Supporting information for:

A solvent-mediated conformational switch in sulfanilamide

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Figure SI01. LA-CP-FTMW rotational spectrum of sulfanilamide in the 6-14 GHz frequency range. The red stars indicate the rotational transitions of the monomer, while a few selected transitions of its water cluster are highlighted using blue triangle marks to illustrate the difference in intensity

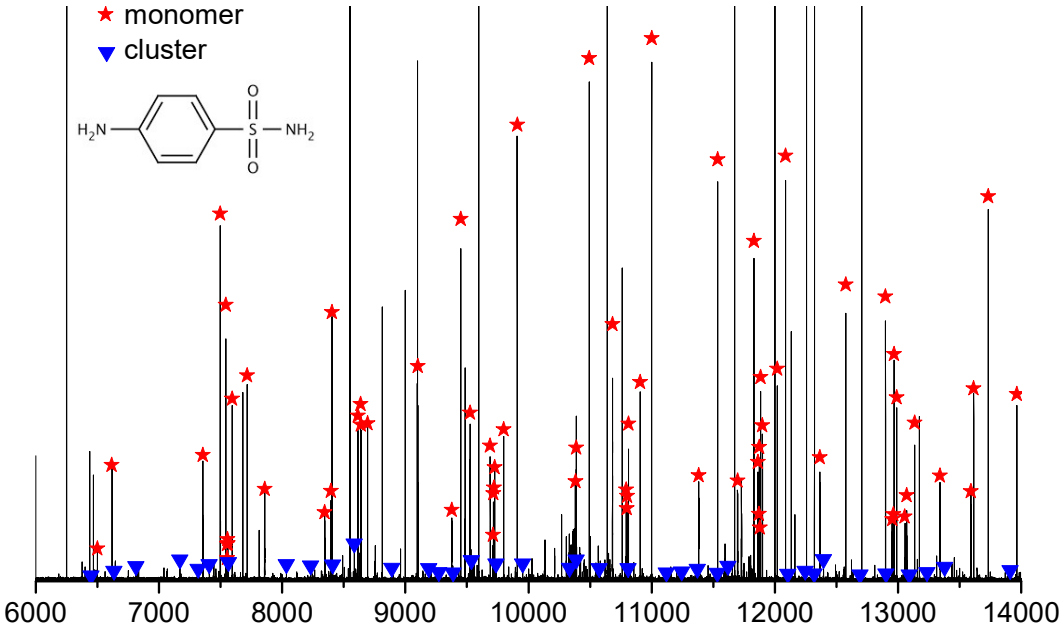

Table SI01. Measured frequencies and residuals (in MHz) for the rotational transitions of rotamer I, corresponding to the e-d conformer, using the LA-CP-FTMW spectrometer.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs} - \nu_{cal}$
1	1	0	0	0	0	3175.558	-0.064
2	1	1	1	1	0	2208.585	0.039
2	1	1	1	0	1	4305.700	0.033
3	0	3	2	0	2	3231.695	-0.042
3	1	3	2	1	2	3157.551	0.042
3	1	2	2	1	1	3312.222	0.010
3	2	1	2	2	0	3239.375	0.014
3	2	2	2	2	1	3235.518	0.014
3	1	2	2	0	2	5461.852	0.013
4	0	4	3	0	3	4304.363	-0.044
4	1	4	3	1	3	4209.059	0.031
4	1	3	3	1	2	4415.175	0.040
4	2	3	3	2	2	4313.251	-0.006
4	2	3	4	1	3	5958.213	0.067
5	0	5	4	0	4	5373.322	-0.048
5	1	5	4	1	4	5259.590	0.034
5	1	4	4	1	3	5517.008	-0.030
5	2	3	4	2	2	5409.582	0.078
5	2	4	4	2	3	5390.359	-0.010
5	3	3	4	3	2	5395.762	0.066
5	4	2	4	4	1	5394.643	-0.001
5	2	4	5	1	4	5831.447	-0.029
6	0	6	5	0	5	6437.663	-0.045
6	1	6	5	1	5	6308.940	-0.051
6	2	5	5	2	4	6466.643	-0.037
6	2	5	6	1	5	5680.448	-0.082
7	2	6	7	1	6	5505.994	0.002
8	2	7	8	1	7	5308.782	0.033
9	2	8	9	1	8	5089.941	0.005
10	2	9	10	1	9	4850.980	-0.002
11	2	10	11	1	10	4593.660	0.003
12	2	11	12	1	11	4320.141	0.010
6	2	4	5	2	3	6499.966	-0.003
6	1	5	5	1	4	6617.646	0.028
7	1	7	6	1	6	7357.157	-0.005
7	0	7	6	0	6	7496.702	0.001
7	2	6	6	2	5	7542.059	0.037
7	2	5	6	2	4	7594.869	0.061
7	3	4	6	3	3	7558.286	0.075
7	3	5	6	3	4	7556.878	0.076
7	4	3	6	4	2	7554.286	-0.009
7	5	3	6	5	2	7552.907	-0.007
7	1	6	6	1	5	7716.553	-0.008
5	1	4	4	0	4	7858.135	0.226
2	2	0	1	1	0	8346.013	-0.119
2	2	1	1	1	1	8396.418	-0.297
8	1	8	7	1	7	8404.021	0.060
8	0	8	7	0	7	8549.908	0.036
8	2	7	7	2	6	8616.259	0.002
8	3	6	7	3	5	8638.163	-0.001
8	3	5	7	3	4	8640.974	-0.003
8	2	6	7	2	5	8694.363	0.016
8	1	7	7	1	6	8813.495	-0.006
6	1	5	5	0	5	9101.634	-0.531
3	2	1	2	1	1	9376.649	-0.284
9	1	9	8	1	8	9449.298	0.019
3	2	2	2	1	2	9526.503	-0.256
9	0	9	8	0	8	9597.005	0.007
9	2	8	8	2	7	9689.182	-0.037
9	4	5	8	4	4	9715.740	-0.044
9	5	5	8	5	4	9712.782	-0.030
9	3	7	8	3	6	9720.027	-0.018
9	3	6	8	3	5	9725.203	0.016
9	2	7	8	2	6	9798.715	0.081
9	1	8	8	1	7	9908.043	0.009
7	1	6	6	0	6	10381.271	0.242
4	2	2	3	1	2	10387.249	-0.325

10	1	10	9	1	9	10493.089	0.038
10	0	10	9	0	9	10638.225	0.022
4	2	3	3	1	3	10682.478	0.055
10	2	9	9	2	8	10760.763	0.003
10	5	6	9	5	5	10793.254	-0.030
10	4	7	9	4	6	10797.133	-0.079
10	4	6	9	4	5	10797.405	0.007
10	3	8	9	3	7	10802.437	0.049
10	3	7	9	3	6	10811.215	0.052
10	2	8	9	2	7	10907.462	0.092
10	1	9	9	1	8	10999.714	-0.002
5	2	3	4	1	3	11381.920	-0.023
11	1	11	10	1	10	11535.253	0.003
11	0	11	10	0	10	11673.966	0.010
8	1	7	7	0	7	11698.074	0.245
11	2	10	10	2	9	11830.726	-0.007
5	2	4	4	1	4	11863.805	0.041
11	6	5	10	6	4	11871.301	-0.060
11	5	7	10	5	6	11874.133	-0.024
11	4	8	10	4	7	11879.319	-0.013
11	3	9	10	3	8	11885.108	0.005
11	3	8	10	3	7	11899.301	0.026
11	2	9	10	2	8	12019.995	0.090
11	1	10	10	1	9	12088.032	-0.026
6	2	4	5	1	4	12364.439	-0.441
12	1	12	11	1	11	12575.869	-0.007
12	0	12	11	0	11	12705.011	-0.012
12	2	11	11	2	10	12898.961	-0.039
12	5	8	11	5	7	12955.369	-0.103
12	4	9	11	4	8	12962.091	-0.008
12	4	8	11	4	7	12962.768	-0.024
12	3	10	11	3	9	12968.050	-0.016
12	3	9	11	3	8	12989.899	-0.035
9	1	8	8	0	8	13056.330	0.339
6	2	5	5	1	5	13070.948	0.060
12	2	10	11	2	9	13135.328	0.045
12	1	11	11	1	10	13172.444	-0.084
7	2	5	6	1	5	13342.059	-0.010
3	3	0	2	2	0	13591.955	0.238
13	1	13	12	1	12	13614.978	0.012
13	0	13	12	0	12	13732.320	-0.039
13	2	12	12	2	11	13965.376	-0.055

Figure SI02. A section of the experimental broadband rotational spectrum of sulfanilamide showing the $8_{08}\leftarrow7_{07}$ rotational transition for the ^{13}C and ^{34}S isotopologues of the eclipsed conformer of SA.

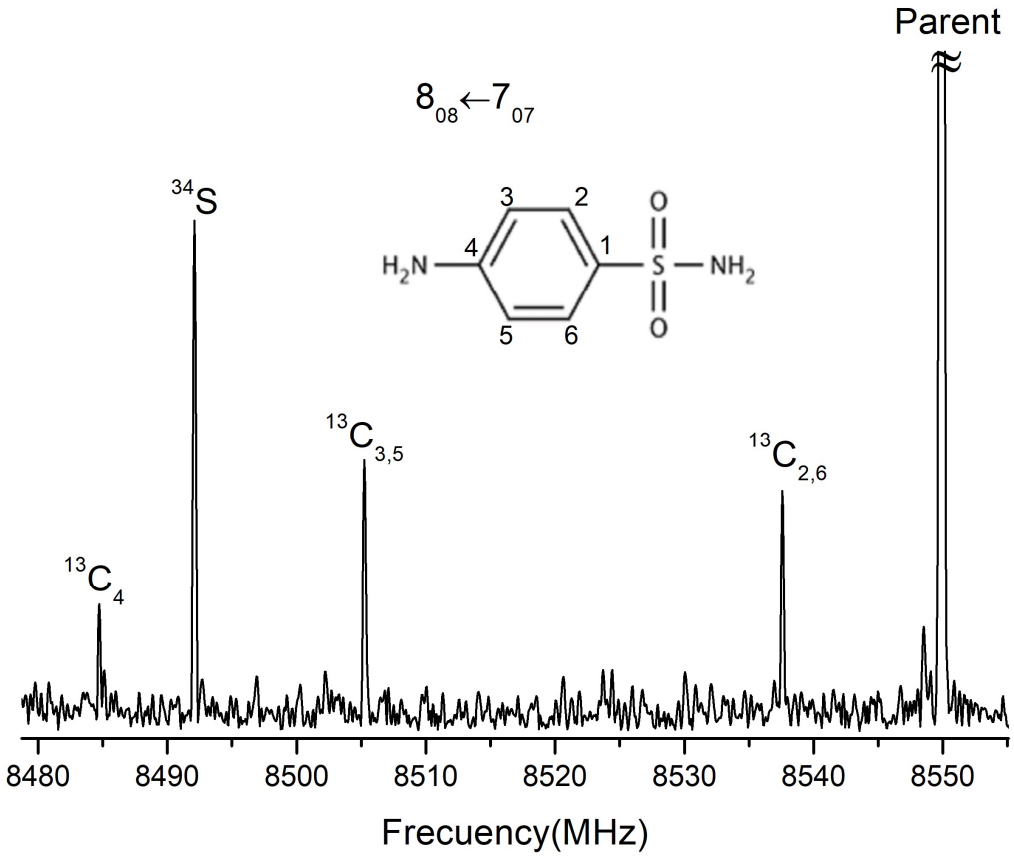

Table SI02. Measured frequencies and residuals (in MHz) for the rotational transitions of the ^{34}S isotopomer of rotamer I, corresponding to the e-d conformer, using the LA-CP-FTMW spectrometer.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs} - \nu_{cal}$
4	1	4	3	1	3	4180.469	-0.037
5	0	5	4	0	4	5336.377	-0.007
5	1	5	4	1	4	5223.998	0.046
5	1	5	4	1	3	5477.823	0.001
5	2	4	4	2	3	5352.895	0.004
6	0	6	5	0	5	6393.617	0.003
6	1	6	5	1	5	6266.322	-0.013
6	2	5	4	2	4	6421.772	-0.005
7	0	7	6	0	6	7445.715	0.018
7	2	6	6	2	5	7489.677	-0.046
7	2	5	6	2	4	7541.061	0.067
7	1	6	6	1	5	7661.922	0.027
8	1	8	7	1	7	8347.451	0.094
8	0	8	7	0	7	8492.080	0.017
8	2	7	7	2	6	8556.652	0.074
8	1	7	7	1	6	8751.230	0.038
9	1	9	8	1	8	9385.742	0.006
9	0	9	8	0	8	9532.567	0.049
9	2	8	8	2	7	9622.184	-0.016
9	2	7	8	2	6	9728.670	0.093
9	1	8	8	1	7	9838.173	0.010
10	1	10	9	1	9	10422.628	0.018
10	0	10	9	0	9	10567.213	0.052
10	2	9	9	2	8	10686.417	-0.024
10	3	7	9	3	6	10735.322	0.019
10	2	8	9	2	7	10829.123	0.045
10	1	9	9	1	8	10922.369	-0.006
11	1	11	10	1	10	11457.914	-0.029
11	0	11	10	0	10	11596.446	0.022
11	2	10	10	2	9	11749.144	-0.015
11	3	8	10	3	7	11815.600	0.009
11	2	9	10	2	8	11933.380	0.025
12	1	12	11	1	11	12491.707	-0.030
12	0	12	11	0	11	12621.048	0.013
12	2	11	11	2	10	12810.173	-0.046
12	3	10	11	3	9	12877.363	-0.051
12	3	9	11	3	8	12898.272	-0.062
12	2	10	11	2	9	13040.533	0.030
12	1	11	11	1	10	13080.573	-0.023
13	1	13	12	1	12	13524.012	-0.013
13	0	13	12	0	12	13641.922	0.027
13	2	12	12	2	11	13869.459	-0.035
8	3	6	7	3	5	8577.896	0.031
8	3	5	7	3	4	8580.546	-0.008
10	3	8	9	3	7	10726.913	-0.000
11	3	9	10	3	8	11802.006	-0.031
11	1	10	10	1	9	12003.323	-0.034
13	3	11	12	3	10	13952.857	-0.040
13	3	10	12	3	9	13983.914	-0.043

Table SI03. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_2$ (=$^{13}C_6$ due to symmetry) isotopomer of rotamer I, corresponding to the e-d conformer, using the LA-CP-FTMW spectrometer.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs} - \nu_{cal}$
6	1	6	5	1	5	6299.407	-0.029
5	1	4	4	1	3	5512.680	-0.038
5	2	3	4	2	2	5404.192	-0.011
5	0	5	4	0	4	5366.679	-0.023
4	1	4	3	1	3	4202.741	-0.027
8	0	8	7	0	7	8537.560	0.034
8	1	8	7	1	7	8391.008	0.056
8	1	7	7	1	6	8806.062	0.019
9	1	9	8	1	8	9434.502	0.034
9	0	9	8	0	8	9582.456	0.041
9	2	8	8	2	7	9677.780	-0.097
9	1	8	8	1	7	9899.330	-0.015
10	1	10	9	1	9	10476.405	0.011
10	0	10	9	0	9	10621.322	0.057
10	2	8	9	2	7	10899.642	0.017
10	1	9	9	1	8	10989.671	-0.001
11	1	11	10	1	10	11516.677	-0.027
11	0	11	10	0	10	11654.645	0.044
11	2	10	10	2	9	11816.371	-0.061
11	2	9	10	2	8	12011.893	0.028
11	1	10	10	1	9	12076.479	-0.032
12	1	12	11	1	11	12555.363	-0.042
12	0	12	11	0	11	12683.287	0.037
12	2	10	11	2	9	13126.909	0.034
7	0	7	6	0	6	7486.450	0.019
7	2	6	6	2	5	7533.433	0.006
7	2	5	6	2	4	7588.246	0.077
7	1	6	6	1	5	7710.262	0.032
8	2	7	7	2	6	8606.317	0.006
10	2	9	9	2	8	10747.937	-0.030
10	3	7	9	3	6	10800.409	0.011
11	3	9	10	3	8	11872.726	0.019
12	2	11	11	2	10	12883.078	-0.050
12	3	9	11	3	8	12977.742	-0.042
13	0	13	12	0	12	13708.183	-0.036

Table SI04. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_3$ (=$^{13}C_5$ due to symmetry) isotopomer of rotamer I, corresponding to the e-d conformer, using the LA-CP-FTMW spectrometer.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs} - \nu_{cal}$
5	1	5	4	1	4	5231.762	0.012
5	0	5	4	0	4	5345.9831	-0.038
5	1	4	4	1	3	5490.7481	-0.010
6	1	6	5	1	5	6275.511	-0.065
6	0	6	5	0	5	6404.635	-0.047
7	0	7	6	0	6	7457.942	0.030
7	2	6	6	2	5	7504.210	0.070
8	0	8	7	0	7	8505.245	0.029
8	1	8	7	1	7	8359.318	0.049
8	1	7	7	1	6	8771.176	0.017
9	1	9	8	1	8	9398.937	0.030
9	0	9	8	0	8	9546.392	0.001
9	1	8	8	1	7	9860.267	0.030
10	0	10	9	0	9	10581.626	0.038
10	1	10	9	1	9	10436.975	-0.001
10	2	9	9	2	8	10706.315	-0.049
11	1	11	10	1	10	11473.428	-0.020
11	0	11	10	0	10	11611.354	0.046
11	2	10	10	2	9	11770.760	-0.013
11	1	10	10	1	9	12029.102	-0.028
12	1	12	11	1	11	12508.327	-0.003
12	0	12	11	0	11	12636.335	-0.016
8	3	6	7	3	5	8595.227	-0.010
8	2	6	7	2	5	8652.605	0.080
9	2	8	8	2	7	9640.332	-0.023
10	2	8	9	2	7	10855.718	0.035
12	2	11	11	2	10	12833.397	-0.047
12	3	10	11	3	9	12903.790	0.005
12	3	9	11	3	8	12926.387	-0.026
13	1	13	12	1	12	13541.653	-0.007
13	0	13	12	0	12	13657.723	0.018
13	2	12	12	2	11	13894.190	-0.051

Table SI05. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_4$ isotopomer of rotamer I, corresponding to the e-d conformer, using the LA-CP-FTMW spectrometer.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs} - \nu_{cal}$
7	0	7	6	0	6	7439.174	-0.001
8	0	8	7	0	7	8484.741	0.075
9	0	9	8	0	8	9524.308	0.045
9	1	8	8	1	7	9829.338	0.069
10	1	10	9	1	9	10413.578	0.006
10	0	10	9	0	9	10558.100	0.039
10	1	9	9	1	8	10912.561	0.032
11	1	11	10	1	10	11447.997	-0.026
11	0	11	10	0	10	11586.490	0.003
12	1	12	11	1	11	12480.912	-0.027
12	0	12	11	0	11	12610.230	-0.029
8	1	8	7	1	7	8340.138	0.041
8	1	7	7	1	6	8743.293	0.028
10	2	9	9	2	8	10676.909	-0.040
11	2	10	10	2	9	11738.734	-0.004
12	2	11	11	2	10	12798.848	-0.027
12	3	9	11	3	8	12886.663	0.010
12	1	11	11	1	10	13068.773	-0.114

Figure SI03. The predicted lowest-energy conformers of glutamine in energetical order from lowest to highest. The first and third lines have the "down" configurations, while the third and fourth lines have their corresponding conformer but with the "up" configuration. The labels are shown in the bottom together with the calculated ΔE_{ZPE} values in cm^{-1}.

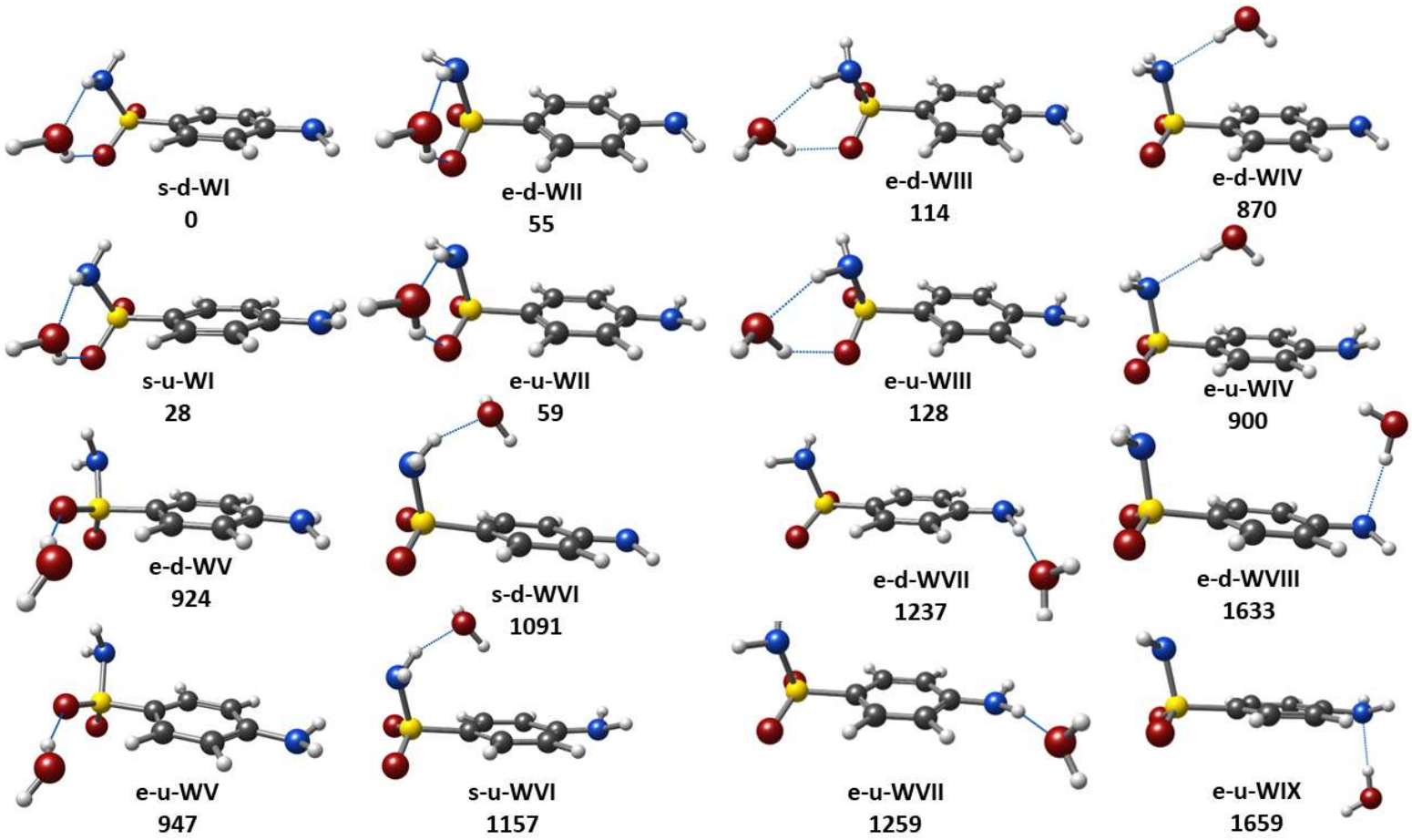

Table SI06. Calculated spectroscopic parameters for the lowest energy conformers of sulfanilamide-water cluster. All the calculations were done using B3LYP-D3(BJ) with the 6-311++G(d,p) basis set. *A*, *B*, and *C* represent the rotational constants (in MHz); μ_a, μ_b, and μ_c are the electric dipole moment components (in D); χ_{aa}, χ_{bb}, and χ_{cc}, are the diagonal elements of the ^{14}N nuclear quadrupole coupling tensor (in MHz); A and S labels make reference to the amino and sulfonil nitrogen atoms, respectively. ΔE is the relative energy (in cm^{-1}) respect to the global minimum. ΔE_{ZPE} is the relative energy (in cm^{-1}) respect to the global minimum, taking into account the zero-point energy (ZPE). ΔG is the Gibbs energies (in cm^{-1}) calculated at 298 K.

Specie	s-d-WI	s-u-WI	e-d-WII	e-u-WII	e-d-WIII	e-u-WIII	e-d-WIV	e-u-WIV	e-d-WV	e-u-WV	s-d-WVI	s-u-WVI	e-u-WVII	e-u-WVII	e-d-WVIII	e-u-WIX
A^a	1407	1407	1467	1466	1922	1901	1366	1374	1135	1134	1345	1347	1802	1798	1648	1755
B	506	506	475	475	410	412	508	509	534	534	517	517	362	361	375	359
C	404	404	396	396	365	366	470	470	393	393	457	457	323	322	370	359
$\lvert\mu_a\rvert$	5.1	5.0	3.4	3.3	5.1	5.0	4.7	4.6	4.0	4.0	8.1	8.0	7.3	7.6	2.0	0.5
$\lvert\mu_b\rvert$	2.9	3.0	1.9	2.4	2.6	2.7	0.7	0.7	1.8	1.8	2.4	3.6	0.7	1.2	0.3	1.2
$\lvert\mu_c\rvert$	1.4	3.0	0.8	2.4	1.0	2.6	0.0	0.3	0.9	2.5	1.1	2.1	2.1	3.6	0.0	5.6
χ_{aa},*NA*	2.66	2.49	2.77	2.21	2.69	2.41	2.70	2.56	2.56	2.61	2.74	2.46	2.59	2.54	1.71	1.39
χ_{bb},*NA*	2.18	2.26	1.67	1.93	2.16	2.24	-4.92	-4.45	2.22	2.22	-2.46	-2.18	1.98	1.96	-3.69	1.73
χ_{cc},*NA*	-4.83	-4.75	-4.44	-4.14	-4.85	-4.65	2.22	1.89	-4.78	-4.84	-0.28	-0.28	-4.58	-4.50	1.98	-3.13
χ_{aa},*NS*	-3.99	-3.99	-2.35	-2.37	-1.73	-1.83	-3.09	-3.08	-2.80	-2.86	-4.55	-4.57	-2.89	-3.38	-4.39	-1.27
χ_{bb},*NS*	0.78	0.78	1.30	1.30	-0.77	-0.54	1.65	1.57	0.19	0.25	1.89	1.86	1.16	1.12	2.78	1.52
χ_{cc},*NS*	3.21	3.21	1.05	1.07	2.50	2.38	1.45	1.51	2.61	2.61	2.66	2.71	1.73	2.26	1.61	-0.25
ΔE^b	0	41	154	159	243	263	1144	1131	1175	1201	1302	1379	1644	1682	1905	1933
$\Delta E_{ZPE}{}^c$	0	28	55	59	114	128	870	900	924	947	1091	1157	1237	1259	1633	1659
ΔG^d	283	304	0	3	18	6	1144	800	642	691	1008	1103	665	693	784	729

Table SI07. Measured frequencies and residuals (in MHz) for the rotational transitions of rotamer II, corresponding to the s-WI conformer, using the LA-CP-FTMW spectrometer.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs} - \nu_{cal}$
7	3	4	6	3	3	6448.807	0.213
7	2	5	6	2	4	6635.755	0.069
8	0	8	7	0	7	6813.917	0.098
8	2	7	7	2	6	7170.192	0.006
8	3	6	7	3	5	7318.686	0.039
8	3	5	7	3	4	7408.802	0.013
8	1	7	7	1	6	7462.613	0.014
3	3	1	2	2	0	7507.873	-0.026
9	1	9	8	1	8	7563.386	-0.040
6	2	5	5	1	4	7565.108	-0.363
9	0	9	8	0	8	7610.924	0.069
8	2	6	7	2	5	7616.914	0.009
9	2	8	8	2	7	8035.138	0.011
7	2	6	6	1	5	8184.506	0.107
9	3	7	8	3	6	8232.431	-0.009
9	4	6	8	4	5	8245.525	0.066
9	4	5	8	4	4	8257.785	0.040
9	1	8	8	1	7	8317.371	-0.032
10	0	10	9	1	9	8328.290	-0.031
10	1	10	9	1	9	8378.405	-0.059
9	3	6	8	3	5	8387.216	0.061
4	3	2	3	2	1	8399.474	0.117
4	3	1	3	2	1	8402.269	0.156
10	0	10	9	0	9	8409.605	-0.001
4	3	2	3	2	2	8438.717	-0.202
4	3	1	3	2	2	8441.640	-0.036
9	2	7	8	2	6	8585.915	-0.023
10	2	9	9	2	8	8890.802	0.056
10	3	8	9	3	7	9140.937	-0.015
10	1	9	9	1	8	9145.949	0.021
11	0	11	10	1	10	9160.437	-0.023
11	1	11	10	1	10	9190.790	-0.037
10	4	6	9	4	5	9199.311	-0.017
11	0	11	10	0	10	9210.552	-0.051
11	1	11	10	0	10	9240.951	-0.019
5	3	3	4	2	2	9260.327	-0.023
5	3	2	4	2	2	9271.376	0.069
10	3	7	9	3	6	9382.449	0.005
5	3	2	4	2	3	9387.779	-0.016
10	2	8	9	2	7	9537.288	-0.051
11	2	10	10	2	9	9737.294	0.039
11	1	10	10	1	9	9952.645	-0.019
12	0	12	11	1	11	9983.194	0.008
12	1	12	11	1	11	10001.277	-0.029
12	0	12	11	0	11	10013.484	-0.069
12	1	12	11	0	11	10031.564	-0.107
11	3	9	10	3	8	10042.403	0.008
6	3	4	5	2	3	10073.570	-0.020
11	4	8	10	4	7	10102.382	-0.007
6	3	3	5	2	3	10106.135	0.087
11	4	7	10	4	6	10152.441	0.050
4	4	1	3	3	0	10334.808	-0.027
4	4	0	3	3	1	10335.223	-0.023
6	3	4	5	2	4	10336.364	-0.036
6	3	3	5	2	4	10368.892	0.033
11	3	8	10	3	7	10388.806	-0.001
11	2	9	10	2	8	10466.878	-0.045
12	2	11	11	2	10	10575.306	0.025
12	1	11	11	1	10	10745.428	-0.035
13	0	13	12	1	12	10799.821	-0.009
13	1	13	12	1	12	10810.510	-0.001
13	0	13	12	0	12	10817.915	-0.034
7	3	5	6	2	4	10825.118	0.044
13	1	13	12	0	12	10828.609	-0.021
7	3	4	6	2	4	10904.655	0.045
12	3	10	11	3	9	10935.301	0.029
12	5	8	11	5	7	11008.614	-0.033

12	4	8	11	4	7	11120.061	-0.043
5	4	2	4	3	1	11243.501	-0.047
5	4	1	4	3	2	11246.518	0.067
7	3	5	6	2	5	11324.319	-0.021
12	2	10	11	2	9	11370.891	-0.046
12	3	9	11	3	8	11396.787	0.008
7	3	4	6	2	5	11403.887	0.005
13	2	12	12	2	11	11405.775	-0.014
8	3	6	7	2	5	11508.059	0.031
13	1	12	12	1	11	11532.615	0.070
14	1	14	13	1	13	11618.904	0.016
14	0	14	13	0	13	11623.347	0.011
14	1	14	13	0	13	11629.569	0.000
8	3	5	7	2	5	11677.631	-0.082
13	5	8	12	5	7	11955.524	0.031
13	4	10	12	4	9	11957.485	0.006
13	4	9	12	4	8	12105.241	0.032
6	4	3	5	3	2	12146.987	0.012
6	4	2	5	3	3	12158.848	0.194
14	2	13	13	2	12	12229.949	-0.009
13	2	11	12	2	10	12246.158	-0.056
14	1	13	13	1	12	12319.950	0.095
8	3	6	7	2	6	12346.873	0.024
13	3	10	12	3	9	12396.105	-0.041
15	0	15	14	1	14	12423.178	0.042
15	1	15	14	1	14	12426.767	0.026
15	0	15	14	0	14	12429.390	0.021
14	3	12	13	3	11	12691.288	-0.038
14	4	11	13	4	10	12879.840	-0.007
14	5	9	13	5	8	12903.790	-0.097
15	2	14	14	2	13	13049.021	-0.019
14	2	12	13	2	11	13091.330	-0.002
5	5	0	4	4	1	13157.779	-0.034
16	1	16	15	1	15	13234.326	0.054
16	0	16	15	0	15	13235.863	0.056
14	3	11	13	3	10	13378.397	-0.068
16	1	15	15	1	14	13904.817	0.040
15	2	13	14	2	12	13908.189	-0.003
8	4	5	7	3	4	13909.923	-0.093
8	4	4	7	3	4	13917.835	-0.038

Table SI08. Measured frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of the rotamer I, corresponding to the e-d conformer, using the LA-MB-FTMW spectrometer.

J'	K'_{-1}	K'_{+1}	I'	F'	J''	K''_{-1}	K''_{+1}	I''	F''	ν_{obs}	$\nu_{obs} - \nu_{cal}$
3	1	2	2	3	2	0	2	1	2	5462.734	0.003
3	1	2	3	2	2	0	2	2	1	5460.758	0.001
3	1	2	3	3	2	0	2	3	2	5460.914	0.003
3	1	2	3	4	2	0	2	3	3	5462.309	-0.002
3	1	3	4	3	2	0	2	3	2	5462.115	0.001
3	1	3	4	3	2	0	2	3	3	5462.866	-0.000
3	1	3	4	4	2	0	2	3	3	5461.958	-0.004
3	1	3	4	5	2	0	2	3	4	5461.910	-0.003
4	1	4	3	2	3	1	3	2	1	4209.095	0.002
4	1	4	4	4	3	1	3	3	3	4208.993	-0.005
4	1	4	4	4	3	1	3	3	4	4209.144	-0.002
4	1	4	5	5	3	1	3	4	4	4208.900	0.001
4	1	4	5	6	3	1	3	4	5	4209.007	0.003
4	2	3	3	3	3	2	2	3	2	4312.841	-0.003
4	2	3	3	4	3	2	2	3	4	4313.105	-0.005
4	2	3	4	3	3	2	2	3	3	4313.671	-0.002
4	2	3	4	5	3	2	2	3	4	4313.593	-0.000
4	2	3	5	4	3	2	2	3	3	4313.407	0.002
4	2	3	5	5	3	2	2	4	4	4312.924	-0.002
4	2	3	5	6	3	2	2	4	5	4313.256	0.001
5	0	5	4	5	4	0	4	3	4	5373.424	0.002
5	0	5	5	4	4	0	4	4	3	5373.404	0.004
5	0	5	5	6	4	0	4	4	5	5373.438	0.003
5	0	5	6	6	4	0	4	5	5	5373.331	-0.003
5	0	5	6	7	4	0	4	5	6	5373.350	0.000
5	2	3	4	4	4	2	2	3	3	5409.331	-0.001
5	2	3	4	5	4	2	2	3	4	5409.511	-0.001
5	2	3	5	4	4	2	2	4	3	5409.663	0.001
5	2	3	5	5	4	2	2	4	4	5409.463	0.001
5	2	3	5	6	4	2	2	4	5	5409.643	0.000
5	2	3	6	6	4	2	2	5	5	5409.345	-0.000
5	2	3	6	7	4	2	2	5	6	5409.526	0.003

Figure SI04. Comparison of the intensity dependence of selected *c*-type transitions of rotamer I, corresponding to the e-d conformer, using different polarization levels: a) 1dBm and b) -6.5 dBm

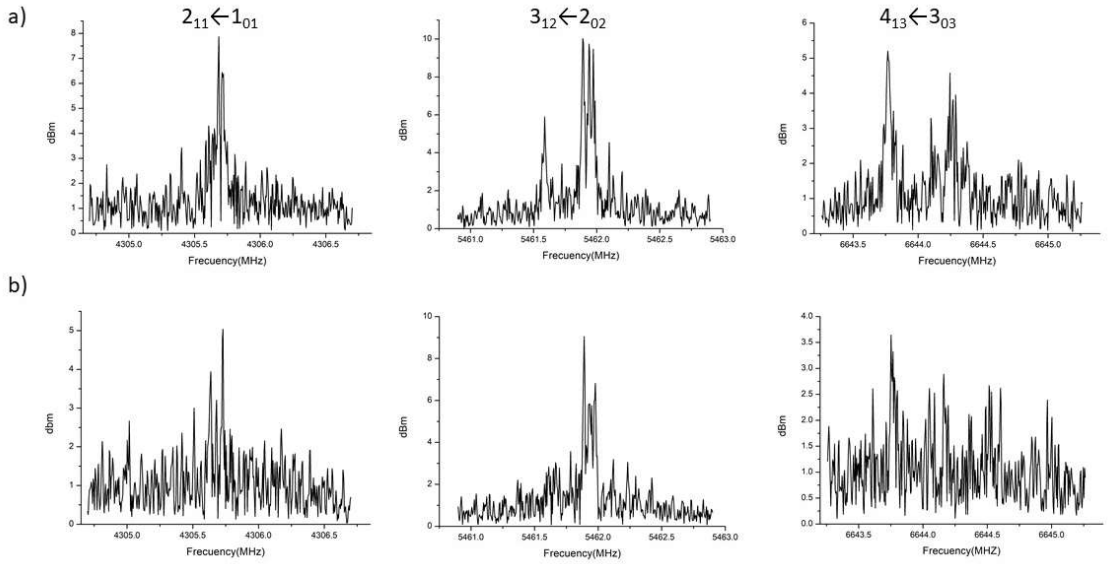

Figure SI05. Comparison of the intensity dependence of selected *a*-type transitions of rotamer I, corresponding to the e-d conformer, using different polarization levels: a) 1dBm and b) -6.5 dBm

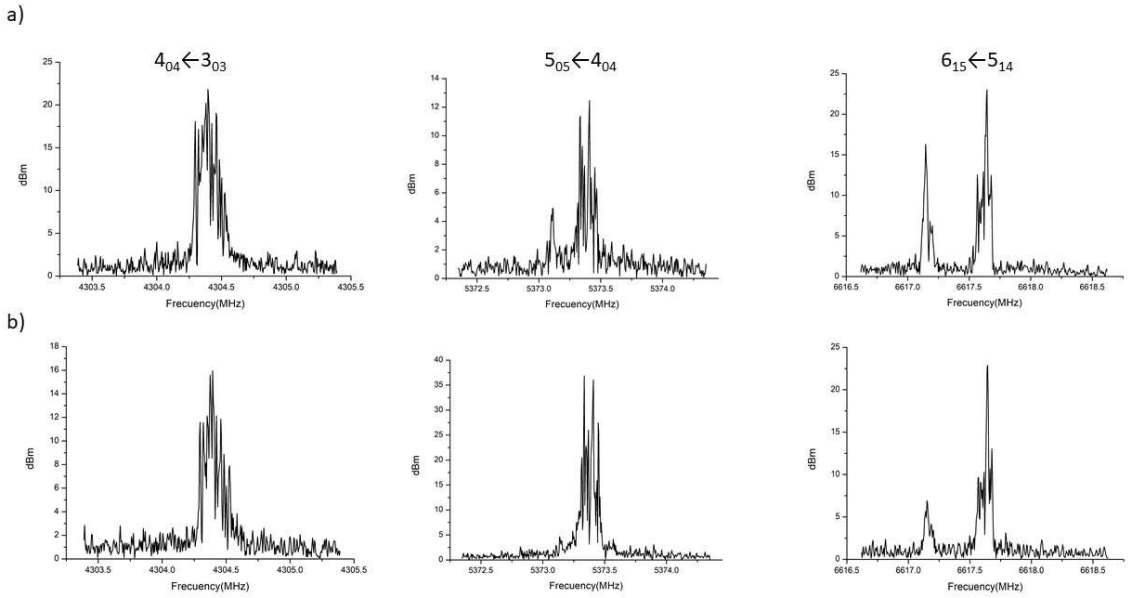

Figure SI06. (a) Relaxed PES rotating the C-C-N-H dihedral angle of SA. This scan shows that the interconversion between the *up* and *down* conformers is lower than 100 cm^{-1}. (b) Relaxed PES rotating the C-S-N-H dihedral angle of SA. This scan shows that the interconversion between the *staggered* and *eclipsed* conformers is higher than 1000 cm^{-1}. (c) Interconversion between the staggered and eclipsed conformers of SA through the transition state using the qst3 method. All the calculations were done using B3LYP-D3(BJ)/6-311++G(d,p). (b) and (c) show only the relevant portion of the molecule for an easier visualization.

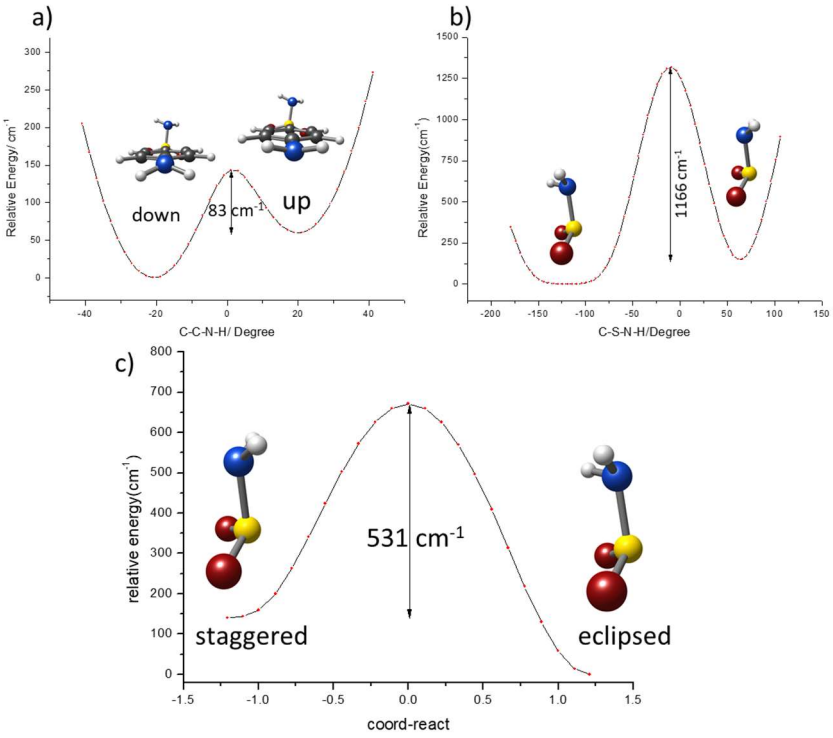

Figure SI07. (a)Interconversion between the staggered and eclipsed conformers of SA-Water through the transition state using the qst3 method. (b) Relaxed PES rotating the H-O-H-O dihedral angle of SA-Water. This scan shows that the interconversion between the *e-WI* and *e-WII* conformers is lower than 28 cm^{-1}. All the calculations were done using B3LYP-D3(BJ)/6-311++G(d,p).

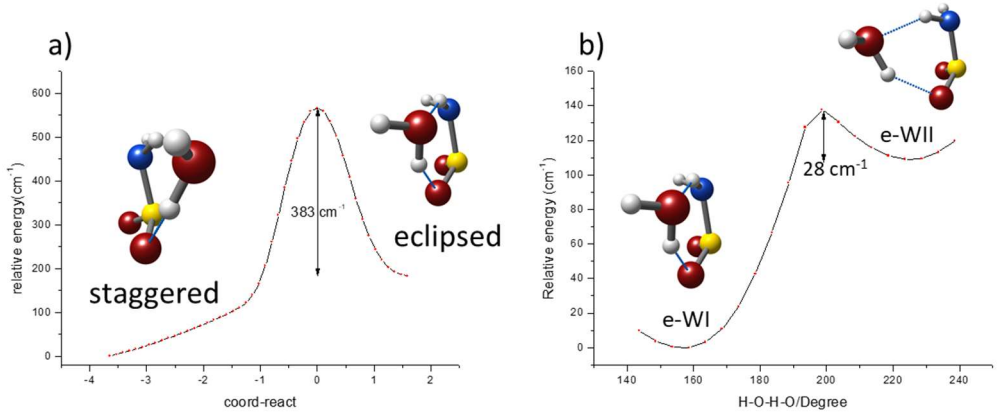

Table SI09. Comparison of the bond strengths of sulfanilamide-water with similar systems.

Specie	Energy/D_0 (kJ mol^{-1})	Method	Reference
SA-WATER staggered	39.0	B3LYP-D3(BJ)/6-311++G(d,p)	This work
SA-WATER eclipsed	33.6	B3LYP-D3(BJ)/6-311++G(d,p)	This work
BA-WATER	37.7	B3LYP-D3(BJ)/6-311++G(d,p)	Ref1 – recalculated
Phenol-water	21.33 / 23.9	B3LYP-D3(BJ)/6-311++G(d,p) // MATI[2]	Ref2
Indole-water	15.97 / 20.4	B3LYP-D3(BJ)/6-311++G(d,p) // MATI[2]	Ref2

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