

Water-carbon disulfide dimers: observation of a new isomer, determination of an A rotational constant for the known isomer, and ab initio structure theory

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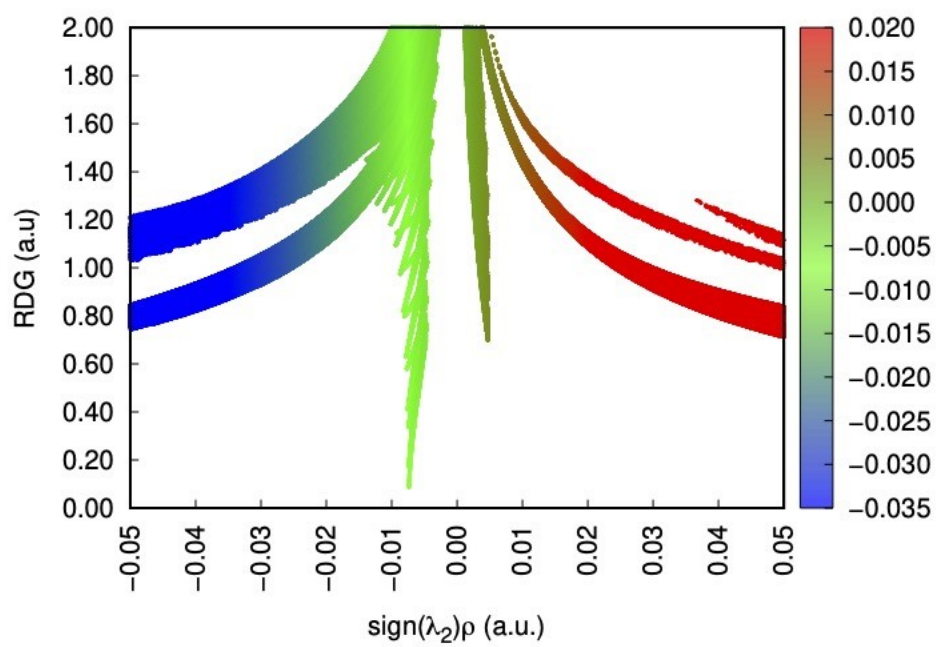
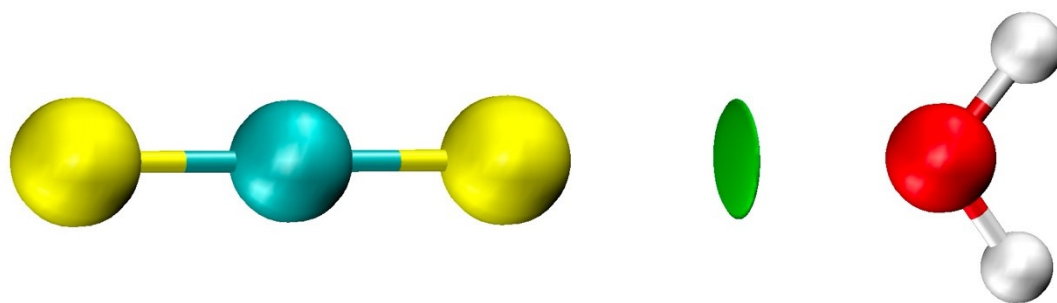


Figure S1. NCI and RDG scatter plots of Isomer 1.

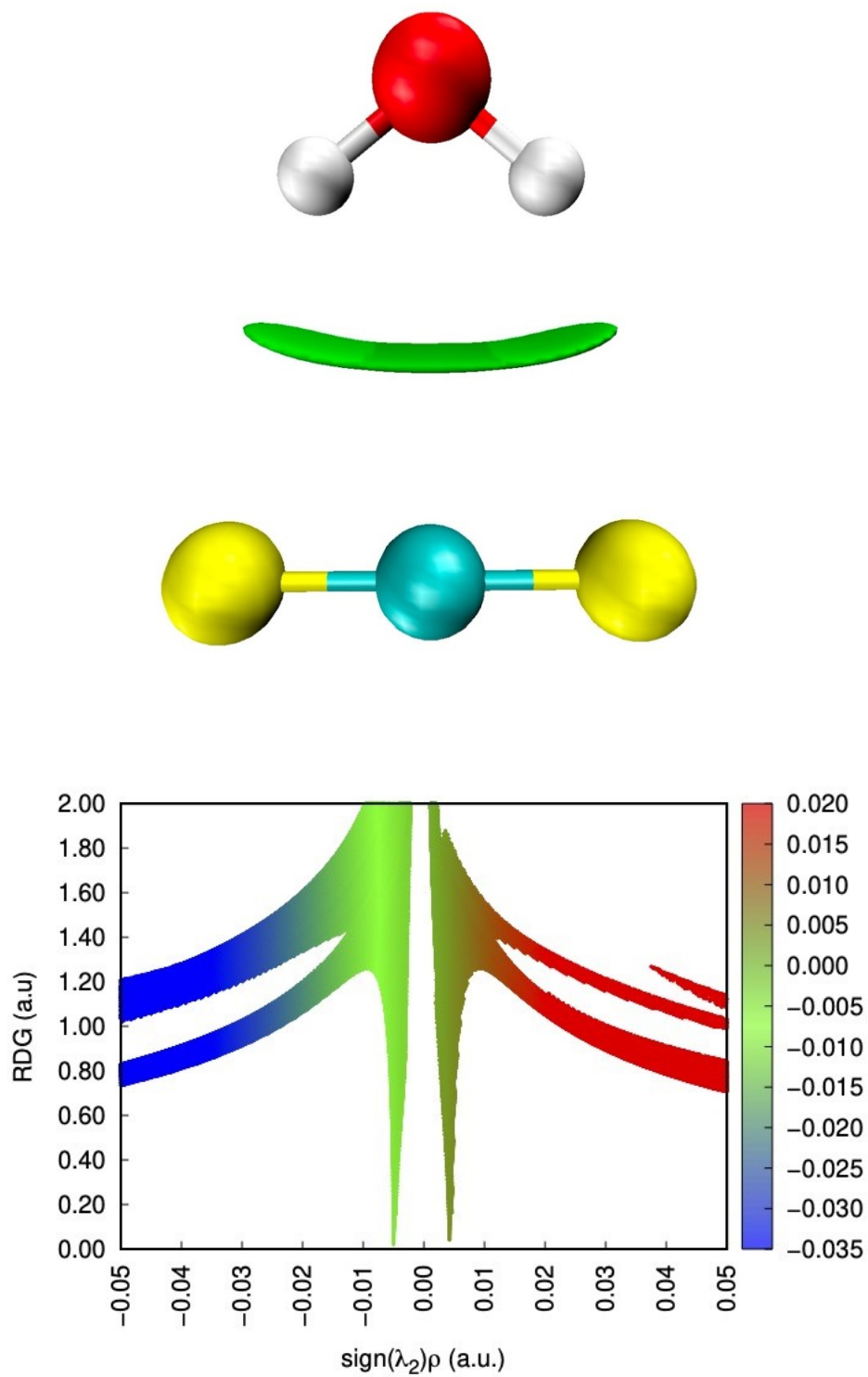


Figure S2. NCI and RDG scatter plots of Isomer 2.

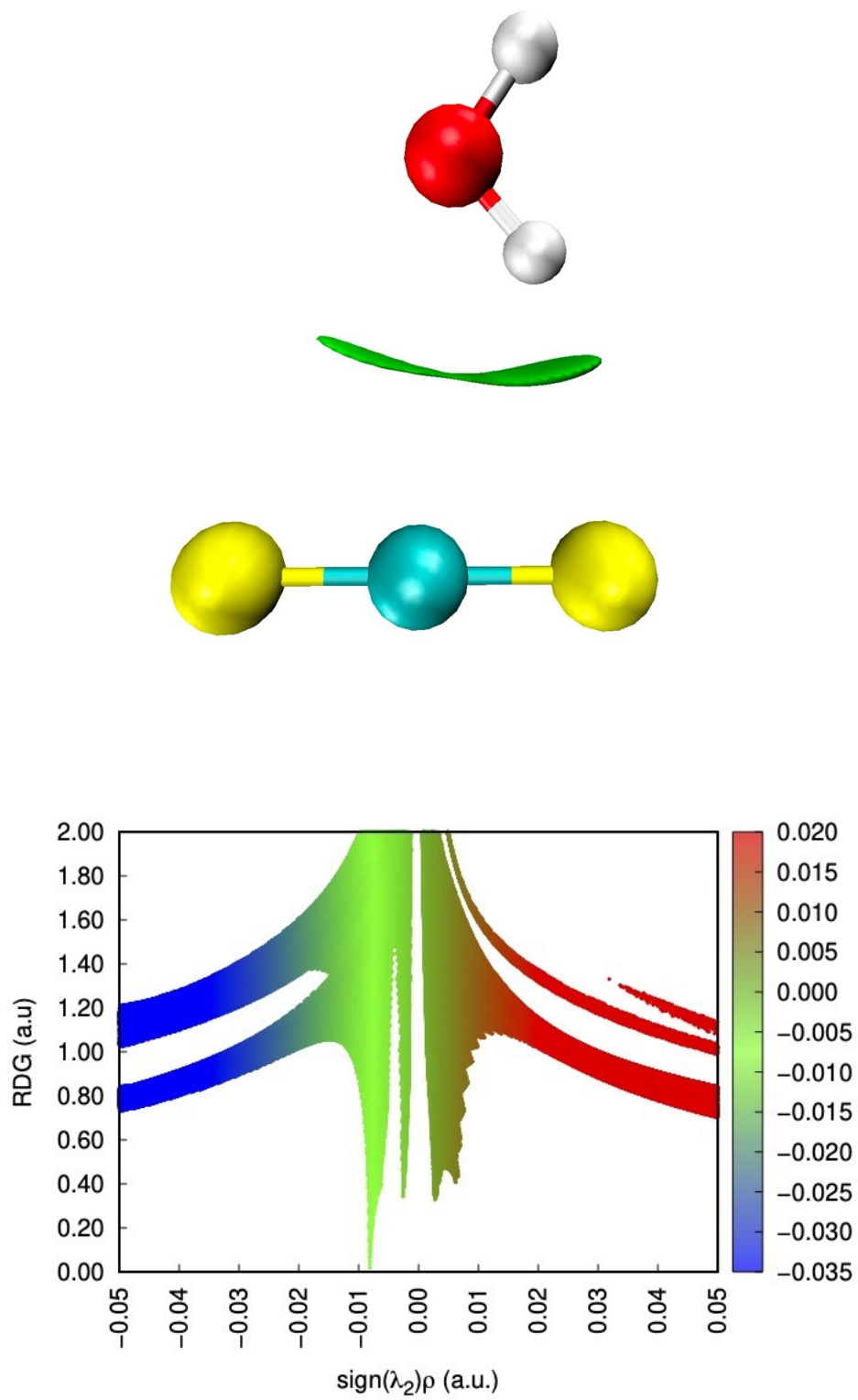


Figure S3. NCI and RDG scatter plots of Isomer 3

Table S1. Structural data of isomer 1.

 Geometry optimized at revDSD-PBEP86-D3BJ/jun-cc-pVT(+d)Z level.

	(Angstrom)		
C	0.000000	0.000000	1.006606
S	0.000000	0.000000	2.567634
S	0.000000	-0.000000	-0.550619
O	0.000000	-0.000000	-3.713570
H	-0.000000	0.760420	-4.301659
H	-0.000000	-0.760420	-4.301659

 Geometry optimized at CCSD(T)-F12b/cc-pVTZ-F12 level.

	(Angstrom)		
C	0.0000000000	0.0000000000	1.0044270350
S	0.0000000000	0.0000000000	2.5645890828
S	0.0000000000	0.0000000000	-0.5516364522
O	0.0000000000	0.0000000000	-3.7065978688
H	0.0000000000	-0.7583404431	-4.2935801385
H	0.0000000000	0.7583404431	-4.2935801385

 Geometry optimized at CCSD(T)-F12b/cc-pVQZ-F12 level.

	(Angstrom)		
C	0.0000000000	0.0000000000	1.0017178544
S	0.0000000000	0.0000000000	2.5611720153
S	0.0000000000	0.0000000000	-0.5535716694
O	0.0000000000	0.0000000000	-3.7042969990
H	0.0000000000	-0.7583829118	-4.2906998407
H	0.0000000000	0.7583829118	-4.2906998407

Table S2. Structural data of isomer 2.

 Geometry optimized at revDSD-PBEP86-D3BJ/jun-cc-pVT(+d)Z level.

	(Angstrom)		
C	0.000000	-0.000000	-0.715760
S	0.000000	1.557955	-0.712218
S	-0.000000	-1.557955	-0.712218
O	0.000000	0.000000	2.826902
H	0.000000	0.758173	2.235163
H	-0.000000	-0.758173	2.235163

 Geometry optimized at CCSD(T)-F12b/cc-pVTZ-F12 level.

	(Angstrom)		
C	0.0000000000	0.0000000000	-0.7087054943
S	0.0000000000	1.5570479117	-0.7039350107
S	0.0000000000	-1.5570479117	-0.7039350107
O	0.0000000000	0.0000000000	2.8014614911
H	0.0000000000	0.7561112472	2.2105823673
H	0.0000000000	-0.7561112472	2.2105823673

 Geometry optimized at CCSD(T)-F12b/cc-pVQZ-F12 level.

	(Angstrom)		
C	0.0000000000	0.0000000000	-0.7126922287
S	0.0000000000	1.5562690903	-0.7079099248
S	0.0000000000	-1.5562690903	-0.7079099248
O	0.0000000000	0.0000000000	2.8049508268
H	0.0000000000	0.7562747062	2.2148059808
H	0.0000000000	-0.7562747062	2.2148059808

Table S3. Structural data of isomer 3.

Geometry optimized at revDSD-PBEP86-D3BJ/jun-cc-pVT(+d)Z level.

(Angstrom)

C	-0.000000	0.715495	0.000000
S	-1.542765	0.887474	0.000000
S	1.552885	0.536411	0.000000
O	-0.131746	-2.685214	0.000000
H	0.591469	-2.049874	0.000000
H	0.300577	-3.543545	0.000000

Geometry optimized at CCSD(T)-F12b/cc-pVTZ-F12 level.

(Angstrom)

C	0.6651810480	0.2474818962	0.0000000000
S	1.3400731495	-1.1492453678	0.0000000000
S	-0.0218612529	1.6508171773	0.0000000000
O	-2.4530481662	-1.0514182065	0.0000000000
H	-2.1202823018	-0.1505344879	0.0000000000
H	-3.4070282767	-0.9548622413	0.0000000000

Table S4. Harmonic Frequencies and Intensities for the CS₂-D₂O isomers.^a

Isomer 1		Isomer 2		Isomer 3	
Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
2883.6 [2885.9]	39.4	2873.8 [2874.2]	11.8	2873.7 [2875.8]	70.9
2754.4 [2760.5]	6.8	2749.8 [2753.3]	12.1	2743.8 [2749.8]	8.6
1566.6 [1552.7]	690.1	1572.2 [1557.7]	621.2	1573.7 [1559.4]	636.4
1203.9 [1208.2]	43.0	1205.1 [1208.0]	72.2	1202.7 [1207.5]	38.2
671.0 [669.3]	1.0	673.5 [671.6]	0.0	673.6 [671.7]	0.3
409.0 [404.9]	4.5	405.7 [402.8]	3.7	403.6 [400.1]	4.8
407.6 [403.7]	4.0	398.1 [395.0]	4.0	398.3 [395.2]	4.0
78.0 [80.6]	27.8	97.6 [105.3]	91.3	124.2 [125.6]	34.5
72.4 [73.8]	0.8	75.5 [81.8]	32.0	101.7 [107.5]	54.3
52.2 [47.8]	114.5	68.1 [71.2]	0.2	69.9 [69.7]	6.6
25.3 [25.5]	10.7	63.3 [70.0]	0.0	30.5 [37.5]	5.4
19.8 [22.8]	6.0	25.8 [31.7]	11.9	26.8 [21.3]	71.2

^a Frequencies (in cm⁻¹) and intensities (in km/mol) are computed at revDSD level of theory; between square parentheses are reported the corresponding frequency data obtained by CCSD(T)-F12b calculations.

Table S5. Observed and fitted line positions of CS₂-D₂O (cm⁻¹).

Note: Blank Kc values indicate an unresolved asymmetry doublet, where Calc equals the mean of the calculated doublet line positions.

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*****
J'   Ka'  Kc'   J''  Ka'' Kc''   Obs       Calc      Obs-Calc
*****
12   0    12   13   0    13   2667.7709 2667.7709 0.0000
10   0    10   11   0    11   2667.8978 2667.8976 0.0002
9    0    9    10   0    10   2667.9611 2667.9609 0.0001
7    1    8    8    1    8    2667.9948 2667.9944 0.0005
8    0    8    9    0    9    2668.0245 2668.0244 0.0001
6    1    7    7    1    7    2668.0581 2668.0579 0.0002
7    0    7    8    0    8    2668.0881 2668.0879 0.0003
5    1    6    6    1    6    2668.1219 2668.1215 0.0004
6    0    6    7    0    7    2668.1516 2668.1514 0.0003
5    0    5    6    0    6    2668.2152 2668.2149 0.0003
3    1    4    4    1    4    2668.2492 2668.2488 0.0005
4    0    4    5    0    5    2668.2789 2668.2785 0.0004
2    1    3    3    1    3    2668.3130 2668.3125 0.0005
3    0    3    4    0    4    2668.3424 2668.3422 0.0002
1    1    2    2    1    2    2668.3762 2668.3762 0.0000
2    0    2    3    0    3    2668.4060 2668.4059 0.0001
1    0    1    2    0    2    2668.4696 2668.4696 0.0000
0    0    0    1    0    1    2668.5332 2668.5334 -0.0002
2    1    1    1    1    0    2668.6310 2668.6313 -0.0003
1    0    1    0    0    0    2668.6609 2668.6610 -0.0001
3    1    2    2    1    1    2668.6948 2668.6952 -0.0004
2    0    2    1    0    1    2668.7247 2668.7249 -0.0002
4    1    3    3    1    2    2668.7586 2668.7591 -0.0005
3    0    3    2    0    2    2668.7887 2668.7888 -0.0001
5    1    4    4    1    3    2668.8226 2668.8230 -0.0005
4    0    4    3    0    3    2668.8528 2668.8528 0.0000
6    1    5    5    1    4    2668.8869 2668.8870 -0.0001
5    0    5    4    0    4    2668.9164 2668.9168 -0.0004
7    1    6    6    1    5    2668.9508 2668.9509 -0.0001
6    0    6    5    0    5    2668.9807 2668.9808 -0.0001
8    1    7    7    1    6    2669.0149 2669.0149 0.0000
7    0    7    6    0    6    2669.0447 2669.0449 -0.0002
9    1    8    8    1    7    2669.0786 2669.0789 -0.0003
8    0    8    7    0    7    2669.1088 2669.1090 -0.0001
10   1    9    9    1    8    2669.1431 2669.1430 0.0001
9    0    9    8    0    8    2669.1729 2669.1731 -0.0002
10   0    10   9    0    9    2669.2371 2669.2373 -0.0001
11   0    11   10   0    10   2669.3014 2669.3015 -0.0001
12   0    12   11   0    11   2669.3658 2669.3657 0.0000
13   0    13   12   0    12   2669.4301 2669.4300 0.0001
14   0    14   13   0    13   2669.4942 2669.4943 -0.0001

9    0    9    10   1    10   2775.8845 2775.8842 0.0003
8    0    8    9    1    9    2775.9459 2775.9460 -0.0001
7    0    7    8    1    8    2776.0081 2776.0080 0.0001

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6	0	6	7	1	7	2776.0702	2776.0702	-0.0001
5	0	5	6	1	6	2776.1328	2776.1327	0.0001
4	0	4	5	1	5	2776.1955	2776.1953	0.0002
3	0	3	4	1	4	2776.2582	2776.2582	0.0000
2	0	2	3	1	3	2776.3213	2776.3213	0.0000
1	0	1	2	1	2	2776.3847	2776.3845	0.0001
0	0	0	1	1	1	2776.4479	2776.4480	-0.0001
2	0	2	1	1	1	2776.6401	2776.6397	0.0004
3	0	3	2	1	2	2776.7038	2776.7039	-0.0001
4	0	4	3	1	3	2776.7684	2776.7684	0.0000
5	0	5	4	1	4	2776.8329	2776.8331	-0.0002
6	0	6	5	1	5	2776.8976	2776.8980	-0.0005
7	0	7	6	1	6	2776.9627	2776.9631	-0.0004
8	0	8	7	1	7	2777.0282	2777.0284	-0.0002
9	0	9	8	1	8	2777.0940	2777.0939	0.0000
10	0	10	9	1	9	2777.1598	2777.1596	0.0002
15	1	15	16	0	16	2790.1804	2790.1805	-0.0001
14	1	14	15	0	15	2790.2459	2790.2458	0.0000
13	1	13	14	0	14	2790.3110	2790.3111	-0.0001
12	1	12	13	0	13	2790.3763	2790.3762	0.0001
11	1	11	12	0	12	2790.4412	2790.4413	-0.0001
10	1	10	11	0	11	2790.5061	2790.5062	-0.0001
9	1	9	10	0	10	2790.5709	2790.5711	-0.0002
8	1	8	9	0	9	2790.6358	2790.6358	0.0000
7	1	7	8	0	8	2790.7004	2790.7005	-0.0001
6	1	6	7	0	7	2790.7649	2790.7650	-0.0001
5	1	5	6	0	6	2790.8294	2790.8294	-0.0001
3	1	3	4	0	4	2790.9579	2790.9580	-0.0001
2	1	2	3	0	3	2791.0223	2791.0221	0.0002
1	1	1	2	0	2	2791.0861	2791.0861	-0.0001
1	1	1	0	0	0	2791.2777	2791.2776	0.0002
2	1	2	1	0	1	2791.3411	2791.3412	0.0000
4	1	4	3	0	3	2791.4681	2791.4680	0.0001
5	1	5	4	0	4	2791.5314	2791.5313	0.0001
6	1	6	5	0	5	2791.5945	2791.5944	0.0001
7	1	7	6	0	6	2791.6576	2791.6575	0.0002
8	1	8	7	0	7	2791.7206	2791.7204	0.0001
9	1	9	8	0	8	2791.7833	2791.7832	0.0000
10	1	10	9	0	9	2791.8459	2791.8460	0.0000
11	1	11	10	0	10	2791.9086	2791.9086	0.0000
12	1	12	11	0	11	2791.9710	2791.9711	0.0000
13	1	13	12	0	12	2792.0334	2792.0334	0.0000
14	1	14	13	0	13	2792.0957	2792.0957	0.0000
15	1	15	14	0	14	2792.1579	2792.1578	0.0000
16	1	16	15	0	15	2792.2199	2792.2199	0.0001
17	1	17	16	0	16	2792.2815	2792.2818	-0.0003
18	1	18	17	0	17	2792.3440	2792.3436	0.0004
3	2		4	1		2805.4686	2805.4681	0.0005
2	2		1	1		2805.8509	2805.8509	0.0000
3	2		2	1		2805.9145	2805.9145	0.0000
4	2		3	1		2805.9779	2805.9781	-0.0002
5	2		4	1		2806.0414	2806.0417	-0.0003
7	2	6	6	1	5	2806.1669	2806.1667	0.0002
7	2	5	6	1	6	2806.1704	2806.1707	-0.0003

8	2	7	7	1	6	2806.2296	2806.2295	0.0001
8	2	6	7	1	7	2806.2349	2806.2349	0.0000
9	2	8	8	1	7	2806.2918	2806.2921	-0.0004
9	2	7	8	1	8	2806.2991	2806.2990	0.0001
10	2	9	9	1	8	2806.3545	2806.3546	-0.0001
10	2	8	9	1	9	2806.3636	2806.3632	0.0003
1	0	1	0	0	0	2176.8932	2176.8931	0.0002
2	0	2	1	0	1	2176.9562	2176.9565	-0.0002
0	0	0	1	0	1	2176.7658	2176.7656	0.0001
2	0	2	3	0	3	2176.6376	2176.6375	0.0001
1	0	1	2	0	2	2176.7017	2176.7016	0.0001
3	0	3	4	0	4	2176.5732	2176.5731	0.0001
4	0	4	5	0	5	2176.5086	2176.5085	0.0001
5	0	5	6	0	6	2176.4439	2176.4438	0.0001
6	0	6	7	0	7	2176.3790	2176.3789	0.0001
7	0	7	8	0	8	2176.3139	2176.3137	0.0001
9	0	9	10	0	10	2176.1832	2176.1830	0.0003
3	0	3	2	0	2	2177.0196	2177.0197	-0.0002
4	0	4	3	0	3	2177.0825	2177.0828	-0.0003
5	0	5	4	0	4	2177.1455	2177.1456	-0.0001
6	0	6	5	0	5	2177.2081	2177.2083	-0.0001
7	0	7	6	0	6	2177.2706	2177.2708	-0.0001
8	0	8	7	0	7	2177.3330	2177.3330	-0.0001
9	0	9	8	0	8	2177.3952	2177.3951	0.0000
10	0	10	9	0	9	2177.4570	2177.4570	-0.0001
11	0	11	10	0	10	2177.5190	2177.5187	0.0003
12	0	12	11	0	11	2177.5803	2177.5802	0.0000
10	0	10	11	0	11	2176.1170	2176.1173	-0.0003
11	0	11	12	0	12	2176.0513	2176.0514	-0.0001
1	1		2	1		2176.6939	2176.6942	-0.0003
2	1		3	1		2176.6303	2176.6300	0.0003
3	1		4	1		2176.5663	2176.5657	0.0006
4	1		5	1		2176.5017	2176.5011	0.0005
5	1		6	1		2176.4363	2176.4364	-0.0001
6	1		7	1		2176.3714	2176.3715	-0.0001
7	1		8	1		2176.3068	2176.3064	0.0004
2	1		1	1		2176.9482	2176.9489	-0.0007
3	1		2	1		2177.0118	2177.0121	-0.0003
5	1		4	1		2177.1378	2177.1379	-0.0001
6	1		5	1		2177.2006	2177.2005	0.0001
7	1		6	1		2177.2630	2177.2630	0.0000
8	1		7	1		2177.3251	2177.3252	-0.0001
9	1		8	1		2177.3872	2177.3872	-0.0001
10	1		9	1		2177.4490	2177.4491	-0.0001

Table S6. Observed and fitted line positions of CS₂-HDO (cm⁻¹).

```

*****
J'   Ka'  Kc'   J''  Ka'' Kc''  Obs      Calc      Obs-Calc
*****
10    0   10    11    0   11   2176.2298  2176.2300  -0.0002
 9    0    9    10    0   10   2176.2984  2176.2981   0.0003
 8    0    8     9    0    9   2176.3658  2176.3659  -0.0001
 7    0    7     8    0    8   2176.4334  2176.4335  -0.0001
 6    0    6     7    0    7   2176.5012  2176.5010   0.0002
 5    0    5     6    0    6   2176.5681  2176.5682  -0.0002
 4    0    4     5    0    5   2176.6358  2176.6353   0.0005
 3    0    3     4    0    4   2176.7019  2176.7022  -0.0002
 2    0    2     3    0    3   2176.7688  2176.7688  -0.0001
 1    0    1     2    0    2   2176.8351  2176.8353  -0.0002
 0    0    0     1    0    1   2176.9015  2176.9016   0.0000
 1    0    1     0    0    0   2177.0341  2177.0336  0.0006*
 2    0    2     1    0    1   2177.0993  2177.0992   0.0000
 3    0    3     2    0    2   2177.1647  2177.1647   0.0000
 4    0    4     3    0    3   2177.2300  2177.2300   0.0000
 5    0    5     4    0    4   2177.2952  2177.2951   0.0001
 6    0    6     5    0    5   2177.3600  2177.3600   0.0000
 7    0    7     6    0    6   2177.4247  2177.4247   0.0000
 8    0    8     7    0    7   2177.4891  2177.4892   0.0000
 9    0    9     8    0    8   2177.5534  2177.5534  -0.0001
10    0   10     9    0    9   2177.6176  2177.6175   0.0001
11    0   11    10    0   10   2177.6813  2177.6814  -0.0001
12    0   12    11    0   11   2177.7451  2177.7451   0.0000
13    0   13    12    0   12   2177.8086  2177.8086   0.0000
*****

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*given a reduced weight in the fit.

Table S7. Observed and fitted line positions of CS₂-H₂O (cm⁻¹).

Note: Blank Kc indicates an unresolved asymmetry doublet, where Calc equals the mean of the calculated doublet line positions.

```

*****
J'  Ka'  Kc'      J''  Ka''  Kc''      Obs      Calc      Obs-Calc
*****
14  1      15  1      1597.1770  1597.1764  0.0006
13  0    13  14  0    14  1597.1900  1597.1891  0.0009
13  1      14  1      1597.2457  1597.2451  0.0006
12  0    12  13  0    13  1597.2586  1597.2578  0.0007
12  1      13  1      1597.3143  1597.3139  0.0005
11  0    11  12  0    12  1597.3272  1597.3266  0.0006
11  1      12  1      1597.3826  1597.3826  0.0000
10  0    10  11  0    11  1597.3953  1597.3953  0.0000
10  1      11  1      1597.4513  1597.4513  0.0000
 9  0      10  0    10  1597.4642  1597.4641  0.0001
 9  1      10  1      1597.5202  1597.5200  0.0002
 8  0      9   9   0    9   1597.5329  1597.5328  0.0001
 8  1      9   9   1      1597.5889  1597.5887  0.0002
 7  0      8   8   0    8   1597.6017  1597.6015  0.0002
 7  1      8   8   1      1597.6572  1597.6574 -0.0002
 6  0      6   6   0    7   1597.6699  1597.6702 -0.0003
 6  1      7   7   1      1597.7260  1597.7261 -0.0001
 5  0      5   5   0    6   1597.7388  1597.7389 -0.0002
 5  1      6   6   1      1597.7948  1597.7947  0.0001
 4  0      4   4   0    5   1597.8077  1597.8076  0.0001
 4  1      5   5   1      1597.8635  1597.8634  0.0002
 3  0      3   3   0    4   1597.8763  1597.8763  0.0001
 3  1      4   4   1      1597.9321  1597.9320  0.0001
 2  0      2   2   0    3   1597.9448  1597.9449 -0.0001
 2  1      3   3   1      1598.0007  1598.0006  0.0001
 1  0      1   1   0    2   1598.0136  1598.0135  0.0000
 1  1      2   2   1      1598.0693  1598.0692  0.0001
 0  0      0   0   0    1   1598.0822  1598.0821  0.0000
 1  0      1   0   0    0   1598.2193  1598.2193  0.0000
 2  0      2   1   0    1   1598.2878  1598.2879 -0.0001
 2  1      1   1   1      1598.3435  1598.3434  0.0001
 3  0      3   2   0    2   1598.3565  1598.3564  0.0000
 3  1      2   2   1      1598.4120  1598.4119  0.0001
 4  0      4   3   0    3   1598.4249  1598.4249  0.0000
 4  1      3   3   1      1598.4803  1598.4804 -0.0001
 5  0      5   4   0    4   1598.4932  1598.4934 -0.0002
 5  1      4   4   1      1598.5488  1598.5489  0.0000
 6  0      6   5   0    5   1598.5618  1598.5619 -0.0001
 6  1      5   5   1      1598.6173  1598.6173  0.0000
 7  0      7   6   0    6   1598.6302  1598.6304 -0.0001
 7  1      6   6   1      1598.6856  1598.6857 -0.0001
 8  0      8   7   0    7   1598.6985  1598.6988 -0.0003
 8  1      7   7   1      1598.7538  1598.7541 -0.0004
 9  0      9   8   0    8   1598.7670  1598.7672 -0.0002
 9  1      8   8   1      1598.8225  1598.8225  0.0000

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10	0	10	9	0	9	1598.8355	1598.8356	-0.0001
10	1		9	1		1598.8909	1598.8909	0.0000
11	0	11	10	0	10	1598.9038	1598.9040	-0.0001
11	1		10	1		1598.9591	1598.9592	-0.0001
12	0	12	11	0	11	1598.9722	1598.9723	-0.0001
12	1	12	11	1	11	1599.0264	1599.0265	-0.0001
12	1	11	11	1	10	1599.0282	1599.0285	-0.0002
13	0	13	12	0	12	1599.0403	1599.0406	-0.0003
13	1	13	12	1	12	1599.0947	1599.0947	0.0000
13	1	12	12	1	11	1599.0965	1599.0969	-0.0004
14	0	14	13	0	13	1599.1087	1599.1089	-0.0002
14	1	14	13	1	13	1599.1626	1599.1628	-0.0003
14	1	13	13	1	12	1599.1650	1599.1652	-0.0003
15	0	15	14	0	14	1599.1769	1599.1772	-0.0002
15	1	15	14	1	14	1599.2305	1599.2310	-0.0005
15	1	14	14	1	13	1599.2334	1599.2336	-0.0001
8	1		9	1		2176.4128	2176.4129	-0.0001
7	1		8	1		2176.4826	2176.4832	-0.0006
6	1		7	1		2176.5532	2176.5533	0.0000
5	1		6	1		2176.6230	2176.6231	-0.0001
4	1		5	1		2176.6928	2176.6927	0.0001
3	1		4	1		2176.7623	2176.7622	0.0001
2	1		3	1		2176.8315	2176.8314	0.0001
1	1		2	1		2176.9004	2176.9004	0.0001
2	1		1	1		2177.1742	2177.1742	0.0000
3	1		2	1		2177.2421	2177.2421	0.0000
4	1		3	1		2177.3098	2177.3098	0.0000
5	1		4	1		2177.3773	2177.3772	0.0000
6	1		5	1		2177.4445	2177.4445	0.0000
7	1		6	1		2177.5116	2177.5115	0.0000
8	1		7	1		2177.5784	2177.5783	0.0001
9	1		8	1		2177.6450	2177.6449	0.0000
10	1		9	1		2177.7114	2177.7113	0.0001
12	1		11	1		2177.8435	2177.8434	0.0001
