573314	0.9993527

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_4$

Isomer: mo-2-a

Na	1.6652214	0.2240653	0.3840526
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S	-1.0083283	-0.1335817	0.0125522
O	-2.2876527	-0.8164775	-0.0735876
O	-1.1582702	1.3561983	-0.1361072
O	-0.2882945	-0.4047554	1.3051813
O	-0.0512772	-0.5830880	-1.0882800
H	0.2146213	2.0741262	-0.1565226
O	1.1928406	2.4068486	-0.2003982
H	1.3138157	2.6162697	-1.1317762
H	1.1130780	-1.6582505	-0.7022879
O	1.9533173	-2.0442468	-0.2876125
H	1.6016038	-2.5358730	0.4635698

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_4$

Isomer: mo-2-b

Na	1.7163685	0.0336939	-0.0367558
S	-0.9862544	-0.0236420	0.0064060
O	-2.3677758	0.4166279	0.0871713
O	-0.8864187	-1.5133389	-0.1907434
O	-0.2448880	0.6271856	-1.1511189
O	-0.1888532	0.3294752	1.2392842
H	0.5539802	-2.0445727	-0.1203273
O	1.5631503	-2.2586515	-0.0180811
H	1.6138800	-2.7171130	0.8260872
H	0.9278735	2.2516642	0.8481253
O	1.3944643	2.4272358	0.0138972
H	0.7228256	2.0406769	-0.6083742

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_5$

Isomer: 5-2a

Na	-0.3917549	1.6441618	0.0220087
Na	0.4564008	-1.5430055	-0.1997137
S	2.3316309	0.7244421	0.1764791
S	-2.6646526	-0.2313279	-0.3282606
O	1.8317104	1.9508114	-0.5009342
O	1.2297109	0.2634191	1.1105223
O	2.5061729	-0.3834276	-0.8326387
O	3.5837179	0.9600670	0.9042117
O	-1.3219682	-0.2255399	-1.0287957
O	-3.0718268	-1.6231301	-0.0533169
O	-2.4337454	0.5046675	0.9830545
O	-3.6503304	0.5061661	-1.1304787
O	-2.5186469	3.0221882	-0.0499707
H	-2.6695035	2.2901710	0.5910716
H	-2.9443145	2.6149465	-0.8232367
O	-0.7569116	-0.6650617	2.9307454
H	-1.4423650	-0.2637740	2.3512950
H	0.0726114	-0.3196773	2.5526012
O	-0.9279726	-2.9079167	1.1465109

H	-0.8620409	-2.3335685	1.9361803
H	-1.7594956	-2.5895269	0.7182356
H	4.5341598	-1.0723264	-0.8059552
O	5.3586291	-0.9447736	-0.3089994
H	5.0413542	-0.2483656	0.2960556
H	-0.1518094	-0.8935952	-2.5040973
O	0.6702007	-1.3611411	-2.7356869
H	1.3840844	-0.8337738	-2.3231959

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_5$

Isomer: 5-1b

Na	0.2399944	-1.5178071	0.0529321
Na	-0.8569715	1.4109292	-0.6354685
S	-2.5539999	-0.7496575	0.2119903
S	2.3418775	0.5460920	-0.5468697
O	-2.0062168	-2.0166780	-0.3417045
O	-1.4398109	-0.1367975	1.0461142
O	-2.8187747	0.2322108	-0.8993233
O	-3.7642438	-0.9695132	1.0146667
O	1.0428560	0.2891526	-1.2542780
O	2.6721152	1.9825662	-0.5908611
O	2.1414268	0.0963989	0.8872595
O	3.4077078	-0.2901989	-1.1566868
O	4.2137120	-1.6821782	1.3133803
H	3.4762510	-1.0443656	1.4507031
H	4.5078687	-1.3637783	0.4449108
O	0.2983984	1.5532856	2.4731120
H	1.0393522	1.0804483	2.0354278
H	-0.4716584	1.0063264	2.2231058
O	0.3256250	3.2913244	0.2074612
H	0.2931478	2.9234612	1.1154255
H	1.2010038	2.9780951	-0.1203230
H	-4.8396611	0.6392045	-0.9970480
O	-5.6899786	0.5231465	-0.5377854
H	-5.3627981	-0.0384710	0.1884811
H	2.5710242	-2.0502283	-1.0503393
O	2.2374748	-2.8247080	-0.5474986
H	2.8273041	-2.7921609	0.2266237

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_5$

Isomer: 5-1c

Na	0.1574324	-1.5722607	0.1135650
Na	-0.8096384	1.4020767	-0.6082834
S	-2.5927888	-0.7520352	0.0639010

S	2.4366974	0.7024539	-0.4062653
O	-2.0265899	-2.0116648	-0.4936301
O	-1.5310662	-0.1846505	0.9933343
O	-2.7668900	0.2645882	-1.0317590
O	-3.8575461	-0.9792279	0.7736849
O	1.1355978	0.2287913	-0.9948768
O	2.5232405	2.1739255	-0.5095624
O	2.4433721	0.2848432	1.0442382
O	3.5709135	0.0610180	-1.1122202
O	2.1364164	-2.4218249	1.1016549
H	2.3327460	-1.4589062	1.2351115
H	2.8404120	-2.6833416	0.4803986
O	0.2653997	1.4468782	2.5140492
H	1.0668161	1.0541688	2.1048742
H	-0.4631873	0.8738831	2.2092624
O	0.1812963	3.3242285	0.3446803
H	0.1543015	2.9170730	1.2343108
H	1.0757596	3.0568121	0.0184478
H	-4.7833804	0.6540777	-1.2944008
O	-5.6682157	0.5066151	-0.9171805
H	-5.3943679	-0.0619284	-0.1745284
H	4.0988759	-1.4969372	-0.8895134
O	4.4663703	-2.3926271	-0.6312061
H	5.0669910	-2.1721749	0.0884788

Cluster: $(\text{NaSO}_4^-)_2(\text{H}_2\text{O})_5$

Isomer: 5-3f

Na	-0.4379007	1.3429930	-1.0034423
Na	0.4366155	-1.4741895	0.6356800
S	-2.3705941	-0.6023193	0.0448536
S	2.3069872	0.6847026	-0.2837285
O	-2.5374742	0.8860125	0.1928939
O	-1.2991080	-0.7977008	-1.0084724
O	-1.8422567	-1.1818269	1.3141819
O	-3.6314984	-1.2329074	-0.3565415
O	1.2196781	0.8717670	0.7666992
O	2.4808156	-0.8031770	-0.4330127
O	1.7793957	1.2610431	-1.5482752
O	3.5595878	1.3179086	0.1390884
H	0.0726124	2.4402239	1.0849046
O	-0.7339496	2.9493931	0.8758647
H	-1.4565614	2.2967045	0.9566209
H	0.8075316	0.0306318	2.5077464
O	0.3681661	-0.6801084	3.0118121

H	-0.5507557	-0.6727775	2.6811624
H	-4.5651929	1.4315386	-0.3105838
O	-5.3797319	1.0272895	-0.6495598
H	-5.0701366	0.1028103	-0.6772700
H	4.5941755	-1.2978084	-0.2067276
O	5.4270434	-0.8627076	0.0343202
H	5.0772541	0.0384171	0.1649624
H	-0.1088303	-2.2066593	-1.6248578
O	0.7046538	-2.7371197	-1.5263607
H	1.4220935	-2.0749870	-1.4882227