SUPPORTING INFORMATION

The chemical fate of paroxetine metabolites. Dehydration of radicals derived from 4-(4-fluorophenyl)-3-(hydroxymethyl)piperidine

Davor Šakić,[a] Florian Achrainer,[b] Valerije Vrček,[a,*] and Hendrik Zipse[b]

[a] University of Zagreb, Faculty of Pharmacy and Biochemistry, A. Kovačića 1, HR-10000 Zagreb, Croatia

[b] Department of Chemistry, LMU München, Butenandtstrasse 13, D-81377 München, Germany

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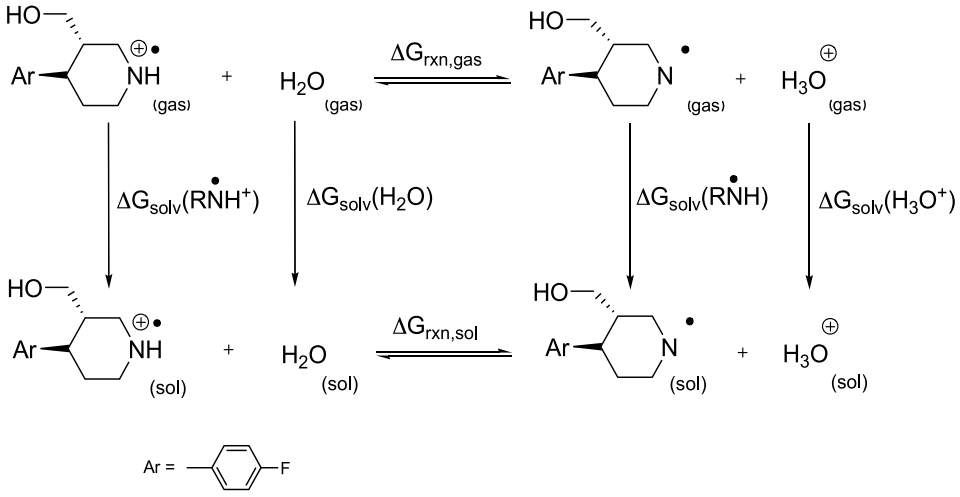
For the calculation of pKa value of radical cation **1b** in water, we have made use of the thermodynamic cycle shown in Scheme S3 and Equations (1) and (2). According to the free-energy cycle (Scheme S3) the overall expression for the reaction free energy for proton transfer from the radical cation to the solvent is:

$$\Delta G_{rxn,sol} = \Delta G_{rxn,gas} + \Delta G_{solv}(RN\cdot) + \Delta G_{solv}(H_3O^+) - \Delta G_{solv}(RNH+/\cdot) - \Delta G_{solv}(H_2O) \quad (1)$$

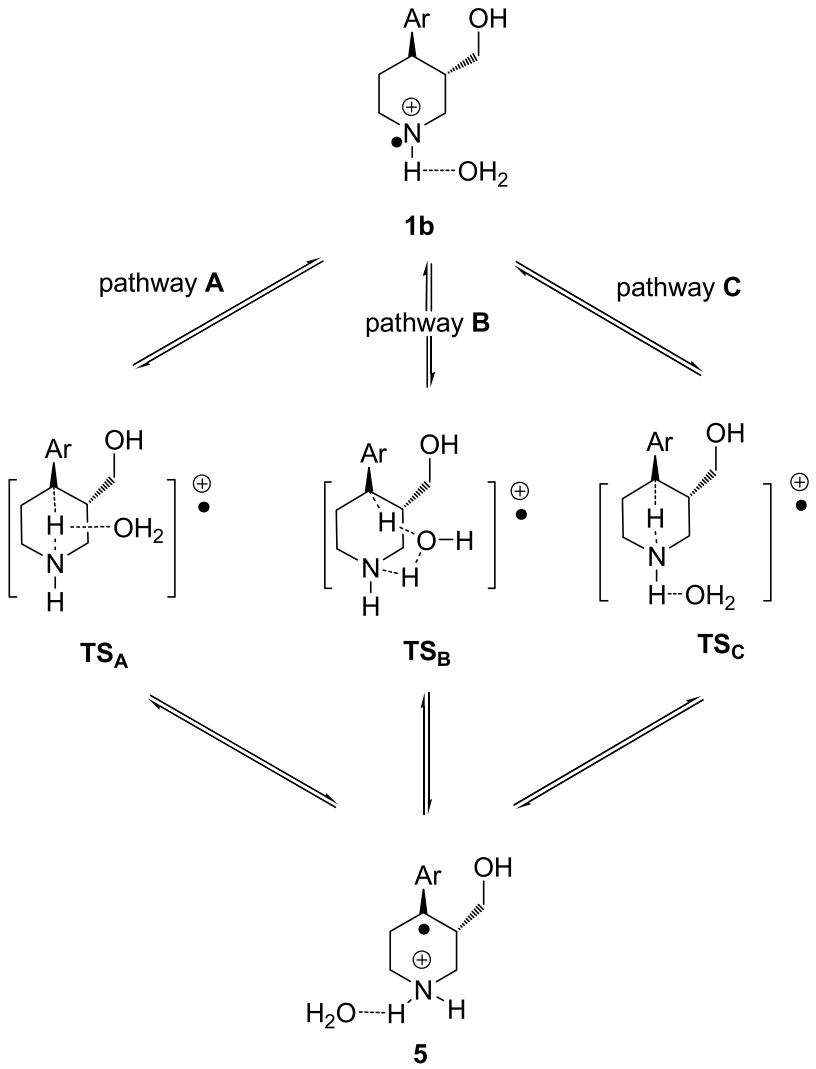
and

$$pK_a = \Delta G_{rxn,sol}/2.303RT - \log [H_2O] \quad (2)$$

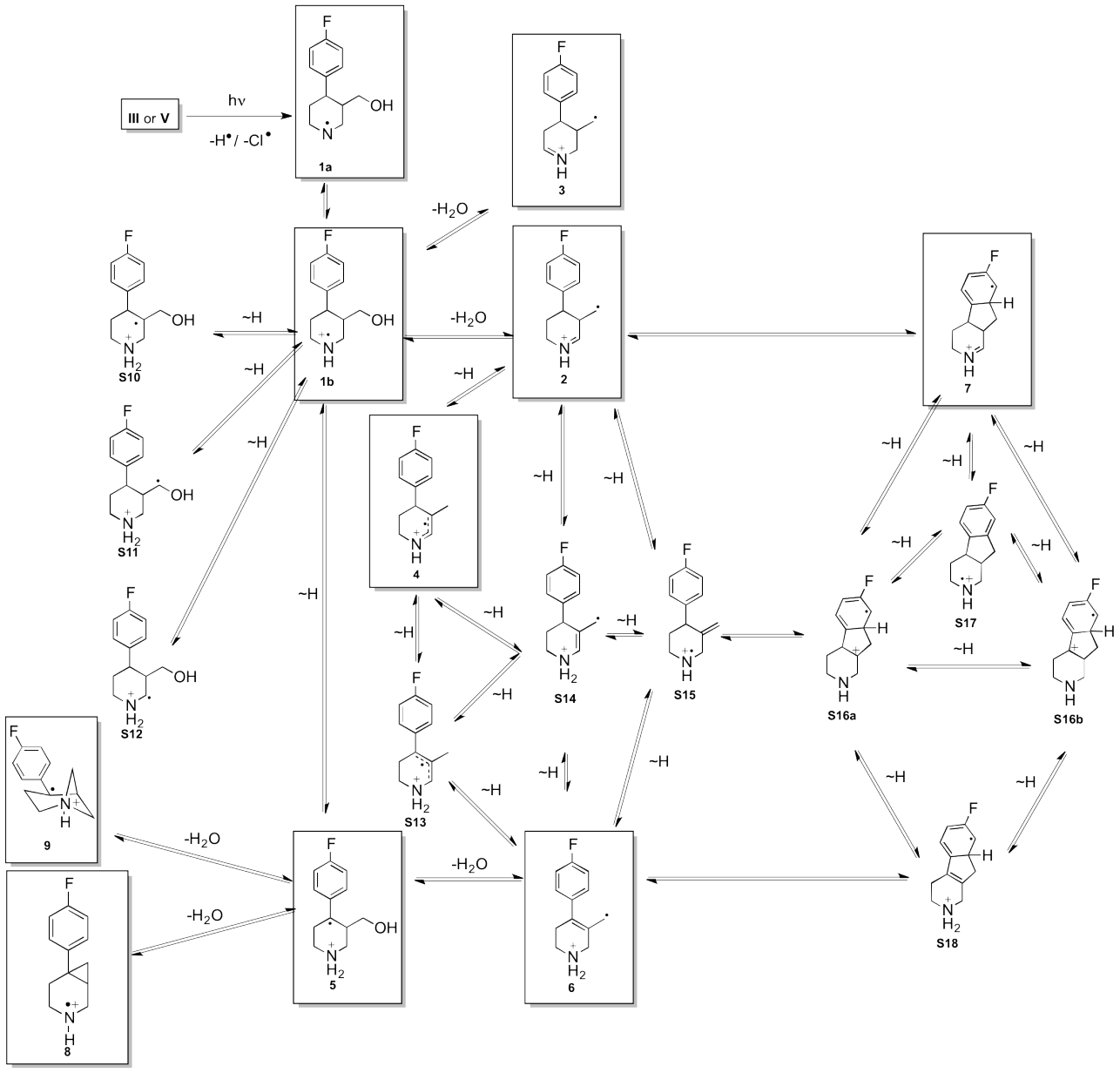


Scheme S1. Free-energy cycle for the calculation of pKa values of paroxetine-derived radical cation **1b** in aqueous solution, calculated at the G3(MP2)-RAD level.
The Gibbs energies of solvation (ΔG_{solv}) for all species are calculated at the CPCM/UAHF/B3LYP/6-31G(d) level (corresponding numbers are in Table S1) using Gaussian03 default parameters (see Ref 24).

In each case, three different water-assisted pathways have been considered: pathway **A** in which the water molecule is bound to the migrating hydrogen throughout the reaction step, pathway **B** in which the water molecule is directly involved in forming *n*-membered ring transition states, and pathway **C** in which a "spectator" water molecule is bound to the amine hydrogen throughout the reaction step. The representative case of 1,4-[N<->C]-hydrogen migration is shown in Scheme S4.



Scheme S2. Different pathways for water-assisted 1,4-[N<->C]-H shifts in paroxetine-derived radical cation **1b**.



Scheme S3. Rearrangement reactions of paroxetine-derived radical cations.
Structures in boxes are discussed in the main text. "~H" denotes hydrogen atom migration.

Table S1. Calculated Gibbs free energies and thermal corrections (in Hartree, at 298.15 K), free energies of solvation (in kcal/mol) and relatives energies (in kJ/mol) for all structures involved in rearrangements of paroxetine-derived radicals presented in Scheme S3.

		B3LYP/ 6-31G(d)		B2K-PLYP/ Def2-TZVPPD		B2-PLYP/ Def2-TZVPPD		B2-PLYPD / aug-cc-pvDz		G3(MP2)RAD	
Structure[a]	**CPCM/ UAKS (kJ/mol)**	**G (Hartree)**	**ΔG + ΔGsolv (kJ/mol)**	**G (Hartree)**	**ΔG + ΔGsolv (kJ/mol)**	**G (Hartree)**	**ΔG + ΔGsolv (kJ/mol)**	**G (Hartree)**	**ΔG + ΔGsolv (kJ/mol)**	**G (Hartree)**	**ΔG + ΔGsolv (kJ/mol)**
1a	-26.36	-695.84039		-695.44304		-695.56661		-693.95859		-695.0203	
1b	-199.62	-696.21156	0.00	-695.79943	0.00	-695.92504	0.00	-694.30959	0.00	-695.3762	0.00
2	-195.98	-696.21865	-14.97	-695.82125	-53.66	-695.94634	-52.29	-694.33484	-62.64	-695.39656	-49.81
3	-198.99	-696.21863	-17.93	-695.8224	-59.70	-695.94714	-57.38	-694.33643	-69.83	-695.39692	-53.76
4	-186.82	-696.26152	-118.35	-695.85858	-142.49	-695.98546	-145.83	-694.37117	-148.87	-695.4315	-132.39
5	-208.70	-696.22925	-55.52	-695.81855	-59.29	-695.95109	-77.49	-694.33601	-78.44	-695.40017	-72.00
6	-205.23	-696.23451	-65.85	-695.82873	-82.53	-695.96029	-98.15	-694.35004	-111.81	-695.40608	-84.03
7	-198.24	-696.21281	-1.90	-695.80948	-25.02	-695.93602	-27.44	-694.32909	-49.80	-695.39349	-44.00
8	-187.53	-696.20385	32.33	-695.79882	13.68	-695.9243	14.03	-694.30953	12.26	-695.4323	-135.20
9	-197.69	-696.20947	7.43	-695.80388	-9.76	-695.93203	-16.43	-694.3238	-35.36	-695.38732	-27.26
TS_1b_2	-205.98	-696.15592	139.73	-695.74942	129.96	-695.87633	126.55	-694.26109	120.99	-695.32256	139.50
TS_1b_3	-210.58	-696.16113	121.44	-695.75891	88.80	-695.88151	96.72	-694.27444	81.34	-695.33316	95.45
TS_1b_5	-187.69	-696.18019	94.31	-695.76801	-37.85	-695.89064	-30.03	-694.28476	77.14	-695.34023	-25.89
TS_2_4	-186.48	-696.18803	74.92	-695.78872	47.82	-695.91619	42.94	-694.30479	25.74	-695.36255	55.55
TS_2_7	-195.60	-696.18202	81.57	-695.77342	76.22	-695.8462	214.94	-694.29944	30.66	-695.36092	48.09
TS_5_6	-220.92	-696.12518	205.50	-695.71392	202.96	-695.84501	188.56	-694.23508	174.33	-695.29507	191.47
TS_5_8	-189.74	-696.16645	128.32	-695.75023	139.04	-695.88296	120.35	-694.26403	129.50	-695.33188	126.24
TS_5_9	-202.42	-696.15212	153.28	-695.73975	160.70	-695.86981	149.03	-694.25889	130.32	-695.32296	143.79
H_2O	-27.36	-76.405441		-76.39280		-76.41278		-76.25738		-76.36031	
1a	-49.62	-772.24426		-771.83584		-771.97939		-770.20997		-771.38061	
1b + H_2O	-226.40	-772.617	0.00	-772.19223	0.00	-772.33782	0.00	-770.56698	0.00	-771.73651	0.00
1b	-192.63	-772.63199	-5.59	-772.20799	-7.63	-772.34993	1.98	-770.58365	-10.01	-771.74931	0.17
2	-187.57	-772.62731	11.77	-772.21468	-20.12	-772.35874	-16.10	-770.59358	-31.03	-771.75688	-14.64
3	-192.84	-772.63168	-4.97	-772.21691	-31.26	-772.36084	-26.88	-770.59635	-43.56	-771.75840	-23.90
4	-184.35	-772.6727	-104.17	-772.25102	-112.31	-772.39708	-113.55	-770.62934	-121.68	-771.79145	-102.20
5	-193.05	-772.64887	-50.32	-772.22137	-43.18	-772.36711	-43.55	-770.60418	-64.34	-771.77041	-55.66
6	-190.41	-772.65144	-54.42	-772.2296	-62.13	-772.37951	-73.47	-770.61749	-96.64	-771.78053	-79.58
7	-192.46	-772.6253	12.16	-772.20352	4.28	-772.34920	4.04	-770.58854	-22.69	-771.75440	-13.02
8	-187.65	-772.61492	44.22	-772.194	34.10	-772.33794	38.43	-770.57038	29.82	-771.73415	44.94
9	-194.43	-772.6144	38.81	-772.19862	15.19	-772.33966	27.15	-770.57977	-1.63	-771.74532	8.85
TS_1b_2	-200.96	-772.58529	108.71	-772.16829	88.30	-772.30948	99.84	-770.54730	77.11	-771.70860	98.72
TS_1b_3	-217.19	-772.5783	110.82	-772.15975	94.47	-772.30111	105.59	-770.54120	76.90	-771.70076	103.08
TS_1b_5	-319.95	-772.55732	63.14	-772.1322	64.04	-772.27721	65.58	-770.51756	36.19	-771.68197	49.64
TS_2_4	-179.91	-772.60103	88.42	-772.1843	67.28	-772.33114	64.02	-770.56512	51.36	-771.72485	77.10
TS_2_7	-191.67	-772.59423	94.52	-772.16721	100.42	-772.31787	87.11	-770.55888	55.99	-771.72187	73.17
TS_5_6	-221.17	-772.54741	187.95	-772.11413	210.28	-772.26145	205.73	-770.50197	175.91	-771.65995	206.25
TS_5_8	-245.81	-772.56055	128.82	-772.1447	105.36	-772.29645	89.20	-770.52452	92.07	-771.69386	92.58
TS_5_9	-195.60	-772.56209	174.97	-772.13393	183.86	-772.28295	174.86	-770.51850	158.08	-771.68481	166.53
S10	-257.15	-772.59509	26.78								
S11	-263.09	-772.59697	15.90								
S12	-267.86	-772.60096	0.65								
S13	-249.28	-772.64308	-85.77								
S14	-260.62	-772.62347	-45.62								
S15	-258.07	-772.61412	-18.51								
S16a	-209.07	-696.1608	93.71								
S16b	-219.07	-696.20051	-52.37								
S17	-236.81	-696.23763	-224.07								
S18	-269.28	-696.22226	-319.57								
STS_1b_S10	-230.37	-772.56448	133.93								
STS_1b_S11	-236.73	-772.57144	109.28								

		B3LYP/ 6-31G(d)		B2K-PLYP/ Def2-TZVPPD		B2-PLYP/ Def2-TZVPPD		B2-PLYPD / aug-cc-pvDz		G3(MP2)RAD	
Structure[a]	**CPCM/ UAKS (kJ/mol)**	**G (Hartree)**	**ΔG + ΔGsolv (kJ/mol)**	**G (Hartree)**	**ΔG + ΔGsolv (kJ/mol)**	**G (Hartree)**	**ΔG + ΔGsolv (kJ/mol)**	**G (Hartree)**	**ΔG + ΔGsolv (kJ/mol)**	**G (Hartree)**	**ΔG + ΔGsolv (kJ/mol)**
STS_1b_S12	-329.66	-772.53534	111.15								
STS_2_S14	-246.19	-696.15531	-47.15								
STS_2_S15	-247.15	-696.17989	-115.71								
STS_3_S14	-246.19	-696.15531	-47.15								
STS_4_S13	-199.20	-696.18417	73.67								
STS_4_S14	-228.28	-696.11848	124.46								
STS_6_S13	-243.63	-696.13973	4.43								
STS_6_S14	-244.35	-696.13836	5.06								
STS_6_S15	-208.87	-696.18837	22.19								
STS_6_S18	-258.24	-696.1879	-183.14								
STS_7_16b	-239.24	-696.12594	59.01								
STS_7_S16a	-276.23	-696.15305	-166.90								
STS_S13_ S14	-239.20	-696.13933	24.05								
STS_S14_ S15	-246.52	-696.15418	-45.58								
STS_S15_ S16a	-249.49	-696.15175	-51.64								
STS_S16a_ S16b	-238.40	-696.15599	-16.38								
STS_S16b_ S18	-217.44	-696.15825	65.41								

[a] First section corresponds to structures without explicit water molecules, next section contains structures with explicit water molecule and the last section presents structures in Scheme S3 that were not discussed in the article.

B3LYP/6-31G(d) Cartesian coordinates for structures presented in Scheme S3 and Table S1

1b

C -1.654533 0.609276 -0.121880
C -3.153446 0.187593 0.065993
C -2.572209 -2.198925 -0.038877
C -1.044392 -1.857506 -0.229878
C -0.716420 -0.488996 0.416491
H -3.371847 0.118976 1.139903
H -3.811855 0.926914 -0.389441
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H -2.829277 -3.117863 -0.570162
H -0.462954 -2.668452 0.222252
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H -0.894693 -0.580713 1.497455
N -3.359004 -1.109533 -0.523921
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O -2.334044 2.880927 -0.022967
H -2.276000 3.727323 0.446863
C 0.772304 -0.254453 0.209186
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C 1.295751 0.217164 -1.013800
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H 1.287519 -0.974665 2.184127
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H 3.741993 -0.679211 1.874564
H 3.078826 0.754453 -2.119918
F 4.831630 0.201073 -0.302083

2

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4

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5

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H 1.674105 2.543065 -0.199056
C -0.440631 0.687764 0.528720
C -1.237709 1.856087 -0.042163
C -0.794907 -0.607757 -0.239875
H -0.756190 0.537648 1.577912
C -2.736985 1.563558 0.138442
H -1.002334 1.995865 -1.103838
H -1.011693 2.798683 0.466682
C -2.257308 -0.833904 -0.267367
H -3.356424 2.159259 -0.538636
H -3.067338 1.780976 1.160727
H -2.699925 -1.811721 -0.458261
C 0.169514 -1.688625 0.312947
H 0.427195 -2.429808 -0.447594
H -0.266154 -2.216535 1.166850
N -3.090154 0.140893 -0.111976
H -4.100925 -0.100365 -0.164384
O -5.587892 -0.999081 -0.342078
H -6.184557 -1.205922 0.394334
H -6.155428 -0.953385 -1.127525
H -0.517096 -0.446601 -1.297770

8
C -1.110991 -1.202124 -0.209146
C -2.168760 -0.630629 -1.215727
C -2.523500 1.436133 0.100355
C -1.118244 1.244481 0.686461
C -0.359828 -0.050646 0.476366
H -1.621163 -0.078855 -1.992929
H -2.752296 -1.431278 -1.673560
H -1.626963 -1.848266 0.507884
H -0.423253 -1.827079 -0.786680
H -2.445285 2.219893 -0.675652
H -3.242687 1.793454 0.843893
N -3.047795 0.251604 -0.519271
C -0.882228 0.350488 1.869835
H -1.710331 -0.231020 2.267657
H -0.528504 2.156646 0.667374
C 1.115279 -0.025561 0.219167
C 1.740668 1.015710 -0.488166
C 1.906633 -1.101604 0.676898
C 3.109620 0.995386 -0.732231
H 1.152900 1.848840 -0.862026
C 3.275123 -1.136812 0.445814
H 1.442094 -1.908959 1.236704
C 3.858390 -0.083298 -0.258872
H 3.605038 1.790124 -1.279435
H 3.895766 -1.951553 0.802675
H -0.161803 0.678321 2.612892
H -4.034626 -0.025573 -0.371396
F 5.173650 -0.105408 -0.486418
O -5.667738 -0.672120 -0.287929
H -6.100912 -1.091160 0.471213
H -6.387332 -0.398269 -0.877059

9
C 0.902031 1.518947 0.118511
C 2.400028 1.427765 -0.272266
C 2.170743 -0.980862 -0.869929
C 1.117890 -0.994234 0.282442
C 0.188397 0.177258 0.130189
H 2.565522 1.645497 -1.330541
H 3.012676 2.113081 0.318458
H 0.829850 1.995595 1.108065
H 0.422978 2.216390 -0.575578
H 1.878080 -0.613374 -1.854696
H 2.768525 -1.891876 -0.945638
N 2.943214 0.040130 -0.043274
H 3.982403 0.009991 -0.118464
C 2.319367 -0.598927 1.192883
H 2.938503 -1.444939 1.496502
H 2.170634 0.094513 2.021525
H 0.637931 -1.945404 0.499188
C -1.229147 0.067064 0.061457
C -1.894446 -1.194748 -0.003118
C -2.059680 1.228784 0.054979
C -3.273859 -1.289334 -0.071418
H -1.321894 -2.115878 -0.017654
C -3.440091 1.139691 -0.010187
H -1.613991 2.215281 0.120819
C -4.035990 -0.120123 -0.073880
H -3.772883 -2.251000 -0.126390
H -4.064974 2.026469 -0.007883
F -5.369756 -0.210553 -0.138471
O 5.713382 -0.283545 -0.216944
H 6.358632 -0.141421 0.492824
H 6.234799 -0.318175 -1.033815

TS_1b_3
N -3.092145 -1.206978 -0.181567
C -2.097804 -0.910006 -1.230452
C -1.380727 0.406599 -0.863750
C -0.587510 0.285744 0.493530
C -2.343123 1.592769 -0.860651
C -2.666118 -1.030048 1.145926
C -1.191817 -0.844272 1.378551
H -2.615266 -0.830754 -2.192171
H -1.357560 -1.714938 -1.322392
H -0.668754 0.637602 -1.665569
H -0.741735 1.227924 1.037371
H -2.853207 1.760496 -1.810716
H -1.888989 2.520221 -0.513488
H -3.288588 -1.508902 1.896413
H -0.995489 -0.638239 2.434186
H -0.678500 -1.794559 1.156277
O -3.503381 1.381400 0.114962
H -3.150285 0.860666 0.934925
C 0.914198 0.149312 0.289148
C 1.486488 -1.007830 -0.263341
C 1.762461 1.210106 0.635082
C 2.860662 -1.105028 -0.470245
H 0.866464 -1.858857 -0.534545
C 3.140502 1.131224 0.438330
H 1.346961 2.114534 1.073613
C 3.669132 -0.029141 -0.115283
H 3.310527 -1.996550 -0.893821
H 3.801832 1.946919 0.709964
F 4.992119 -0.117831 -0.309524
H -4.039498 0.635524 -0.268461
H -3.702990 -1.999535 -0.365666

S10 with 1 H_2O
C -1.641201 -0.386594 -0.210252
C -2.572173 -0.574630 -1.238105
C -3.942744 -0.560567 -0.970542
C -4.398990 -0.356651 0.331578
C -3.479140 -0.166816 1.365724
C -2.111180 -0.183059 1.096278
H -2.225754 -0.736351 -2.256594
H -4.650977 -0.709235 -1.780399
H -5.464412 -0.345503 0.541410
H -3.826925 -0.006736 2.382237
H -1.405790 -0.029529 1.910781
C -0.148309 -0.438481 -0.509524
C 0.612353 0.821974 -0.160895
C 0.507442 -1.674681 0.167565
H -0.040712 -0.588856 -1.601035
C 2.103136 0.774872 -0.249733
C 2.019429 -1.723986 -0.022475
H 0.272676 -1.675747 1.239343
H 0.075308 -2.591980 -0.244923
H 2.558580 1.664497 0.186756
H 2.469157 0.673750 -1.284763
H 2.482789 -2.548438 0.525464
H 2.303148 -1.807750 -1.075889
C -0.041537 2.169816 -0.232553
H -0.441255 2.327911 -1.254156
H -0.912138 2.197065 0.439733
O 0.916783 3.163175 0.102712
H 0.489548 4.031374 0.052378
N 2.645171 -0.443232 0.473871
H 3.684382 -0.492571 0.361538
H 2.442960 -0.339367 1.474311
O 5.372841 -0.756524 0.008238
H 6.026316 -1.107767 0.632938
H 5.887386 -0.272536 -0.656214

S11 with 1 H_2O
C -1.599294 -0.281451 -0.190862
C -2.478088 0.249335 -1.143013
C -3.859849 0.132425 -0.984742
C -4.383515 -0.518383 0.132628
C -3.517938 -1.050509 1.090330
C -2.137574 -0.932686 0.928554
H -2.077658 0.761187 -2.014990
H -4.525342 0.549470 -1.735168
H -5.458316 -0.611650 0.257336
H -3.917038 -1.559017 1.963358
H -1.482558 -1.356214 1.687797
C -0.096544 -0.155489 -0.389815
C 0.573188 0.719153 0.717557
C 0.584478 -1.538849 -0.487363
H 0.071322 0.364838 -1.341499
C 2.105727 0.762577 0.529683
C 2.089650 -1.436341 -0.699883
H 0.382377 -2.129762 0.416471
H 0.156739 -2.104416 -1.321830
H 2.604105 1.257107 1.367369
H 2.362072 1.290587 -0.392253
H 2.586279 -2.410050 -0.701768
H 2.340175 -0.917935 -1.629939
C 0.039780 2.115508 0.733376
H -0.114382 2.670037 1.654648
O 0.276121 2.815845 -0.420231
H -0.126038 3.696505 -0.359121
N 2.710714 -0.621530 0.410851
H 3.742442 -0.547155 0.254277
H 2.575359 -1.118598 1.297919

O 5.426703 -0.483754 -0.189975
H 6.140529 -1.027114 0.178016
H 5.868345 0.217951 -0.692592
H 0.353874 0.276476 1.698944

S12 with 1 H_2O
C 1.240414 -0.345274 0.184814
C 1.851835 0.168484 1.337861
C 3.243990 0.238554 1.439499
C 4.043365 -0.211494 0.389099
C 3.445446 -0.729230 -0.762550
C 2.056587 -0.794026 -0.864872
H 1.235858 0.509519 2.167753
H 3.698954 0.640630 2.339964
H 5.125222 -0.158986 0.464964
H 4.061858 -1.079767 -1.585074
H 1.612538 -1.193396 -1.773707
C -0.277003 -0.420747 0.100046
C -0.874459 0.444127 -1.049708
C -0.780157 -1.875470 -0.054305
H -0.673783 -0.027870 1.048182
C -2.278551 0.052312 -1.328438
C -2.296614 -1.987384 0.146160
H -0.508158 -2.251108 -1.046362
H -0.292322 -2.527703 0.676316
H -3.518053 1.906891 1.849881
H -2.730797 -2.799887 -0.439076
H -2.567847 -2.125073 1.195612
C -0.741386 1.987247 -0.784943
O 0.563841 2.462388 -0.970692
H 1.145863 2.072264 -0.297799
N -3.005956 -0.691764 -0.294607
H -3.135233 -0.084909 0.554636
H -0.298449 0.270463 -1.970946
H -3.947837 -0.919790 -0.624315
H -1.133552 2.204165 0.223199
H -1.362107 2.526530 -1.507254
O -3.221446 0.985612 1.919296
H -3.339919 0.743853 2.851413
H -2.870511 0.389933 -2.169946

S13 with 1 H_2O
C 1.477424 0.631512 -0.344209
C 0.588106 -0.401496 0.037870
C 1.156177 -1.621941 0.475476
C 2.532119 -1.794707 0.555901
C 3.358419 -0.742768 0.172207
C 2.856014 0.471313 -0.286726
H 1.083343 1.562861 -0.734064
H 0.519326 -2.437452 0.803095
H 2.968562 -2.720726 0.914404
H 3.549261 1.253001 -0.587077
C -0.863117 -0.237727 -0.055172
C -1.555657 0.962858 0.261746
C -1.668639 -1.416982 -0.571060
C -2.903266 1.101708 0.012641
C -3.151350 -1.338029 -0.237721
H -1.535842 -1.502313 -1.661846
H -1.288215 -2.360224 -0.167400
H -3.497010 1.966178 0.276190
H -3.741899 -2.089262 -0.767016
H -3.332629 -1.425415 0.835824
H -4.680193 0.115751 -0.368583
C -0.893226 2.145086 0.945272
H -0.075551 1.824608 1.593963
H -0.484297 2.855475 0.219151
N -3.671288 0.023368 -0.632695
F 4.693811 -0.913053 0.246438
H -3.628558 0.108477 -1.657433
H -6.648735 0.340544 1.050393
O -6.313251 0.363751 0.141174
H -1.620834 2.689232 1.554670
H -7.076685 0.583276 -0.414681
H 5.925084 0.971157 -0.193536
O 5.699519 1.855138 -0.521645
H 6.331426 2.014665 -1.238722

S14 with 1 H_2O
C 1.364429 -1.855303 0.278624
C 0.588065 -0.709791 0.066087
C 1.237424 0.506096 -0.199493
C 2.626513 0.587438 -0.255492
C 3.358725 -0.575553 -0.038352
C 2.758169 -1.798509 0.227794
H 0.882039 -2.807181 0.487669
H 0.656692 1.412839 -0.353266
H 3.152593 1.518553 -0.448993
H 3.370641 -2.678194 0.393808
C -0.932044 -0.799660 0.088081
C -1.585617 0.168121 1.086329
C -1.522649 -0.631355 -1.328966
H -1.195703 -1.809411 0.432277
C -2.754035 0.839020 0.781116
C -3.039665 -0.529077 -1.297474
H -1.101329 0.259502 -1.813069
H -1.235388 -1.484350 -1.951227
H -3.249468 1.526530 1.455786
H -3.486002 -0.437343 -2.290520
H -3.500651 -1.374166 -0.779483
H -4.474071 0.698018 -0.367143
H -3.237925 1.533941 -1.100289
C -1.024441 0.342964 2.353395
H -1.490198 0.988742 3.091185
H -0.103595 -0.155862 2.630420
N -3.435250 0.707085 -0.519321
F 4.710171 -0.514486 -0.081802
O -6.169400 0.527684 -0.142267
H -6.869463 1.019936 -0.598309
H -6.597558 0.109538 0.620646
H 5.523719 1.542585 -0.220224
O 5.218959 2.447553 -0.389780
H 5.765162 2.748852 -1.131309

S15 with 1 H_2O
C 1.384554 -1.936045 -0.097984
C 0.523675 -0.829786 -0.057988
C 1.080880 0.462913 -0.092555
C 2.458931 0.655773 -0.137864
C 3.275413 -0.470632 -0.159721
C 2.766371 -1.766644 -0.141946
H 0.975524 -2.942814 -0.080843
H 0.434171 1.335935 -0.074276
H 2.915254 1.642306 -0.150757
H 3.444300 -2.613249 -0.157077
C -0.983165 -1.046042 -0.029586
C -1.719136 -0.464839 1.169504
C -1.591194 -0.494880 -1.345662
H -1.169183 -2.131396 -0.022711
C -3.241659 -0.660272 1.111494
C -3.156484 -0.645553 -1.346620
H -1.342095 0.563706 -1.467346
H -1.202742 -1.033409 -2.216294
H -3.492818 -1.729425 1.110196
H -3.591132 -0.135466 -2.208752
H -3.404279 -1.714351 -1.375551
H -4.026466 0.900343 -0.163141
C -1.164518 0.146380 2.220192
H -1.760085 0.563568 3.027495
H -0.084604 0.210640 2.321311
N -3.673918 -0.078115 -0.141450
F 4.613267 -0.306322 -0.199844
H -3.749725 -0.168513 1.942072
O -4.652805 2.496761 -0.484672
H -5.600571 2.685051 -0.566099
H -4.239564 3.343230 -0.255556
H 5.319138 1.862816 0.082210
O 4.853372 2.712831 0.107024
H 5.366347 3.285746 -0.482545

S16a
F -3.921416 1.752586 -0.223546
C -2.910061 0.885417 -0.232239
C -2.857105 -0.103706 0.707205
C -1.922927 1.068826 -1.245365
C -1.753468 -1.099007 0.675521
H -3.643913 -0.188516 1.450404
C -0.817730 0.230070 -1.306906
H -2.046799 1.891971 -1.941008
C -0.715568 -0.852402 -0.413690
H -2.177729 -2.113879 0.623633
H -0.024725 0.429008 -2.018760
C 0.465297 -1.808549 -0.243249
C 1.627690 -1.778889 -1.246395
C 0.476374 -0.838359 0.873662
H 0.114662 -2.811558 0.014163
C 2.769896 -0.860149 -0.785395
H 1.264030 -1.463804 -2.229501
H 1.999666 -2.800877 -1.367205
C 1.522036 0.220404 0.969892
H 3.434732 -0.644814 -1.626008
H 3.370543 -1.382928 -0.017907
H 1.097207 1.172140 1.309595
H 2.182366 -0.130030 1.798212
C -0.681577 -1.014844 1.841367
H -0.830130 -0.140471 2.478377
H -0.626604 -1.914276 2.464273
O 4.058184 2.534960 0.574524
H 4.971554 2.414127 0.875961
H 4.046459 3.423344 0.186785
H 2.939433 1.118134 -0.167609
N 2.219912 0.399513 -0.283446

S16b
F 4.910468 -0.565490 -0.469266
C 3.650567 -0.275865 -0.131999
C 2.770255 -1.267755 0.158692
C 3.313271 1.120183 -0.090113
C 1.397337 -0.904723 0.611759
H 3.096477 -2.303285 0.163192
C 2.023667 1.524468 0.152424
H 4.100885 1.835916 -0.303649
C 1.015445 0.540641 0.362317
H 1.390215 -1.069537 1.708995
H 1.767742 2.578719 0.098788
C -0.350385 0.657434 0.264503
C -1.171966 1.873090 -0.035112
C -0.993480 -0.697972 0.308017
H -1.436944 -0.881584 1.299535

C -2.683147 1.628396 0.083075
H -0.934994 2.200193 -1.059683
H -0.899882 2.717618 0.610525
C -2.186079 -0.726846 -0.707576
H -3.228730 2.427083 -0.438514
H -2.977515 1.708268 1.143073
H -2.729895 -1.674043 -0.662668
C 0.168105 -1.682420 0.047903
H 0.299233 -1.837897 -1.029384
H 0.026300 -2.657354 0.520772
N -3.107325 0.339038 -0.430550
H -4.057727 0.042701 -0.189301
O -5.566384 -1.027851 0.081381
H -6.240540 -1.087912 -0.612791
H -6.051500 -1.157139 0.910541
H -1.756524 -0.634580 -1.716570

S17
F -4.929034 -0.347835 0.685672
C -3.657969 -0.081846 0.375004
C -2.793709 -1.146887 0.119708
C -3.253793 1.259642 0.322230
C -1.482960 -0.834956 -0.212103
H -3.160911 -2.166012 0.181765
C -1.932461 1.560537 -0.000227
H -3.981723 2.035553 0.533235
C -1.049394 0.514893 -0.272469
H -1.609393 2.596533 -0.041480
C 0.409772 0.541426 -0.662466
C 1.347948 1.625155 -0.139346
C 0.852752 -0.848414 -0.150555
C 2.797894 1.265436 -0.615329
H 1.313994 1.679061 0.954966
H 1.118263 2.620616 -0.534088
C 2.272752 -1.174768 -0.696571
H 3.547890 1.922439 -0.171753
H 2.820505 1.384162 -1.710234
H 2.216975 -1.219683 -1.795764
C -0.328097 -1.772171 -0.509854
H -0.362325 -2.702526 0.064689
H -0.298011 -2.038879 -1.577144
N 3.139299 -0.098453 -0.298699
O 5.280480 -0.278466 1.474513
H 6.190062 -0.467595 1.197415
H 5.273023 -0.398011 2.436361
H 2.671896 -2.117807 -0.317017
H 0.479122 0.535764 -1.766356
H 0.920640 -0.795199 0.944274
H 3.905955 -0.269283 0.376752

S18
F 4.668996 -0.161824 0.733032
C 3.415024 -0.129194 0.244860
C 2.709100 1.030903 0.272939
C 2.900548 -1.364572 -0.251799
C 1.367456 1.060601 -0.393677
H 3.162348 1.941060 0.652019
C 1.555842 -1.453705 -0.630457
H 3.548724 -2.233633 -0.246689
C 0.764853 -0.316345 -0.602949
H 1.518084 1.487904 -1.407454
H 1.132738 -2.426654 -0.868753
C -0.663559 -0.166478 -0.626104
C -1.675632 -1.221164 -0.992327
C -1.007471 1.076819 -0.178551
C -3.060577 -0.601933 -1.180728
H -1.718335 -2.000337 -0.219923
H -1.400144 -1.724607 -1.926134
C -2.415648 1.543900 -0.011263
H -3.853345 -1.353205 -1.183610
H -3.123724 -0.014404 -2.100641
H -2.746252 2.225886 -0.806473
C 0.204272 1.887324 0.230874
H 0.289969 1.926810 1.328327
H 0.184133 2.923700 -0.125044
N -3.351966 0.351229 -0.038202
H -3.261604 -0.175581 0.863065
O -3.008463 -1.197815 2.249185
H -3.683697 -1.626784 2.797916
H -2.204494 -1.179688 2.791382
H -2.578860 2.052548 0.946100
H -4.320278 0.680389 -0.102352

STS_1b_S10 with 1 H_2O
C -1.647381 -0.364096 -0.202026
C -2.706182 -0.303213 -1.116039
C -4.023602 -0.168822 -0.673068
C -4.297270 -0.088255 0.692115
C -3.248606 -0.144266 1.613324
C -1.933957 -0.283643 1.169412
H -2.503329 -0.369061 -2.182751
H -4.832908 -0.129216 -1.396109
H -5.321177 0.015541 1.038445
H -3.454084 -0.083088 2.678033
H -1.130643 -0.328538 1.902323
C -0.223211 -0.525858 -0.713716
C 0.703705 0.664262 -0.433028
C 0.441049 -1.831749 -0.170569
H -0.266777 -0.606679 -1.811464
C 2.066131 0.508499 -1.102753
C 1.974666 -1.847913 -0.332962
H 0.209499 -1.915382 0.896576
H 0.003988 -2.706111 -0.660215
H 2.670705 1.411068 -1.024483
H 2.083224 0.101819 -2.117595
H 2.440230 -2.534584 0.377226
H 2.274715 -2.136905 -1.347936
C 0.178750 2.048782 -0.165809
H -0.362833 2.364900 -1.079490
H -0.558685 2.024712 0.645500
O 1.275024 2.896167 0.117369
H 0.942201 3.793634 0.271493
N 2.505310 -0.490728 -0.081696
H 3.459525 -0.407703 0.332090
H 1.477211 0.133026 0.621811
O 5.036589 -0.470397 1.075135
H 5.258653 -0.009747 1.898769
H 5.875853 -0.571115 0.600343

STS_1b_S11 with 1 H_2O
C 1.255207 -0.319935 0.179131
C 1.959285 0.268586 1.244430
C 3.350572 0.382554 1.203206
C 4.061719 -0.100259 0.098480
C 3.376160 -0.697696 -0.961992
C 1.987640 -0.808127 -0.923417
H 1.417000 0.623256 2.118999
H 3.879112 0.841491 2.033263
H 5.143691 -0.016281 0.069892
H 3.924144 -1.082363 -1.816676
H 1.471375 -1.295344 -1.746999
C -0.259963 -0.425504 0.237553
C -0.956290 0.236396 -0.981942
C -0.768896 -1.881944 0.382852
H -0.589343 0.104223 1.141645
C -2.350404 -0.364866 -1.245757
C -2.278894 -1.906589 0.683100
H -0.546867 -2.440646 -0.533555
H -0.232271 -2.385050 1.192029
H -3.001394 0.356081 -1.753497
H -2.703866 -2.861791 0.349936
H -2.458608 -1.821999 1.759335
C -1.023125 1.788739 -0.837504
O 0.169142 2.420539 -0.623092
H 0.747904 1.896956 -0.025009
N -2.983641 -0.767283 0.021493
H -2.967299 0.634006 0.931018
H -0.345319 0.084816 -1.885511
H -3.956306 -1.022144 -0.143592
H -1.716558 1.921014 0.114962
H -1.522332 2.292965 -1.671878
O -2.679112 1.530638 1.347863
H -3.450933 2.125185 1.377253
H -2.244963 -1.220951 -1.929071

STS_1b_S12 with 1 H_2O
C 1.335340 -0.363085 0.209025
C 2.047402 0.025901 1.353260
C 3.442668 0.106904 1.335854
C 4.145519 -0.206613 0.172844
C 3.447619 -0.599599 -0.971895
C 2.055574 -0.675516 -0.954662
H 1.508662 0.258812 2.269598
H 3.975610 0.409443 2.232515
H 5.229520 -0.146029 0.156638
H 3.988105 -0.844418 -1.881531
H 1.532689 -0.977229 -1.859202
C -0.184363 -0.452795 0.252274
C -0.878153 0.573444 -0.679328
C -0.700688 -1.870308 -0.072053
H -0.493601 -0.221970 1.283873
C -2.360534 0.326842 -0.824487
C -2.198985 -1.970004 0.197418
H -0.488393 -2.124625 -1.117693
H -0.184743 -2.610431 0.548344
H -3.229723 1.126830 0.536835
H -2.611665 -2.929616 -0.123321
H -2.385158 -1.881396 1.275083
C -0.619564 2.056283 -0.292385
O 0.657118 2.520133 -0.639631
H 1.318466 2.050368 -0.105233
N -2.975241 -0.901382 -0.502890
H -4.062028 -0.130418 0.754801
H -0.456624 0.459933 -1.693893
H -3.580841 -1.258240 -1.239747
H -0.833870 2.181094 0.785556
H -1.322382 2.696132 -0.839562
O -3.980453 0.778102 1.222063
H -4.809215 1.298804 1.151199
H -2.872456 0.858039 -1.628676

STS_2_4
C -2.096622 -0.163000 -1.310125
C -1.133573 -0.178845 -0.292513
C -1.565937 -0.125366 1.042489
C -2.920908 -0.057395 1.357435
C -3.848900 -0.045859 0.319204
C -3.458001 -0.097841 -1.013961
H -1.784429 -0.207035 -2.350709

H -0.845147 -0.144979 1.857882
H -3.265935 -0.018874 2.385084
H -4.210195 -0.088569 -1.795378
C 0.346083 -0.270110 -0.639378
C 1.145959 0.983488 -0.243252
C 1.018122 -1.527500 -0.042483
H 0.426547 -0.329074 -1.733728
C 2.544854 0.831999 0.023896
C 2.509729 -1.590113 -0.368575
H 0.884505 -1.541496 1.045094
H 0.525948 -2.421499 -0.435582
H 3.156690 1.692865 0.283419
H 3.003872 -2.391598 0.187091
H 2.679275 -1.776070 -1.437240
H 4.178641 -0.318067 0.210859
C 0.573738 2.317424 -0.495444
H 1.180944 3.209318 -0.388718
H -0.489314 2.399572 -0.676981
N 3.169467 -0.327361 -0.008029
F -5.153797 0.018653 0.615739
H 0.684472 1.557767 0.728741
O 5.823552 0.219674 0.640291
H 6.549067 0.256649 -0.002260
H 6.247278 0.026060 1.490884

H 0.905835 0.536969 -1.758605
H 3.344240 0.683435 -2.216140
H 4.196361 -0.689869 1.753605
C -0.335730 -0.319816 0.557812
C -1.131111 0.983054 0.401579
C -0.967400 -1.464614 -0.270909
H -0.438060 -0.602888 1.615570
C -2.492012 0.915957 -0.033032
C -2.462760 -1.626867 0.002845
H -0.805309 -1.293351 -1.343167
H -0.464355 -2.404716 -0.028519
H -3.181138 1.749829 0.060850
H -2.912923 -2.404959 -0.618599
H -2.643006 -1.877553 1.057586
H -4.210044 -0.307319 -0.268284
C -0.605282 2.210167 0.681217
H -1.200741 3.115573 0.606200
H 0.428721 2.318970 0.988182
N -3.169775 -0.364575 -0.268570
F 5.194879 0.087175 -0.508496
H -2.684536 0.387109 -1.206239
O -5.857660 0.245315 -0.269519
H -6.430678 0.202922 0.512153
H -6.453302 0.149720 -1.029365

H 0.905835 0.536969 -1.758605
H 3.344240 0.683435 -2.216140
H 4.196361 -0.689869 1.753605
C -0.335730 -0.319816 0.557812
C -1.131111 0.983054 0.401579
C -0.967400 -1.464614 -0.270909
H -0.438060 -0.602888 1.615570
C -2.492012 0.915957 -0.033032
C -2.462760 -1.626867 0.002845
H -0.805309 -1.293351 -1.343167
H -0.464355 -2.404716 -0.028519
H -3.181138 1.749829 0.060850
H -2.912923 -2.404959 -0.618599
H -2.643006 -1.877553 1.057586
H -4.210044 -0.307319 -0.268284
C -0.605282 2.210167 0.681217
H -1.200741 3.115573 0.606200
H 0.428721 2.318970 0.988182
N -3.169775 -0.364575 -0.268570
F 5.194879 0.087175 -0.508496
H -2.684536 0.387109 -1.206239
O -5.857660 0.245315 -0.269519
H -6.430678 0.202922 0.512153
H -6.453302 0.149720 -1.029365

STS_2_7
C 1.269698 1.654627 0.778271
C 2.727166 1.551536 0.293680
C 2.397453 -0.891614 0.045529
C 0.950290 -0.800688 0.379940
C 0.429378 0.614319 0.028243
H 2.881728 2.109890 -0.636640
H 3.433244 1.945821 1.031135
H 1.211055 1.488518 1.860016
H 0.919086 2.674141 0.590363
H 0.625516 0.763450 -1.045669
N 3.151772 0.156696 0.006667
C -0.014185 -1.807865 -0.201768
H -0.034345 -2.809700 0.220509
H -0.190181 -1.758556 -1.274068
C -1.080061 0.533096 0.168577
C -1.935750 1.370495 -0.529110
C -1.576357 -0.709510 0.712506
C -3.292242 1.052634 -0.690169
H -1.548546 2.270417 -1.001976
C -2.953895 -1.028143 0.536561
H -1.132460 -1.101451 1.628290
C -3.760715 -0.161426 -0.175981
H -3.971289 1.703608 -1.229222
H -3.385036 -1.916544 0.985018
F -5.054060 -0.469379 -0.348837
O 5.655169 -0.768391 -0.690035
H 6.054419 -0.709858 -1.572153
H 6.398181 -0.896020 -0.079609
H 4.148802 0.002267 -0.246510
H 2.883968 -1.840930 -0.174877
H 0.923952 -0.915159 1.480867

STS_2_S15
C 2.081906 -0.346769 1.297081
C 1.146275 -0.212860 0.262824
C 1.611648 0.043047 -1.037402
C 2.974077 0.159984 -1.301048
C 3.874814 0.016314 -0.248889
C 3.449927 -0.235660 1.050947
H 1.744413 -0.548182 2.310921
H 0.911550 0.156178 -1.861299
H 3.345293 0.355438 -2.301318
H 4.181466 -0.343985 1.844390
C -0.337297 -0.367112 0.559420
C -1.132611 0.942884 0.369314
C -1.000598 -1.488745 -0.278041
H -0.427824 -0.646889 1.616930
C -2.564858 0.804111 0.114213
C -2.484401 -1.652644 0.049359
H -0.886294 -1.271667 -1.345754
H -0.482117 -2.431540 -0.084484
H -2.127790 1.023271 1.349430
H -2.963112 -2.356805 -0.637221
H -2.621991 -2.043970 1.067611
H -4.200005 -0.331628 -0.197559
C -0.531040 2.212548 0.334010
H -1.121677 3.111902 0.187593
H 0.533918 2.315301 0.492357
N -3.178910 -0.369801 -0.071579
F 5.186610 0.125267 -0.497496
H -3.154480 1.693657 -0.100240
O -5.852538 0.363488 -0.420093
H -6.556404 0.286157 0.242725
H -6.308818 0.335476 -1.275560

STS_4_S13
C -1.518850 0.529253 -0.948968
C -0.925455 -0.025964 0.225210
C -1.746893 -0.828855 1.066571
C -3.083283 -1.032320 0.780465
C -3.620587 -0.454382 -0.377420
C -2.849092 0.321622 -1.252478
H -0.903301 1.108764 -1.629036
H -1.334398 -1.271702 1.965522
H -3.723366 -1.624127 1.425751
H -3.307343 0.735959 -2.143876
C 0.484390 0.190105 0.482531
C 1.190891 1.469034 0.030962
C 1.207449 -0.375012 1.730605
H 1.256066 -0.519332 -0.318508
C 2.444111 1.153951 -0.331885
C 2.657097 -0.680860 1.251367
H 1.192665 0.354262 2.547910
H 0.741210 -1.292042 2.099344
H 3.253300 1.813927 -0.622912
H 3.418938 -0.137973 1.818254
H 2.886998 -1.748604 1.284949
H 3.413044 -0.707748 -0.766522
C 0.620858 2.846391 0.185113
H 1.318889 3.598239 -0.194549
H -0.331591 2.961291 -0.342376
N 2.687954 -0.257429 -0.181408
F -4.902453 -0.654045 -0.657706
H 0.424840 3.071859 1.241235
O 4.701087 -1.699547 -1.545914
H 4.574486 -2.211157 -2.359417
H 5.653453 -1.524612 -1.501688

STS_2_S14
C 2.092028 -0.515236 1.252594
C 1.151905 -0.176311 0.271487
C 1.613209 0.257286 -0.981298
C 2.975851 0.348749 -1.252328
C 3.881428 0.000292 -0.253358
C 3.461165 -0.430421 0.999514
H 1.756975 -0.852374 2.230637

STS_3_S14
C 2.092028 -0.515236 1.252594
C 1.151905 -0.176311 0.271487
C 1.613209 0.257286 -0.981298
C 2.975851 0.348749 -1.252328
C 3.881428 0.000292 -0.253358
C 3.461165 -0.430421 0.999514
H 1.756975 -0.852374 2.230637

STS_4_S14
C -2.065718 1.347791 -0.348871
C -1.221909 0.229428 -0.265539
C -1.796809 -1.027134 -0.021682
C -3.174523 -1.166529 0.138813
C -3.978043 -0.034313 0.053687
C -3.443429 1.227071 -0.190297
H -1.643418 2.330639 -0.543779

H -1.184882 -1.923004 0.030951
H -3.629506 -2.134226 0.320301
H -4.101543 2.086527 -0.257905
C 0.270659 0.444168 -0.423690
C 1.117102 0.474739 0.824489
C 1.034100 -0.697937 -1.234475
H 0.441226 1.382680 -0.964076
C 2.475661 0.948396 0.577982
C 2.572463 -0.592700 -1.234854
H 0.736438 -1.659623 -0.808704
H 0.679028 -0.672691 -2.268841
H 2.760322 1.912896 0.166502
H 3.013963 -1.541869 -1.551609
H 2.909257 0.187210 -1.927587
H 4.165289 -0.210323 0.115465
C 1.075867 -0.496321 1.825951
H 1.652888 -0.337709 2.738438
H 0.212401 -1.148592 1.920162
N 3.128638 -0.264897 0.136482
F -5.301925 -0.163444 0.204610
H 2.176045 -0.934638 1.092248
O 5.927155 0.223909 0.089064
H 6.483371 0.134932 0.878355
H 6.536214 0.121831 -0.658385

H 1.568726 -2.221058 -0.638203
H 3.990745 -2.020896 -0.190050
H 3.490634 2.110799 0.839570
C -0.321152 -0.266296 -0.452997
C -1.162151 0.762399 -0.735250
C -1.022345 -1.620379 -0.409367
C -2.580887 0.611521 -1.072617
C -2.374361 -1.505282 0.305388
H -1.159515 -2.042234 -1.415471
H -0.435752 -2.348870 0.156544
H -2.801280 0.584039 -2.142214
H -2.891686 -2.465839 0.365870
H -2.242299 -1.113183 1.315334
H -3.998423 -0.171953 0.307617
C -1.135017 2.249124 -0.798801
H -0.537005 2.785066 -1.537544
H -1.260300 2.769196 0.153112
N -3.319003 -0.541277 -0.399463
F 5.165759 0.154604 0.580394
H -3.867193 -1.045409 -1.103149
H -2.566358 2.003456 -0.965485
O -4.906523 0.352249 1.690531
H -5.666704 -0.115938 2.069659
H -5.051560 1.288443 1.898138

H 1.434756 -1.720876 -1.557843
H 3.819520 -1.847075 -0.921385
H 3.285775 1.370460 1.873750
C -0.456647 0.014472 -0.536652
C -1.152814 1.345630 -0.542626
C -1.115570 -0.955109 -1.546817
H -1.300620 -0.413734 0.412704
C -2.596725 1.146422 -0.081918
C -2.607494 -1.080588 -1.110600
H -1.018347 -0.575399 -2.568976
H -0.640648 -1.938049 -1.509376
H -2.796569 1.661590 0.863071
H -3.300014 -0.683916 -1.860823
H -2.885479 -2.114594 -0.898118
C -0.628495 2.525025 -0.905395
H -1.232080 3.429144 -0.924328
H 0.407722 2.622446 -1.211387
N -2.715177 -0.301577 0.141073
F 4.944883 -0.320882 0.834345
H -3.330782 1.488396 -0.822164
O -4.703098 -0.882828 2.070432
H -4.560535 -1.332710 2.917024
H -5.659435 -0.923833 1.918249
H -3.436630 -0.595098 0.820526

STS_5_6
C 0.682873 -0.350431 -0.075525
C 1.362229 0.763581 -0.639901
C 2.747025 0.861681 -0.639816
C 3.495873 -0.161725 -0.061832
C 2.884238 -1.283483 0.493427
C 1.499075 -1.374683 0.479486
H 0.792489 1.525304 -1.162408
H 3.257677 1.701366 -1.100060
H 3.497415 -2.063411 0.932584
H 1.041515 -2.245748 0.936825
C -0.759184 -0.451151 -0.081143
C -1.389884 -1.811967 0.146389
C -1.638146 0.736420 -0.030489
C -2.800973 -1.957821 -0.420623
H -1.434530 -2.050085 1.226369
H -0.790893 -2.609730 -0.306360
C -3.044220 0.543905 -0.498972
H -1.147000 2.160837 -0.652656
H -3.284616 -2.879432 -0.087959
H -2.808572 -1.926526 -1.513676
H -3.726334 1.335206 -0.176965
C -1.426794 1.737066 1.052462
H -0.562501 1.569075 1.692116
H -2.286143 2.110913 1.610096
O -1.065703 2.998833 0.135661
H -0.143883 3.309862 0.268085
N -3.657199 -0.794565 0.028200
H -3.131047 0.424126 -1.583527
H -3.694435 -0.771098 1.053924
H -4.620598 -0.908951 -0.307061
F 4.832756 -0.068751 -0.050310

STS_6_S14
C 1.766471 -1.273077 -0.366697
C 1.079655 -0.058263 -0.135954
C 1.825481 1.029051 0.376290
C 3.188246 0.923852 0.618164
C 3.826041 -0.286967 0.356664
C 3.129543 -1.390814 -0.131274
H 1.239791 -2.145553 -0.737705
H 1.328029 1.967165 0.592752
H 3.762148 1.759181 1.004702
H 3.659517 -2.318524 -0.318178
C -0.372289 0.059331 -0.342542
C -1.113207 1.381038 -0.296970
C -1.121458 -0.888514 -1.298001
H -1.142396 -0.124840 0.804563
C -2.228476 0.901620 0.566969
C -2.537232 -1.180465 -0.786326
H -1.154104 -0.434795 -2.297127
H -0.620380 -1.853162 -1.402974
H -2.734249 1.518402 1.308166
H -3.196204 -1.581110 -1.559787
H -2.508663 -1.881074 0.050966
H -3.999788 -0.219999 0.374627
H -3.568660 0.634517 -1.002177
C -0.869749 2.594777 -0.789165
H -1.547310 3.425608 -0.609274
H 0.023515 2.809278 -1.368393
N -3.194006 0.071991 -0.226898
F 5.139355 -0.394603 0.583070
O -5.201238 -0.921066 1.409618
H -6.151939 -0.979526 1.227264
H -5.113699 -1.028973 2.369346

STS_6_S18
C 1.096352 0.460620 0.251384
C 1.631688 -0.794978 0.730048
C 3.019643 -1.045853 0.564232
C 3.802416 -0.090134 -0.060249
C 3.301831 1.146400 -0.485305
C 1.933946 1.405557 -0.331827
H 1.154181 -1.255931 1.592174
H 3.484518 -1.939445 0.966266
H 3.972221 1.864538 -0.943582
H 1.526271 2.334456 -0.722437
C -0.366386 0.453966 0.155517
C -1.225705 1.687089 0.292566
C -0.862568 -0.775880 -0.126847
C -2.688616 1.319166 0.527211
H -1.132399 2.331409 -0.594440
H -0.888540 2.297196 1.138365
C -2.336577 -1.049655 -0.261908
H -3.364543 2.166349 0.388451
H -2.843497 0.903785 1.526499
H -2.558976 -1.675191 -1.132075
C 0.118457 -1.867888 -0.331543
H 0.570863 -1.940299 -1.320448
H -0.066817 -2.832842 0.139621
N -3.113188 0.239915 -0.442302
H -2.765269 -1.547058 0.616798
H -2.960967 0.581572 -1.397109
H -4.135639 0.039762 -0.338712
F 5.113498 -0.327650 -0.213607
O -5.760655 -0.499974 -0.053776
H -6.366144 -0.850057 -0.725695
H -6.316085 -0.299469 0.715443

STS_6_S13
C 1.685796 1.068420 0.257736
C 1.109863 -0.153575 -0.155412
C 1.963946 -1.267554 -0.302399
C 3.329975 -1.170019 -0.064694
C 3.853625 0.054562 0.340194
C 3.046812 1.178049 0.508584
H 1.056723 1.938070 0.412520

STS_6_S15
C 1.520858 0.793281 0.766921
C 0.960125 -0.077749 -0.210598
C 1.816027 -1.044814 -0.801458
C 3.155210 -1.123916 -0.460861
C 3.659917 -0.240896 0.499334
C 2.855134 0.717259 1.122636
H 0.883280 1.520748 1.257201

STS_7_16b
F -4.781920 -0.368641 0.394574
C -3.486857 -0.111255 0.163409
C -2.674684 -1.103961 -0.297576
C -3.038751 1.206023 0.446312
C -1.248493 -0.787587 -0.627278
H -3.079438 -2.087633 -0.511498
C -1.669942 1.517450 0.330455

H -3.752420 1.934143 0.814391
C -0.792502 0.548519 -0.094045
H -1.189297 -0.733216 -1.736941
H -1.318600 2.491841 0.658004
C 0.678249 0.567076 -0.057807
C 1.647376 1.609214 0.494897
C 1.135140 -0.930994 -0.030399
H 0.959853 0.731421 -1.261089
C 2.879384 1.611905 -0.470337
H 1.949681 1.343416 1.512316
H 1.176949 2.596821 0.516373
C 1.903285 -0.415796 -1.214702
H 3.785861 1.991871 0.002559
H 2.667086 2.228963 -1.350092
H 1.636026 -0.649558 -2.248319
C -0.136853 -1.782902 -0.177599
H -0.383962 -2.199859 0.803061
H -0.012250 -2.618902 -0.871581
N 3.112198 0.208570 -0.900393
H 3.542191 -0.286232 -0.106142
O 4.134802 -1.284157 1.437481
H 4.647102 -2.083360 1.235141
H 4.584923 -0.895272 2.204106
H 1.787659 -1.199558 0.799475

H 0.922624 1.446055 -1.281797
H 3.313344 1.131764 -1.892859
H 3.792919 -1.655525 1.329800
C -0.434230 0.253544 0.786689
C -1.244463 1.352181 0.151487
C -1.308690 -0.977413 0.974320
H -0.486899 1.262254 1.800812
C -2.308024 1.146355 -0.622044
C -1.837829 -1.365881 -0.412809
H -0.754734 -1.831965 1.371683
H -2.143296 -0.777221 1.656819
H -3.040021 1.885509 -0.925262
H -1.005267 -1.554331 -1.093630
H -2.493667 -2.238798 -0.387646
H -3.672100 -0.404213 -0.758230
C -0.888248 2.472028 1.043102
H -1.650229 3.160010 1.405307
H 0.112821 2.887127 0.927939
N -2.671148 -0.238157 -1.024169
F 4.944610 -0.448171 -0.649326
O -5.227547 -0.934101 -0.204993
H -5.676214 -0.584180 0.580483
H -5.931600 -1.299745 -0.763207
H -2.633115 -0.329203 -2.045857

H 0.541466 0.690836 -1.433287
H 2.401520 2.296581 -0.947018
H 4.364708 -1.176431 0.595906
C -0.372354 -1.220243 0.403358
C -1.061542 0.109643 0.610348
C -1.128598 -2.062607 -0.672249
H -0.379323 -1.819819 1.329249
C -2.539036 0.187525 0.625462
C -2.625400 -2.072031 -0.335542
H -0.986657 -1.620444 -1.664436
H -0.722672 -3.079345 -0.690822
H -2.837672 -0.086656 1.667688
H -3.165925 -2.659887 -1.083672
H -2.774819 -2.568435 0.642937
C -0.128417 1.243103 0.546533
H -0.570099 2.176807 0.185347
H 0.398280 1.440272 1.487670
N -3.131682 -0.703296 -0.375273
F 4.652722 1.230486 -0.211459
H -2.905319 1.207083 0.462684
O -4.440054 2.640057 -0.113004
H -4.760229 2.812974 -1.011136
H -5.011653 3.182535 0.451267
H -4.144350 -0.674584 -0.291605

STS_7_S16a

F 4.908826 -0.623056 -0.576923
C 3.663878 -0.281443 -0.209799
C 2.799457 -1.255283 0.196100
C 3.327615 1.092466 -0.293466
C 1.438576 -0.867125 0.686607
H 3.129786 -2.286947 0.256740
C 1.998064 1.494726 -0.011473
H 4.076758 1.800588 -0.626975
C 1.084766 0.580557 0.426174
H -0.722630 0.788344 1.621313
H 1.713674 2.529300 -0.185195
C -0.412217 0.704251 0.548427
C -1.207025 1.793698 -0.214225
C -0.903048 -0.647310 0.213171
H 1.399466 -1.049136 1.780785
C -2.719547 1.677766 0.049539
H -0.981380 1.687197 -1.281162
H -0.857947 2.783642 0.089583
C -2.303741 -0.782618 -0.117036
H -3.258051 2.155923 -0.779621
H -2.982693 2.229522 0.959081
H -2.762295 -1.762587 0.051080
C 0.207551 -1.633755 0.089691
H 0.385501 -1.833585 -0.979829
H -0.022400 -2.599900 0.554309
N -3.159575 0.282975 0.217422
H -4.128197 0.078404 -0.033751
O -5.570545 -1.116803 -0.460636
H -6.105824 -1.091180 -1.268880
H -6.206368 -1.306070 0.246894
H -2.021431 -0.817987 -1.231199

STS_S14_S15

C -2.106739 -0.506733 -1.224935
C -1.147738 -0.195414 -0.252735
C -1.585738 0.219280 1.015164
C -2.943512 0.318385 1.308492
C -3.867710 -0.002542 0.317628
C -3.470801 -0.413849 -0.949405
H -1.790184 -0.829948 -2.213751
H -0.864554 0.475993 1.787236
H -3.293576 0.636998 2.284508
H -4.219870 -0.654363 -1.696086
C 0.332325 -0.340371 -0.569462
C 1.114828 0.976943 -0.520892
C 1.023481 -1.382318 0.347070
H 0.407936 -0.718307 -1.600397
C 2.537425 0.905797 -0.387569
C 2.467737 -1.645655 -0.071685
H 0.993409 -1.042056 1.388346
H 0.474713 -2.327419 0.302917
H 3.175235 0.245831 -1.313609
H 3.005317 -2.252804 0.662153
H 2.515956 -2.170914 -1.032319
H 4.189060 -0.285350 0.201043
C 0.540006 2.208773 -0.623515
H 1.137671 3.115849 -0.606601
H -0.532850 2.321589 -0.724440
N 3.228169 -0.376173 -0.190771
F -5.176245 0.090628 0.594882
H 3.148689 1.761089 -0.115768
O 5.721603 0.278698 0.783953
H 6.562848 0.106000 0.332599
H 5.945010 0.352013 1.725075

STS_S16a_S16b

F -4.974838 -0.525700 0.439479
C -3.703937 -0.240608 0.125960
C -2.818087 -1.257049 -0.074707
C -3.360395 1.136322 0.051383
C -1.432372 -0.923091 -0.532642
H -3.146764 -2.289592 -0.021052
C -2.016886 1.510250 -0.152538
H -4.132732 1.876691 0.225249
C -1.072283 0.539043 -0.366037
H -1.378645 -1.156437 -1.618977
H -1.739351 2.558170 -0.080164
C 0.394863 0.626899 -0.312928
C 1.233357 1.877339 -0.063172
C 0.898913 -0.686539 0.005279
H 0.808313 0.139842 -1.331233
C 2.624879 1.478779 0.465055
H 0.705657 2.500727 0.667212
H 1.313157 2.455834 -0.988229
C 2.353702 -0.903695 0.164740
H 2.563637 1.328664 1.559004
H 3.338452 2.285704 0.285130
H 2.696071 -1.781443 -0.397830
C -0.226880 -1.669051 0.116954
H -0.400991 -1.801409 1.199930
H -0.013326 -2.655655 -0.302922
N 3.085703 0.276754 -0.230634
H 4.089356 0.108081 -0.123471
O 5.756797 -0.852050 0.082798
H 6.379336 -0.758293 0.820083
H 6.320292 -0.950289 -0.700118
H 2.467544 -1.181758 1.240053

STS_S13_S14

C 1.811602 -0.810094 1.115590
C 0.978998 0.064259 0.384827
C 1.540760 0.768321 -0.699350
C 2.875870 0.599840 -1.054783
C 3.659973 -0.278590 -0.313022
C 3.145272 -0.988205 0.771350
H 1.416408 -1.342168 1.976552

STS_S15_S16a

C 2.212397 -1.404089 0.406096
C 1.034870 -0.775762 0.066018
C 1.034367 0.614410 -0.452256
C 2.332822 1.294342 -0.535818
C 3.463197 0.631022 -0.144537
C 3.429550 -0.709276 0.301980
H 2.209306 -2.409467 0.816943

STS_S16b_S18

F -4.996382 -0.541322 -0.000431
C -3.692162 -0.261648 -0.117882
C -2.777264 -1.266135 -0.147026
C -3.346695 1.124258 -0.186542
C -1.342780 -0.918725 -0.380958
H -3.098484 -2.302427 -0.117576
C -2.016720 1.521719 -0.186963

H -4.152281 1.850927 -0.172205
C -1.014171 0.544409 -0.159194
H -1.163867 -1.108278 -1.462072
H -1.770447 2.577697 -0.119330
C 0.344471 0.654474 0.183577
C 1.227234 1.850751 0.369035
C 0.911157 -0.644489 0.332953
H 1.714773 -0.432789 -0.772643
C 2.698429 1.551558 -0.091567
H 1.239421 2.095863 1.439062
H 0.842655 2.734812 -0.147362
C 2.317712 -0.696098 0.916622
H 3.390625 2.022908 0.615620
H 2.890398 1.973682 -1.081586
H 2.736831 -1.703409 0.903242
C -0.205410 -1.676112 0.366023
H -0.497798 -1.878186 1.405296
H 0.055933 -2.629341 -0.101117
N 2.955179 0.100905 -0.178867
H 3.934957 -0.145376 -0.391070
O 5.596969 -0.921005 -0.569982
H 6.396471 -0.678218 -0.078706
H 5.919326 -1.289000 -1.406842
H 2.444125 -0.259036 1.914614
H -2.615266 -0.830754 -2.192171
H -1.357560 -1.714938 -1.322392
H -0.668754 0.637602 -1.665569
H -0.741735 1.227924 1.037371
H -2.853207 1.760496 -1.810716
H -1.888989 2.520221 -0.513488
H -3.288588 -1.508902 1.896413
H -0.995489 -0.638239 2.434186
H -0.678500 -1.794559 1.156277
O -3.503381 1.381400 0.114962
H -3.150285 0.860666 0.934925
C 0.914198 0.149312 0.289148
C 1.486488 -1.007830 -0.263341
C 1.762461 1.210106 0.635082
C 2.860662 -1.105028 -0.470245
H 0.866464 -1.858857 -0.534545
C 3.140502 1.131224 0.438330
H 1.346961 2.114534 1.073613
C 3.669132 -0.029141 -0.115283
H 3.310527 -1.996550 -0.893821
H 3.801832 1.946919 0.709964
F 4.992119 -0.117831 -0.309524
H -4.039498 0.635524 -0.268461
H -3.702990 -1.999535 -0.365666
H -0.845147 -0.144979 1.857882
H -3.265935 -0.018874 2.385084
H -4.210195 -0.088569 -1.795378
C 0.346083 -0.270110 -0.639378
C 1.145959 0.983488 -0.243252
C 1.018122 -1.527500 -0.042483
H 0.426547 -0.329074 -1.733728
C 2.544854 0.831999 0.023896
C 2.509729 -1.590113 -0.368575
H 0.884505 -1.541496 1.045094
H 0.525948 -2.421499 -0.435582
H 3.156690 1.692865 0.283419
H 3.003872 -2.391598 0.187091
H 2.679275 -1.776070 -1.437240
H 4.178641 -0.318067 0.210859
C 0.573738 2.317424 -0.495444
H 1.180944 3.209318 -0.388718
H -0.489314 2.399572 -0.676981
N 3.169467 -0.327361 -0.008029
F -5.153797 0.018653 0.615739
H 0.684472 1.557767 0.728741
O 5.823552 0.219674 0.640291
H 6.549067 0.256649 -0.002260
H 6.247278 0.026060 1.490884

TS_1b_2
C -2.776226 -1.884092 0.701764
C -1.272121 -1.805781 0.434911
C -0.766529 -0.345725 0.396902
C -1.562190 0.431781 -0.694112
C -3.046301 0.197297 -0.611703
H -0.741378 -2.354699 1.218622
H -2.996850 -1.585003 1.737699
H -3.141319 -2.905755 0.568737
H -1.023258 0.116553 1.361278
H -1.260564 0.033759 -1.693320
H -2.803156 2.211630 0.718762
H -3.715248 0.775214 -1.245668
H -1.039415 -2.301901 -0.515094
C 0.738951 -0.245591 0.219096
C 1.531087 0.327340 1.224372
C 1.376015 -0.733119 -0.934335
C 2.916901 0.416721 1.094743
H 1.064506 0.695591 2.135819
C 2.758474 -0.651942 -1.083370
H 0.796842 -1.195335 -1.730887
C 3.509942 -0.075296 -0.062655
H 3.535359 0.852791 1.871893
H 3.258678 -1.029092 -1.968919
C -1.141529 1.825404 -0.914823
H -0.122805 2.105898 -0.666778
H -1.612426 2.396207 -1.709193
O -2.096174 2.842971 0.472767
H -1.534943 2.950049 1.261643
N -3.508238 -1.015788 -0.224882
H -4.491625 -1.210386 -0.366547
F 4.839536 0.007693 -0.201195

TS_1b_5
C 1.628714 0.713998 0.276185
C 1.280133 -1.476623 -0.986592
N 2.488614 -1.394812 1.083460
C 2.412293 -2.171295 -0.170901
C 2.900517 0.012341 0.856751
C 0.643862 -0.431904 -0.042041
H 0.568914 -2.219531 -1.347123
H 1.094690 -1.090328 1.035150
H 3.378272 -2.165129 -0.685791
H 3.749387 0.049197 0.166024
H 1.217573 1.334445 1.077551
H 1.677844 -0.974825 -1.875314
H 2.156958 -3.203321 0.081305
H 3.213143 0.454490 1.802832
H 2.920327 -1.868806 1.874980
C -0.791495 -0.215919 -0.017039
C -1.355697 1.008675 0.452270
C -1.703346 -1.240759 -0.414594
C -2.721544 1.209410 0.494068
H -0.710202 1.818289 0.770606
C -3.070733 -1.055421 -0.368578
H -1.329406 -2.200664 -0.750499
C -3.568252 0.173200 0.082042
H -3.150830 2.144553 0.836968
H -3.763582 -1.834453 -0.667422
F -4.881416 0.359228 0.125653
C 1.962589 1.664947 -0.878875
H 1.047392 2.164643 -1.229291
H 2.385341 1.108581 -1.730348
O 2.900014 2.581605 -0.342599
H 3.154264 3.216757 -1.030121

TS_2_7
C 1.269698 1.654627 0.778271
C 2.727166 1.551536 0.293680
C 2.397453 -0.891614 0.045529
C 0.950290 -0.800688 0.379940
C 0.429378 0.614319 0.028243
H 2.881728 2.109890 -0.636640
H 3.433244 1.945821 1.031135
H 1.211055 1.488518 1.860016
H 0.919086 2.674141 0.590363
H 0.625516 0.763450 -1.045669
N 3.151772 0.156696 0.006667
C -0.014185 -1.807865 -0.201768
H -0.034345 -2.809700 0.220509
H -0.190181 -1.758556 -1.274068
C -1.080061 0.533096 0.168577
C -1.935750 1.370495 -0.529110
C -1.576357 -0.709510 0.712506
C -3.292242 1.052634 -0.690169
H -1.548546 2.270417 -1.001976
C -2.953895 -1.028143 0.536561
H -1.132460 -1.101451 1.628290
C -3.760715 -0.161426 -0.175981
H -3.971289 1.703608 -1.229222
H -3.385036 -1.916544 0.985018
F -5.054060 -0.469379 -0.348837
O 5.655169 -0.768391 -0.690035
H 6.054419 -0.709858 -1.572153
H 6.398181 -0.896020 -0.079609
H 4.148802 0.002267 -0.246510
H 2.883968 -1.840930 -0.174877
H 0.923952 -0.915159 1.480867

TS_1b_3
N -3.092145 -1.206978 -0.181567
C -2.097804 -0.910006 -1.230452
C -1.380727 0.406599 -0.863750
C -0.587510 0.285744 0.493530
C -2.343123 1.592769 -0.860651
C -2.666118 -1.030048 1.145926
C -1.191817 -0.844272 1.378551

TS_2_4
C -2.096622 -0.163000 -1.310125
C -1.133573 -0.178845 -0.292513
C -1.565937 -0.125366 1.042489
C -2.920908 -0.057395 1.357435
C -3.848900 -0.045859 0.319204
C -3.458001 -0.097841 -1.013961
H -1.784429 -0.207035 -2.350709

TS_5_6
C 0.682873 -0.350431 -0.075525
C 1.362229 0.763581 -0.639901
C 2.747025 0.861681 -0.639816
C 3.495873 -0.161725 -0.061832
C 2.884238 -1.283483 0.493427
C 1.499075 -1.374683 0.479486
H 0.792489 1.525304 -1.162408

H 3.257677 1.701366 -1.100060
H 3.497415 -2.063411 0.932584
H 1.041515 -2.245748 0.936825
C -0.759184 -0.451151 -0.081143
C -1.389884 -1.811967 0.146389
C -1.638146 0.736420 -0.030489
C -2.800973 -1.957821 -0.420623
H -1.434530 -2.050085 1.226369
H -0.790893 -2.609730 -0.306360
C -3.044220 0.543905 -0.498972
H -1.147000 2.160837 -0.652656
H -3.284616 -2.879432 -0.087959
H -2.808572 -1.926526 -1.513676
H -3.726334 1.335206 -0.176965
C -1.426794 1.737066 1.052462
H -0.562501 1.569075 1.692116
H -2.286143 2.110913 1.610096
O -1.065703 2.998833 0.135661
H -0.143883 3.309862 0.268085
N -3.657199 -0.794565 0.028200
H -3.131047 0.424126 -1.583527
H -3.694435 -0.771098 1.053924
H -4.620598 -0.908951 -0.307061
F 4.832756 -0.068751 -0.050310

TS_5_8
C -1.144140 1.617684 -0.383028
C -2.518841 1.920034 0.257458
C -2.677271 -0.244791 1.261140
C -1.437813 -0.756191 0.512857
C -0.477825 0.332340 0.089542
H -2.352727 2.376753 1.245903
H -3.046308 2.651873 -0.359756
H -1.246460 1.612681 -1.477830
H -0.493702 2.467308 -0.157538
H -2.355467 0.187910 2.222245
H -3.341273 -1.085836 1.488139
N -3.364888 0.713883 0.394956
C -1.657407 -1.185904 -0.900725
H -1.911036 -0.450772 -1.648332
O -3.538684 -1.767364 -1.160497
H -3.859809 -2.460782 -0.555692
H -0.965567 -1.550411 1.090938
C 0.944070 0.153659 0.059759
C 1.582849 -0.990232 0.627283
C 1.789945 1.134337 -0.540360
C 2.956087 -1.143097 0.601871
H 0.997904 -1.763565 1.112072
C 3.164657 0.987374 -0.573811
H 1.358640 2.014309 -1.002466
C 3.735740 -0.150950 -0.000054
H 3.440313 -2.007647 1.042812
H 3.804568 1.730987 -1.036286
H -1.118212 -2.051411 -1.275842
H -4.246218 0.994214 0.824248
H -3.885022 -0.900499 -0.824146
F 5.058196 -0.296552 -0.026752

TS_5_9
C 1.432128 -1.598618 -0.475635
C 2.946181 -1.701183 -0.169989
C 2.901570 0.234237 1.281134
C 1.611306 0.699189 0.596941
C 0.715267 -0.458000 0.223324
H 3.107922 -2.348186 0.704806
H 3.467808 -2.153410 -1.017223
H 1.300502 -1.500042 -1.566180
H 0.974084 -2.560253 -0.220574
H 2.747946 -0.458045 2.119842
H 3.496811 1.084922 1.625851
N 3.542650 -0.374386 0.099524
H 4.557053 -0.439981 0.172561
C 2.233690 1.252352 -0.690290
H 3.006566 2.014421 -0.639698
H 2.147030 0.739969 -1.636314
H 1.102751 1.481763 1.162484
C -0.709749 -0.336935 0.200924
C -1.399621 0.780120 0.770723
C -1.523981 -1.332575 -0.421186
C -2.781567 0.897179 0.712568
H -0.856657 1.538493 1.326703
C -2.902810 -1.220127 -0.480573
H -1.061475 -2.203140 -0.871534
C -3.521659 -0.102507 0.082243
H -3.297591 1.738625 1.163099
H -3.510706 -1.981238 -0.958331
F -4.852075 0.010271 0.021176
O 0.854122 2.444479 -1.269250
H 0.860575 3.310018 -0.819966
H -0.009996 2.029721 -1.059875

1a with 1 H_2O
C 1.417868 0.770810 0.124970
C 2.931742 0.610720 -0.208103
C 2.625953 -1.425758 -1.383129
C 1.097394 -1.430630 -1.128867
C 0.549618 -0.002382 -0.903726
H 3.131063 1.099401 -1.179547
H 3.521752 1.112943 0.561682
H 1.259204 0.341063 1.120521
H 2.841531 -0.883305 -2.320438
H 2.991399 -2.453374 -1.489206
H 0.585469 -1.901759 -1.976531
H 0.907204 -2.040298 -0.240483
H 0.624831 0.534203 -1.862196
N 3.263254 -0.793609 -0.251309
C 1.040231 2.250107 0.189942
H -0.024101 2.338231 0.452238
H 1.177505 2.712174 -0.803736
O 1.864335 2.881446 1.164451
H 1.580092 3.804089 1.243524
C -0.921457 -0.048904 -0.510996
C -1.905428 0.499913 -1.342868
C -1.328097 -0.662961 0.686160
C -3.259015 0.448072 -1.003589
H -1.612959 0.976261 -2.275993
C -2.674484 -0.722167 1.042206
H -0.585639 -1.103949 1.347116
C -3.620282 -0.164330 0.188764
H -4.025025 0.871330 -1.645277
H -2.997205 -1.193181 1.965143
F -4.926674 -0.220829 0.529442
O 2.055483 -1.987676 2.075950
H 2.710928 -1.654723 1.423863
H 2.328434 -2.901484 2.245721

1b with 1 H_2O
C -1.109772 0.722087 -0.598977
C -2.628979 0.879069 -0.223626
C -2.450175 -0.845183 1.539005
C -0.951637 -1.104034 1.171224
C -0.304670 0.174575 0.605281
H -2.684547 1.713256 0.491961
H -3.236620 1.110546 -1.100649
H -1.038733 0.023728 -1.441718
H -2.482707 -0.097279 2.343187
H -2.954499 -1.756262 1.866100
H -0.439281 -1.435282 2.080436
H -0.898731 -1.925165 0.447639
H -0.337345 0.943612 1.386508
N -3.120428 -0.317097 0.386359
H -3.832793 -0.891566 -0.108133
C -0.605557 2.087417 -1.068250
H -1.144879 2.400654 -1.974639
H 0.459551 1.980405 -1.326124
O -0.794423 3.004409 -0.003401
H -0.582548 3.899529 -0.310103
C 1.161921 -0.091425 0.283358
C 2.164976 0.515807 1.054874
C 1.546193 -0.963375 -0.749840
C 3.513916 0.277505 0.801477
H 1.889049 1.192111 1.859637
C 2.889046 -1.214613 -1.017184
H 0.795407 -1.456887 -1.362314
C 3.855475 -0.587968 -0.233361
H 4.295653 0.749301 1.387047
H 3.197040 -1.881618 -1.815225
F 5.149318 -0.824636 -0.486256
O -5.077464 -1.733960 -0.977120
H -6.022854 -1.654186 -0.777341
H -4.991358 -2.536267 -1.514192

2 with 1 H_2O
C 2.413408 -0.400194 1.250016
C 1.494417 -0.319195 0.195954
C 1.971238 0.006589 -1.082949
C 3.324594 0.248450 -1.307850
C 4.206539 0.159978 -0.234864
C 3.772125 -0.162183 1.045468
H 2.068239 -0.654617 2.249278
H 1.286978 0.072349 -1.926260
H 3.702740 0.499914 -2.292953
H 4.489230 -0.222533 1.857075
C 0.020292 -0.594364 0.443003
C -0.862805 0.647458 0.150405
C -0.510400 -1.810993 -0.343009
H -0.099955 -0.825830 1.510370
C -2.313187 0.312531 -0.056305
C -1.958361 -2.111933 0.034181
H -0.442366 -1.629198 -1.422752
H 0.102413 -2.691751 -0.129777
H -3.018858 1.136480 -0.186030
H -2.416318 -2.843383 -0.638078
H -2.039983 -2.504370 1.054984
H -3.814213 -1.009761 -0.119969
C -0.871209 1.659416 1.263647
H -0.605632 1.362287 2.272052
H -1.252151 2.657645 1.082556
N -2.785346 -0.888669 -0.042812
F 5.511475 0.392568 -0.444306
H -0.527561 1.141539 -0.776807
O -5.559125 -1.021603 -0.263519
H -6.167251 -1.255608 0.454390
H -6.046157 -1.198396 -1.082947
O -3.442708 3.196725 -0.347796
H -4.004894 3.680935 0.276404
H -3.425351 3.757537 -1.138751

3 with 1 H_2O
C 0.380716 -1.675315 -0.152756
C 1.863332 -1.763634 -0.152011
C 2.165979 0.547822 0.590932
C 0.710991 0.824559 0.179119
C -0.178477 -0.413665 0.543629
H 0.062968 -1.724856 -1.206379
H -0.020982 -2.593160 0.297495
H -0.083308 -0.564467 1.626867
N 2.633601 -0.794619 0.187743
C 0.240638 2.090522 0.817127
H -0.441128 2.752501 0.298084
H 0.435705 2.281144 1.868736
C -1.651842 -0.215192 0.228994
C -2.604353 -0.264337 1.254682
C -2.092725 0.016965 -1.082971
C -3.962007 -0.088264 0.989772
H -2.286205 -0.442058 2.279020
C -3.444392 0.196787 -1.367975
H -1.380565 0.066547 -1.904411
C -4.360997 0.140082 -0.321976
H -4.705467 -0.125914 1.778712
H -3.794806 0.378184 -2.378401
F -5.664542 0.310216 -0.589698
O 5.288392 -1.037105 -0.139394
H 5.904358 -1.394913 0.517695
H 5.596923 -0.123161 -0.350345
H 3.683009 -0.932907 0.142718
H 2.287377 0.614803 1.679358
H 0.682879 0.941409 -0.913278
H 2.356029 -2.685353 -0.461359
H 2.860865 1.262263 0.139243
O 5.592042 1.615524 -0.707901
H 6.135361 2.216857 -0.173932
H 5.808002 1.838150 -1.627755

4 with 1 H_2O
C 2.634255 -0.441749 1.222969
C 1.617605 -0.268138 0.275508
C 1.961471 0.191123 -1.005870
C 3.284575 0.473343 -1.335661
C 4.268880 0.288549 -0.367993
C 3.965030 -0.166710 0.910040
H 2.390572 -0.801121 2.219924
H 1.192547 0.331518 -1.762594
H 3.563321 0.826998 -2.322523
H 4.759820 -0.300841 1.635856
C 0.173541 -0.604749 0.624673
C -0.775569 0.571683 0.524823
C -0.353461 -1.805441 -0.197905
H 0.158128 -0.895852 1.690041
C -2.115404 0.346923 0.166834
C -1.829456 -2.085387 0.078513
H -0.218040 -1.602079 -1.266129
H 0.236012 -2.696488 0.034627
H -2.819647 1.172235 0.080123
H -2.241403 -2.824148 -0.614341
H -1.982785 -2.470707 1.096464
H -3.643476 -0.923153 -0.279612
C -0.324356 1.950596 0.869435
H -1.155563 2.658759 0.918797
H 0.201866 1.951046 1.833540
N -2.619194 -0.858449 -0.056022
F 5.544468 0.556991 -0.680156
H 0.406179 2.316401 0.136320
O -5.297894 -0.767573 -0.501499
H -5.506543 0.193488 -0.466079
H -5.752406 -1.121956 -1.280272
O -5.306905 1.970442 -0.180921
H -5.785458 2.271867 0.608323
H -5.573252 2.587048 -0.881750

5 **with 1 H_2O**
C -0.828276 -1.210113 0.887605
C -2.214196 -1.563657 0.340734
C -2.291464 0.536161 -0.985264
C -0.925294 0.990194 -0.446372
C -0.094698 -0.175496 0.062882
H -2.147367 -2.123283 -0.596847
H -2.794962 -2.149177 1.057740
H -0.943844 -0.859638 1.925636
H -0.273456 -2.150165 0.940238
H -2.185016 -0.069154 -1.889198
H -2.945290 1.384315 -1.205508
N -2.996963 -0.317102 0.034788
H -3.064288 0.262941 0.888831
H -3.954273 -0.556039 -0.302094
C -1.101143 2.111314 0.602210
H -1.546795 2.997584 0.126719
H -0.122614 2.387370 1.011093
O -1.965133 1.621616 1.642059
H -2.043496 2.290882 2.339579
H -0.426724 1.459599 -1.300259
C 1.333882 -0.172875 -0.039104
C 2.044372 0.818564 -0.783134
C 2.134998 -1.164457 0.606090
C 3.425960 0.814330 -0.886361
H 1.510103 1.607884 -1.299682
C 3.516609 -1.174347 0.508829
H 1.669827 -1.935192 1.209199
C 4.152385 -0.184910 -0.240187
H 3.951494 1.570875 -1.459440
H 4.111692 -1.932309 1.007171
F 5.487876 -0.191054 -0.336467
O -5.533650 -0.857846 -1.027421
H -6.385088 -0.584851 -0.652465
H -5.750594 -1.520845 -1.700688

6 with 1 H_2O
C -2.123044 1.151908 -0.368532
C -1.369692 -0.025695 -0.137184
C -2.090148 -1.230726 0.050528
C -3.478864 -1.258445 0.043368
C -4.173745 -0.071155 -0.174063
C -3.511321 1.135301 -0.388758
H -1.608363 2.083186 -0.577715
H -1.558946 -2.159291 0.233760
H -4.029457 -2.179027 0.205050
H -4.086211 2.034339 -0.583861
C 0.089072 -0.022023 -0.160747
C 0.880786 1.078897 0.301605
C 0.785821 -1.312743 -0.559625
C 2.338089 1.152185 -0.131889
C 2.206599 -1.125501 -1.082909
H 0.825873 -1.994298 0.304914
H 0.213022 -1.833703 -1.333709
H 2.930277 1.764703 0.550600
H 2.747608 -2.073530 -1.133078
H 2.218532 -0.663061 -2.074267
H 3.957549 -0.118456 -0.491442
C 0.444402 2.088052 1.121104
H 1.108791 2.891898 1.423714
H -0.570909 2.126643 1.495564
N 2.970217 -0.208377 -0.172246
F -5.512809 -0.092320 -0.187669
H 2.958808 -0.594361 0.796253
H 2.439435 1.569967 -1.139422
O 5.581524 0.247974 -1.105532
H 6.398912 0.252832 -0.584283
H 5.868146 0.272540 -2.031309
O 2.459159 -1.049756 2.445504
H 2.911379 -1.532460 3.154427
H 1.786132 -0.504475 2.882381

7 with 1 H_2O
F 5.392304 0.050356 -0.882419
C 4.152332 0.141717 -0.366015
C 3.474646 -0.999538 -0.052509
C 3.621345 1.444142 -0.208105
C 2.136159 -0.902657 0.616645
H 3.948194 -1.966802 -0.186566
C 2.273372 1.589572 0.209062
H 4.228642 2.299390 -0.480066
C 1.541458 0.493409 0.561936
H 2.284923 -1.162415 1.684329
H 1.822803 2.579312 0.194226
C 0.058538 0.332633 0.725318
C -0.941468 1.435687 0.393547
C -0.162223 -0.871441 -0.221187
H -0.151119 -0.021425 1.751743
C -2.360824 0.885060 0.609415
H -0.813450 1.766753 -0.644024
H -0.813441 2.315421 1.032635
C -1.577486 -1.312737 -0.210518
H -3.124859 1.464640 0.081704
H -2.629364 0.886860 1.672549
H -1.881029 -2.303935 -0.548921
C 0.985621 -1.860935 0.104277
H 1.289369 -2.434509 -0.775018
H 0.694937 -2.569488 0.886125
N -2.525701 -0.518224 0.150783
H -3.524799 -0.860732 0.097288
O -5.087769 -1.260952 -0.203784
H -5.638262 -1.738521 0.434887
H -5.557078 -0.417589 -0.409876
H 0.010952 -0.512808 -1.252095
O -5.860374 1.302841 -0.759364
H -6.100364 1.481214 -1.682956
H -6.520573 1.784417 -0.235676

8 with 1 H_2O
C 0.778439 0.587018 0.771762
C 1.854627 0.679387 -0.355938
C 1.866896 -1.787295 -0.696070
C 0.424386 -1.802372 -0.194155
C -0.170926 -0.591139 0.501717
H 1.324448 0.852591 -1.304955
H 2.571405 1.485240 -0.183648
H 1.288423 0.495082 1.736237
H 0.228518 1.532469 0.776237
H 1.845928 -1.910441 -1.795896
H 2.466007 -2.618753 -0.307755
N 2.565611 -0.560002 -0.425530
C 0.112625 -1.878700 1.277427
H 0.936268 -1.861977 1.987837
H -0.245756 -2.359825 -0.842118
C -1.593391 -0.200752 0.221064
C -2.154214 -0.296260 -1.061958
C -2.382282 0.320298 1.264939
C -3.463530 0.110804 -1.306068
H -1.563737 -0.690831 -1.884187

C -3.691470 0.729946 1.040313
H -1.967880 0.391894 2.267263
C -4.213168 0.619029 -0.247640
H -3.908911 0.041762 -2.292702
H -4.312425 1.123601 1.837808
H -0.730490 -2.492539 1.579073
H 3.605641 -0.563492 -0.254338
F -5.473126 1.009701 -0.473527
O 5.236461 -0.321356 -0.117404
H 5.798381 -0.751497 0.543953
H 5.406860 0.647404 -0.051494
O 5.177275 2.417785 -0.086049
H 5.537313 2.837419 -0.883927
H 5.501029 2.963381 0.648340

9 with 1 H_2O
C 0.570479 1.302492 -0.406118
C 2.042936 1.031365 -0.811588
C 1.641245 -1.430255 -0.836957
C 0.658907 -1.112648 0.333240
C -0.213133 0.052184 -0.042395
H 2.170005 0.998329 -1.897181
H 2.727711 1.766483 -0.387785
H 0.569374 2.006688 0.439681
H 0.094348 1.839357 -1.232707
H 1.312926 -1.275344 -1.865854
H 2.174240 -2.377700 -0.728864
N 2.514309 -0.307026 -0.298706
H 3.538672 -0.402053 -0.403116
C 1.929716 -0.599883 1.076624
H 2.516804 -1.391410 1.544795
H 1.882469 0.275334 1.721131
H 0.141172 -1.957239 0.781112
C -1.636353 0.029447 -0.007530
C -2.375911 -1.158800 0.274610
C -2.398070 1.211656 -0.255656
C -3.760165 -1.167313 0.304402
H -1.859437 -2.094641 0.458756
C -3.782774 1.209112 -0.224879
H -1.892735 2.149395 -0.458960
C -4.452693 0.018033 0.054362
H -4.315655 -2.075158 0.514555
H -4.354338 2.112680 -0.408799
F -5.791733 0.011178 0.083648
O 5.441892 -0.600068 -0.597778
H 5.900013 -0.313358 -1.404642
H 5.924189 -1.389994 -0.303880
O 4.398744 1.244319 1.278181
H 5.173053 0.840488 0.850603
H 4.752449 1.870387 1.927362

TS_1b_2 with 1 H_2O
C 2.364456 -1.970608 -1.022967
C 0.850538 -1.856371 -0.837520
C 0.462744 -0.465581 -0.291264
C 1.179948 -0.249165 1.072867
C 2.662928 -0.549701 0.986477
H 0.352621 -2.029915 -1.796579
H 2.687504 -1.309333 -1.846214
H 2.647017 -2.991164 -1.296173
H 0.868337 0.273313 -1.001729
H 0.692300 -0.903474 1.816829
H 2.676015 1.544750 0.421286
H 3.249858 -0.425704 1.896812
H 0.506224 -2.636090 -0.147627
C -1.038785 -0.245650 -0.211081
C -1.647714 0.760922 -0.974499
C -1.854738 -1.039932 0.611687
C -3.024820 0.979883 -0.926467
H -1.043061 1.374609 -1.640194
C -3.231488 -0.836980 0.674444
H -1.420792 -1.838673 1.208048
C -3.796870 0.174178 -0.097684
H -3.501330 1.751918 -1.521141
H -3.868442 -1.449320 1.303841
C 1.013547 1.163790 1.616666
H 0.007188 1.570582 1.521979
H 1.384615 1.285699 2.634083
O 1.905563 2.095391 0.820847
H 1.466397 2.487354 0.037139
N 3.054121 -1.621780 0.215629
H 4.029442 -1.887482 0.274647
F -5.121320 0.374498 -0.040666
O 3.415869 2.117074 -1.245933
H 3.656258 1.483501 -1.939780
H 4.112946 2.792983 -1.271898

TS_1b_5 with 1 H_2O
H -1.147089 -1.460457 -2.260377
C -1.159540 -1.571494 -1.164704
C -1.732712 0.747952 -0.421535
N -2.770766 -1.223566 0.643619
C -2.889870 0.244010 0.489025
C -2.603654 -1.861034 -0.682824
C -0.633257 -0.310223 -0.490765
H -0.773644 -1.178603 1.118469
H -3.855346 0.539922 0.062206
H -3.347837 -1.480279 -1.397365
H -0.519060 -2.429958 -0.935293
H -2.134989 0.778487 -1.448111
H -2.817091 0.705265 1.482292
H -2.766994 -2.937382 -0.585283
H -3.616775 -1.581828 1.086903
O -0.424306 -1.643155 2.025158
H 0.262968 -1.088868 2.455351
H -1.228580 -1.726296 2.582626
C 0.791275 -0.101781 -0.345076
C 1.340782 0.889349 0.523200
C 1.724020 -0.946609 -1.016543
C 2.709330 1.032362 0.699936
H 0.683620 1.551720 1.074181
C 3.093099 -0.800666 -0.856489
H 1.366447 -1.702560 -1.705985
C 3.574407 0.187264 0.003026
H 3.119643 1.788589 1.361030
H 3.795184 -1.431898 -1.390935
F 4.891703 0.326001 0.167497
C -1.412055 2.215169 -0.122709
H -1.131944 2.356437 0.934687
H -0.575378 2.560395 -0.746302
O -2.612300 2.913061 -0.412193
H -2.461219 3.863226 -0.291870

TS_2_4 with 1 H_2O
C -2.843465 -0.995970 0.660553
C -1.750105 -0.206701 0.280033
C -1.998097 1.034145 -0.328756
C -3.298935 1.477743 -0.554734
C -4.359848 0.666282 -0.161310
C -4.153122 -0.567488 0.444990
H -2.675216 -1.958632 1.137107
H -1.172308 1.676866 -0.628019
H -3.501440 2.435668 -1.021649
H -5.004786 -1.171290 0.739326
C -0.329886 -0.686149 0.546624
C 0.485668 -0.937741 -0.732288
C 0.450115 0.265710 1.481948
H -0.400037 -1.665195 1.041157
C 1.911845 -0.832405 -0.649505
C 1.882630 -0.211528 1.719114
H 0.471130 1.274218 1.053426
H -0.070525 0.337553 2.441069
H 2.534840 -1.027301 -1.519588
H 2.470543 0.545922 2.244693
H 1.904300 -1.125408 2.327531
H 3.595615 -0.439526 0.371007
C -0.148391 -1.617228 -1.877194
H 0.448611 -1.966265 -2.712016
H -1.227762 -1.669016 -1.917685
N 2.555270 -0.488609 0.444155
F -5.614029 1.088131 -0.375102
H 0.151579 -0.227906 -1.670013
O 5.177546 -0.482651 -0.238178
H 5.793407 -1.175899 0.040838
H 5.712172 0.346530 -0.297105
O 6.603309 1.849379 -0.425693
H 7.246521 2.122259 0.246382
H 7.025429 2.048658 -1.275495

TS_2_7 with 1 H_2O
C -0.583539 -2.053543 0.682381
C -2.054311 -2.106366 0.230855
C -2.051644 0.365447 0.133804
C -0.597152 0.441693 0.452470
C 0.098187 -0.864196 -0.004665
H -2.160225 -2.624286 -0.729388
H -2.687703 -2.631566 0.952550
H -0.518704 -1.955041 1.772101
H -0.108758 -3.003431 0.417521
H -0.097838 -0.966774 -1.084037
N -2.662944 -0.766416 0.038314
C 0.224158 1.607797 -0.045973
H 0.118688 2.566992 0.455479
H 0.396218 1.668305 -1.118380
C 1.586172 -0.595371 0.127625
C 2.530377 -1.251210 -0.646345
C 1.927107 0.651503 0.771810
C 3.831153 -0.746726 -0.790031
H 2.253573 -2.151164 -1.191253
C 3.249352 1.159764 0.615289
H 1.451417 0.905935 1.719297
C 4.147908 0.469585 -0.175514
H 4.578569 -1.255562 -1.388286
H 3.570497 2.055357 1.135953
F 5.388089 0.957262 -0.330266
O -4.924897 2.313848 -0.304010
H -5.091119 2.908055 -1.053636
H -5.334194 2.756205 0.457507
H -3.693855 -0.738979 -0.183041
H -2.664025 1.256296 -0.015094
H -0.572068 0.473433 1.558528
O -5.312339 -0.410379 -0.390278
H -5.405122 0.567796 -0.440817
H -5.836272 -0.780018 -1.116733

TS_5_6 with 1 H_2O
C 0.771144 -0.545272 -0.114453
C 1.401441 0.681905 -0.468914
C 2.781152 0.844593 -0.443326
C 3.580277 -0.228625 -0.055478
C 3.021184 -1.458402 0.285196
C 1.641806 -1.611353 0.251047
H 0.794045 1.495608 -0.846855
H 3.250162 1.776357 -0.743302

H 3.671377 -2.276238 0.578026
H 1.231967 -2.572827 0.540649
C -0.663540 -0.702827 -0.131807
C -1.221612 -2.111995 -0.036097
C -1.581234 0.438398 0.083473
C -2.676739 -2.266972 -0.472699
H -1.143574 -2.485804 1.002903
H -0.641419 -2.816847 -0.642870
C -3.010843 0.210183 -0.285771
H -1.423045 1.713371 -0.998308
H -3.083644 -3.242737 -0.196677
H -2.800381 -2.124591 -1.549955
H -3.695254 0.940296 0.153589
C -1.361422 1.254479 1.322939
H -0.702593 0.801228 2.065033
H -2.281625 1.595320 1.801650
O -0.659370 2.634029 1.085900
H 0.304048 2.481805 1.135805
N -3.525578 -1.200871 0.177800
O -1.372396 2.780171 -1.183862
H -0.748281 2.980791 -1.904432
H -0.926947 2.935532 -0.034176
H -3.202900 0.159575 -1.363774
H -3.453788 -1.273627 1.199181
H -4.513801 -1.328924 -0.068672
F 4.912126 -0.076718 -0.021487

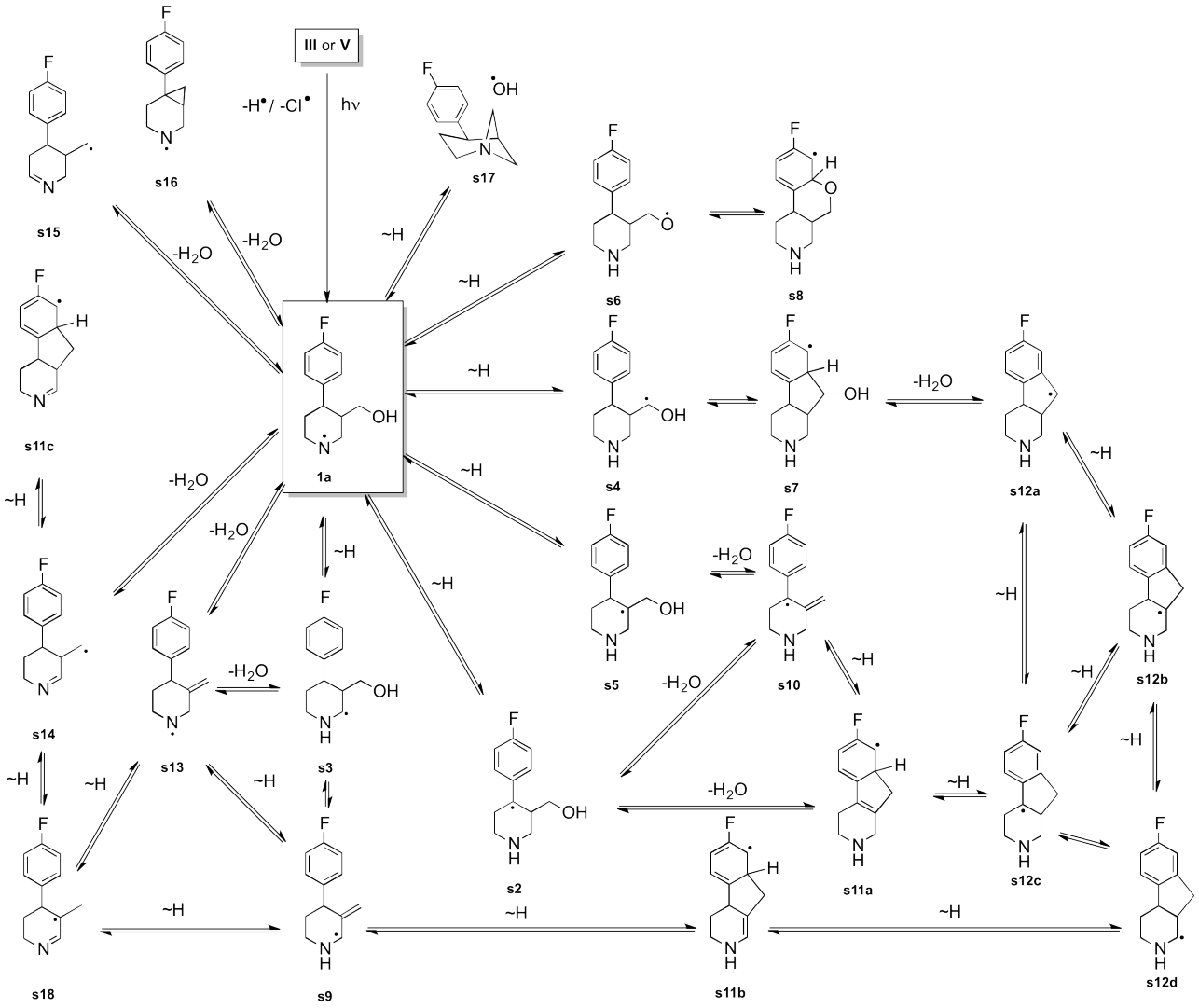
TS_5_8 with 1 H_2O
C -0.655912 -1.473768 0.690844
C -2.105171 -1.748859 0.216975
C -2.253482 0.313850 -0.965005
C -0.926617 0.828585 -0.389131
C 0.017758 -0.260378 0.062621
H -2.059703 -2.305158 -0.733862
H -2.599039 -2.393838 0.948816
H -0.642302 -1.384607 1.786461
H -0.066293 -2.367258 0.466032
H -2.042372 -0.224755 -1.904157
H -2.900435 1.160835 -1.214304
N -2.897305 -0.518081 0.047034
C -0.981256 1.372778 0.996681
H -1.226519 0.726938 1.824056
O -2.883624 2.035488 1.376984
H -3.252967 2.666687 0.734150
H -0.472874 1.544510 -1.074129
C 1.445743 -0.148044 -0.030132
C 2.083794 0.911747 -0.741773
C 2.293720 -1.115201 0.586827
C 3.460128 0.998869 -0.834486
H 1.494126 1.669671 -1.244659
C 3.671929 -1.033882 0.502379
H 1.862737 -1.931845 1.153693
C 4.242482 0.023301 -0.209976
H 3.943691 1.799161 -1.384071
H 4.314860 -1.766981 0.977296
H -0.380180 2.241795 1.249383
H -3.845735 -0.751597 -0.266011
H -3.222891 1.134006 1.120456
F 5.568247 0.105487 -0.297131
O -5.636286 -0.498450 -1.014877
H -6.414940 -0.579695 -0.442682
H -5.921671 -0.870974 -1.863320

TS_5_9 with 1 H_2O
C -0.916011 -1.562283 0.551649
C -2.442564 -1.630750 0.302963
C -2.424780 0.311326 -1.115069
C -1.083348 0.742942 -0.514827
C -0.202484 -0.437116 -0.174508
H -2.643556 -2.266320 -0.574193
H -2.935621 -2.093755 1.161977
H -0.741603 -1.461614 1.636403
H -0.483468 -2.532442 0.283541
H -2.326563 -0.370062 -1.973245
H -3.019620 1.177187 -1.420821
N -3.025193 -0.296648 0.081215
H -4.050485 -0.331691 0.033617
C -1.591172 1.342484 0.800213
H -2.357424 2.112930 0.781573
H -1.491794 0.815340 1.736856
H -0.582378 1.496760 -1.126546
C 1.225493 -0.342021 -0.196638
C 1.918784 0.761457 -0.789260
C 2.040850 -1.350281 0.403296
C 3.304612 0.854002 -0.772210
H 1.373560 1.524368 -1.336978
C 3.422696 -1.262207 0.421331
H 1.575922 -2.211472 0.868735
C 4.044891 -0.156858 -0.161625
H 3.821833 1.684567 -1.241308
H 4.030806 -2.033381 0.882510
F 5.379304 -0.068070 -0.139866
O -0.176656 2.466645 1.272159
H -0.185215 3.314929 0.790239
H 0.657658 2.012069 1.019181
O -5.910613 -0.119049 -0.358589
H -6.398559 -0.671501 -0.988137
H -6.564529 0.118317 0.316443

STS_2_4
C -2.096622 -0.163000 -1.310125
C -1.133573 -0.178845 -0.292513
C -1.565937 -0.125366 1.042489
C -2.920908 -0.057395 1.357435
C -3.848900 -0.045859 0.319204
C -3.458001 -0.097841 -1.013961
H -1.784429 -0.207035 -2.350709
H -0.845147 -0.144979 1.857882
H -3.265935 -0.018874 2.385084
H -4.210195 -0.088569 -1.795378
C 0.346083 -0.270110 -0.639378
C 1.145959 0.983488 -0.243252
C 1.018122 -1.527500 -0.042483
H 0.426547 -0.329074 -1.733728
C 2.544854 0.831999 0.023896
C 2.509729 -1.590113 -0.368575
H 0.884505 -1.541496 1.045094
H 0.525948 -2.421499 -0.435582
H 3.156690 1.692865 0.283419
H 3.003872 -2.391598 0.187091
H 2.679275 -1.776070 -1.437240
H 4.178641 -0.318067 0.210859
C 0.573738 2.317424 -0.495444
H 1.180944 3.209318 -0.388718
H -0.489314 2.399572 -0.676981
N 3.169467 -0.327361 -0.008029
F -5.153797 0.018653 0.615739
H 0.684472 1.557767 0.728741
O 5.823552 0.219674 0.640291
H 6.549067 0.256649 -0.002260
H 6.247278 0.026060 1.490884

STS_2_7
C 1.269698 1.654627 0.778271
C 2.727166 1.551536 0.293680
C 2.397453 -0.891614 0.045529
C 0.950290 -0.800688 0.379940
C 0.429378 0.614319 0.028243
H 2.881728 2.109890 -0.636640
H 3.433244 1.945821 1.031135
H 1.211055 1.488518 1.860016
H 0.919086 2.674141 0.590363
H 0.625516 0.763450 -1.045669
N 3.151772 0.156696 0.006667
C -0.014185 -1.807865 -0.201768
H -0.034345 -2.809700 0.220509
H -0.190181 -1.758556 -1.274068
C -1.080061 0.533096 0.168577
C -1.935750 1.370495 -0.529110
C -1.576357 -0.709510 0.712506
C -3.292242 1.052634 -0.690169
H -1.548546 2.270417 -1.001976
C -2.953895 -1.028143 0.536561
H -1.132460 -1.101451 1.628290
C -3.760715 -0.161426 -0.175981
H -3.971289 1.703608 -1.229222
H -3.385036 -1.916544 0.985018
F -5.054060 -0.469379 -0.348837
O 5.655169 -0.768391 -0.690035
H 6.054419 -0.709858 -1.572153
H 6.398181 -0.896020 -0.079609
H 4.148802 0.002267 -0.246510
H 2.883968 -1.840930 -0.174877
H 0.923952 -0.915159 1.480867

STS_5_6
C 0.682873 -0.350431 -0.075525
C 1.362229 0.763581 -0.639901
C 2.747025 0.861681 -0.639816
C 3.495873 -0.161725 -0.061832
C 2.884238 -1.283483 0.493427
C 1.499075 -1.374683 0.479486
H 0.792489 1.525304 -1.162408
H 3.257677 1.701366 -1.100060
H 3.497415 -2.063411 0.932584
H 1.041515 -2.245748 0.936825
C -0.759184 -0.451151 -0.081143
C -1.389884 -1.811967 0.146389
C -1.638146 0.736420 -0.030489
C -2.800973 -1.957821 -0.420623
H -1.434530 -2.050085 1.226369
H -0.790893 -2.609730 -0.306360
C -3.044220 0.543905 -0.498972
H -1.147000 2.160837 -0.652656
H -3.284616 -2.879432 -0.087959
H -2.808572 -1.926526 -1.513676
H -3.726334 1.335206 -0.176965
C -1.426794 1.737066 1.052462
H -0.562501 1.569075 1.692116
H -2.286143 2.110913 1.610096
O -1.065703 2.998833 0.135661
H -0.143883 3.309862 0.268085
N -3.657199 -0.794565 0.028200
H -3.131047 0.424126 -1.583527
H -3.694435 -0.771098 1.053924
H -4.620598 -0.908950 -0.307061
F 4.832756 -0.068751 -0.050310



Scheme S4. Rearrangement reactions of paroxetine-derived radicals (neutral form). "~H" denotes hydrogen atom migration.

Table S2. Calculated Gibbs free energies and thermal corrections (in Hartree, at 298.15 K), free energies of solvation (in kcal/mol) and relatives energies (in kJ/mol) for all structures involved in rearrangements of paroxetine-derived radicals presented in Scheme S4.

Structure[a]	B3LYP/6-31G(d)		E	G_{298}	ΔG_{solv}	ΔG	
	G	t.c.	B2PLYP(D)/aug-cc-pVdZ // B3LYP/6-31G(d)	B2PLYP(D)/aug-cc-pVdZ // B3LYP/6-31G(d) + t.c.	CPCM/ UAKS// B3LYP/ 6-31G(d)	B3LYP/6-31G(d) + ΔG_{solv}	B2PLYP(D)/aug-cc-pVdZ // B3LYP/6-31G(d) + ΔG_{solv}
s12c	-673.037327	0.238209	-671.426625	-671.188416	-8.33	-95.48	-129.69
s18	-673.031804	0.232234	-671.409357	-671.177123	-9.00	-83.79	-102.85
s12a	-673.021788	0.238975	-671.416294	-671.177319	-8.91	-57.11	-102.98
s12b	-673.019433	0.238336	-671.414163	-671.175827	-7.28	-44.11	-92.25
s12e	-673.018849	0.237868	-671.408283	-671.170415	-7.56	-43.75	-79.21
s9	-673.015985	0.236510	-671.408367	-671.171857	-8.75	-41.21	-87.97
s12d	-673.013148	0.238251	-671.413004	-671.174753	-8.26	-31.71	-93.53
s11	-673.007490	0.237909	-671.397177	-671.159268	-6.84	-10.91	-46.93
s11a	-673.007490	0.237909	-671.397177	-671.159268	-6.84	-10.91	-46.93
s10	-673.004821	0.233910			-8.08	-9.09	
1a	-673.004194	0.244156	-671.386409	-671.142253	-6.30	0.00	0.00
s2	-673.002183	0.241368	-671.386762	-671.145394	-8.62	-4.43	-17.95
s15	-673.001638	0.231218	-671.385923	-671.154705	-7.95	-0.19	-39.60
s3	-673.001304	0.239943	-671.391191	-671.151248	-7.93	0.77	-30.44
s14	-673.000331	0.232009	-671.385401	-671.153392	-7.78	3.95	-35.44
s13	-672.996664	0.236252	-671.381872	-671.145620	-8.19	11.86	-16.75
s4	-672.996538	0.239011	-671.387628	-671.148617	-9.69	5.92	-30.89
s11b	-672.995316	0.237656	-671.384652	-671.146996	-6.62	21.97	-13.79
s5	-672.994579	0.241529	-671.382380	-671.140851	-7.02	22.23	0.67
s6	-672.992880	0.239372	-671.366599	-671.127227	-8.27	21.46	31.21
s7	-672.987697	0.242369	-671.386309	-671.143940	-9.17	31.30	-16.44
s16	-672.987115	0.234963	-671.371519	-671.136556	-6.69	43.21	13.33
s8	-672.986930	0.243604	-671.371027	-671.127423	-8.13	37.67	31.28
TS_1a_s6	-672.980734	0.237417	-671.356184	-671.118767	-8.07	54.19	54.26
TS_s12a_s12c	-672.971652	0.238834			-8.24	77.32	
TS_s12a_s12b	-672.971081	0.239185	-671.352907	-671.113722	-8.22	78.90	66.88
TS_s6_s8	-672.970562	0.243468	-671.353740	-671.110272	-8.61	78.64	74.30
TS_s10_s11a	-672.969791	0.234900	-671.357540	-671.122640	-7.37	85.85	47.02
TS_s9_s11b	-672.969100	0.236387	-671.366588	-671.130201	-8.59	82.56	22.06
TS_s4_s7	-672.965371	0.241976	-671.360110	-671.118134	-8.81	91.43	52.82
TS_1a_s2	-672.954288	0.240002	-671.288985	-671.048983	-7.48	126.09	239.94
TS_1a_s4	-672.941025	0.234927	-671.310900	-671.075973	-7.10	162.50	170.67
TS_s5_s10	-672.940471	0.232311	-671.307815	-671.075504	-8.67	157.39	165.33
TS_s3_s9	-672.939495	0.227044			-6.02	171.04	
TS_1a_s5	-672.932973	0.236947	-671.321482	-671.084535	-7.76	180.88	145.43
TS_1a_s3	-672.932454	0.235537	-671.318333	-671.082796	-9.10	176.64	144.39
TS_s9_s18	-672.928194	0.228187	-671.311862	-671.083675	-10.17	183.35	137.60
TS_s11_s12c	-672.927577	0.235980	-671.285351	-671.049371	-10.66	182.92	225.62
TS_s13_s18	-672.924826	0.227948	-671.301202	-671.073254	-11.99	184.57	157.35
TS_s2_s10	-672.923477	0.236604	-671.300759	-671.064155	-8.15	204.18	197.31
TS_s12a_s12c	-672.922570	0.231340	-671.318676	-671.087336	-8.09	206.81	136.70
TS_s14_s18	-672.922530	0.226656	-671.305331	-671.078675	-10.68	196.08	148.60

Structure[a]	B3LYP/6-31G(d)		E	G_{298}	ΔG_{solv}	ΔG	
	G	t.c.	B2PLYP(D)/aug-cc-pVdZ // B3LYP/6-31G(d)	B2PLYP(D)/aug-cc-pVdZ // B3LYP/6-31G(d) + t.c.	CPCM/ UAKS// B3LYP/ 6-31G(d)	B3LYP/6-31G(d) + ΔG_{solv}	B2PLYP(D)/aug-cc-pVdZ // B3LYP/6-31G(d) + ΔG_{solv}
TS_s7_s12a	-672.921638	0.238374	-671.313432	-671.075058	-9.97	201.40	161.06
TS_1a_s13	-672.912953	0.235049	-671.292207	-671.057158	-7.91	232.82	216.68
TS_s12b_s12c	-672.910114	0.230305			-8.40	238.22	
TS_s12a_s12b	-672.907896	0.228441	-671.296815	-671.068374	-8.19	244.92	186.06
TS_1a_s17	-672.899286	0.237355	-671.278149	-671.040794	-9.10	263.72	254.67
TS_1a_s14	-672.896414	0.234607	-671.271101	-671.036494	-13.11	254.48	249.18
TS_1a_s15	-672.888226	0.233989	-671.266499	-671.032510	-15.36	266.57	250.22
s12c	-596.632491	0.214983	-595.151599	-594.936616	-6.81	-92.73	-93.20
s18	-596.625479	0.212218	-595.135683	-594.923465	-6.90	-74.69	-59.05
s12a	-596.614416	0.218984	-595.141637	-594.922653	-6.72	-44.89	-56.16
s12b	-596.610944	0.216267	-595.135720	-594.919453	-7.06	-37.20	-49.18
s9	-596.610295	0.214340	-595.132008	-594.917668	-7.01	-35.29	-44.29
s12e	-596.609846	0.217401	-595.131619	-594.914218	-6.10	-30.30	-31.42
s12d	-596.608116	0.217896	-595.138627	-594.920731	-6.48	-27.35	-50.11
s11a	-596.598029	0.216578	-595.121937	-594.905359	-6.75	-2.00	-10.88
1a	-596.597795	0.219343	-595.121083	-594.901740	-6.42	0.00	0.00
s11b	-596.585608	0.216024	-595.109151	-594.893127	-6.56	31.41	22.03
s11c	-596.585707	0.214880	-595.106311	-594.891431	-6.73	30.44	25.77
s15	-596.592197	0.209413	-595.109131	-594.899718	-7.06	12.02	2.63
s14	-596.591321	0.210469	-595.108683	-594.898214	-6.70	15.83	8.08
s13	-596.589253	0.212449	-595.102046	-594.889597	-6.73	21.13	30.58
TS_s10_s11a	-596.581662	0.212078	-595.100684	-594.888606	-6.94	40.18	32.31
TS_s11c_s14	-596.558821	0.213235	-595.079661	-594.866426	-6.72	101.07	91.46
s16	-596.579019	0.212347	-595.092180	-594.879833	-6.38	49.46	57.68
TS_s14_s18	-596.566919	0.212005	-595.065975	-594.853970	-5.70	84.08	128.43
TS_s9_s18	-596.526853	0.208650	-595.034867	-594.826217	-5.66	189.44	201.46
TS_s11_s12c	-596.523997	0.216279	-595.010786	-594.794507	-7.02	191.25	279.03
TS_s13_s18	-596.519651	0.208385	-595.024871	-594.816486	-8.48	196.55	215.21
TS_s11_s12b	-596.507097	0.211664			-6.94	235.95	
s12c	-520.225961	0.197731	-518.876755	-518.679024	-3.27		
s18	-520.221967	0.192433	-518.862093	-518.669660	-4.09		
s12a	-520.210721	0.198529	-518.866389	-518.667860	-3.20		
s9	-520.210680	0.193252	-518.859049	-518.665797	-4.21		
s12b	-520.206340	0.196764	-518.860639	-518.663875	-3.31		
s11a	-520.194046	0.196287	-518.846539	-518.650252	-3.45		
s11b	-520.184136	0.196079	-518.835735	-518.639656	-3.30		
s15	-520.189967	0.189704	-518.836126	-518.646422	-3.95		
s14	-520.188685	0.190331	-518.835146	-518.644815	-3.89		
s13	-520.186686	0.192972	-518.829944	-518.636972	-3.88		
s16	-520.176419	0.192647	-518.819547	-518.626900	-3.60		

[a] First section corresponds to structures with one explicit water molecule, next section contains structures without explicit water molecule (eliminated water included), while third section corresponds to structures without any water molecules (eliminated water not included).

B3LYP/6-31G(d) Cartesian coordinates for structures presented in Scheme S4 and Table S2

1a with 1 H_2O
C 1.164769 -0.145690 -1.380793
C 0.714824 0.958008 -0.379200
C 1.894902 1.811558 0.134484
H 0.084323 1.648236 -0.956128
H 1.797276 0.295157 -2.159934
H 0.258915 -0.550547 -1.865317
H 2.407599 2.252539 -0.735765
H 1.475014 2.645036 0.714874
H 3.497958 0.716667 0.420769
O 2.808616 1.144830 0.980263
N 1.887481 -1.214339 -0.733004
C -0.145212 0.333896 0.763052
C 0.550163 -0.921884 1.330304
H 1.420460 -0.586031 1.897623
H -0.111141 -1.464833 2.015723
C 1.061241 -1.896425 0.236737
H 0.207248 -2.356241 -0.288184
H 1.638645 -2.704678 0.699311
H -0.158464 1.074448 1.576081
C -1.606594 0.149618 0.339998
C -2.259949 -1.088952 0.295670
C -2.359401 1.290273 0.009054
C -3.602109 -1.188723 -0.084096
H -1.732686 -1.996413 0.570180
C -3.697118 1.198455 -0.367835
H -1.890900 2.271028 0.060855
C -4.326113 -0.047801 -0.421877
H -4.078726 -2.165352 -0.110793
H -4.251177 2.100968 -0.613036
H -5.369337 -0.124740 -0.715989
O 4.503837 -0.335633 -0.654895
H 3.690140 -0.890993 -0.778001
H 5.066431 -0.851455 -0.057168

H_2O
O 0.000000 0.000000 0.119694
H 0.000000 0.761432 -0.478778
H 0.000000 -0.761432 -0.478778

s10
C -1.465015 0.937719 -0.260620
C -2.966786 1.226092 -0.207204
C -3.415922 -1.021128 0.485459
C -2.012877 -1.515746 0.135212
C -1.022447 -0.396363 -0.115270
H -3.209091 1.975708 -0.969093
H -4.134710 -1.842446 0.393359
H -1.649681 -2.182919 0.928014
H -2.069965 -2.136033 -0.772493
C 0.397313 -0.788000 -0.242524
C 0.985754 -1.680234 0.682014
C 1.209355 -0.311168 -1.291036
C 2.327251 -2.050012 0.577657
H 0.393422 -2.072374 1.504187
C 2.547418 -0.684643 -1.396800
H 0.779685 0.354951 -2.030993
C 3.115845 -1.552277 -0.462958
H 2.755553 -2.728387 1.311240
H 3.148770 -0.287101 -2.208854
H 4.160992 -1.837392 -0.543130
C -0.642273 2.047987 -0.381602
H 0.441808 2.015106 -0.405722
H -1.092583 3.032361 -0.485812
O 2.818957 2.586433 -0.191604
H 2.810437 3.532465 0.017242
N -3.770479 0.035211 -0.456038
O 1.674650 1.325349 2.081403
H 0.772658 1.524149 1.777615
H 2.580903 2.160477 0.659511
H -3.438582 -0.678636 1.539699
H 1.795743 0.396711 1.816904
H -3.190289 1.687722 0.776458
H -4.756276 0.271549 -0.368213

s11a
C 1.698443 -1.536691 -0.019195
C 3.067531 -1.266589 -0.187158
C 3.538561 0.082386 -0.254098
C 2.717130 1.145412 -0.014466
C 1.322008 0.910505 0.486215
C 0.817866 -0.492021 0.194727
H 1.328635 -2.552177 -0.146488
H 3.760980 -2.082026 -0.371005
H 4.576659 0.255146 -0.530450
H 3.088445 2.165610 -0.082731
C -0.617067 -0.429689 0.100413
C -1.020954 0.868911 0.016754
C -1.588080 -1.577622 0.029155
C -2.453116 1.271855 -0.155827
C -3.009724 -1.061603 0.296717
H -1.546993 -2.044156 -0.964623
H -1.327717 -2.355868 0.758710
H -2.540289 2.036524 -0.941597
H -3.746348 -1.831416 0.042337
C 0.151456 1.823867 0.021467
N -3.265463 0.112866 -0.540996
H -2.803743 1.756962 0.781273
H -3.116021 -0.849143 1.378875
H 0.006217 2.696237 0.671473
H -4.250621 0.361764 -0.495626
H 0.333433 2.210823 -0.994372
H 1.351279 1.009327 1.592974

s11a with 1 H_2O
C -1.862462 -1.492929 -0.491378
C -3.205211 -1.458819 -0.078224
C -3.762945 -0.266956 0.482916
C -3.072800 0.909930 0.506715
C -1.756649 1.016176 -0.205884
C -1.108608 -0.334044 -0.456756
H -1.401107 -2.443646 -0.750496
H -3.797043 -2.369320 -0.088743
H -4.756452 -0.317972 0.923275
H -3.507154 1.804135 0.948247
C 0.315343 -0.130671 -0.522629
C 0.625675 1.113746 -0.060821
C 1.368731 -1.117071 -0.951520
C 2.031659 1.613962 0.066967
C 2.690887 -0.378051 -1.200310
H 1.529202 -1.866849 -0.166129
H 1.060796 -1.649689 -1.860198
H 2.181582 2.097257 1.042874
H 3.512861 -1.093698 -1.298439
C -0.602487 1.871296 0.392064
N 2.982648 0.494945 -0.048635
H 2.215305 2.398103 -0.695459
H 2.626411 0.194904 -2.142633
H -0.625212 2.915193 0.053935
H 3.928102 0.863727 -0.128942
H -0.657507 1.893077 1.492734
H -1.961365 1.456404 -1.205708
O 2.957619 -1.635777 1.936778
H 2.147008 -1.516508 2.453457
H 2.998285 -0.822931 1.381597

s11a with 2 H_2O
33

C -2.655793 -1.493109 0.077316
C -3.948983 -1.196542 0.541011
C -4.349205 0.159324 0.759508
C -3.560255 1.211427 0.394854
C -2.309050 0.964964 -0.395600
C -1.804106 -0.462002 -0.274411
H -2.303553 -2.522685 0.081531
H -4.616439 -2.002007 0.832885
H -5.300376 0.344839 1.253977
H -3.874386 2.236323 0.579563
C -0.379756 -0.439784 -0.483001
C 0.077177 0.843318 -0.431713
C 0.542466 -1.615471 -0.670459
C 1.526412 1.202305 -0.548133
C 1.898344 -1.126865 -1.199360
H 0.684676 -2.140937 0.284312
H 0.109489 -2.343276 -1.369094
H 1.809271 1.929686 0.226104
H 2.646072 -1.924170 -1.135850
C -1.037036 1.826088 -0.149427
N 2.368411 0.005955 -0.390256
H 1.704645 1.708892 -1.517651
H 1.795439 -0.853044 -2.264743
H -1.000698 2.724969 -0.777925
H 3.341981 0.235604 -0.614107
H -0.990074 2.168555 0.897251
H -2.564276 1.116902 -1.466660
O 3.610082 -0.516517 2.051209
H 3.332994 0.125547 2.722137
H 2.948373 -0.413237 1.311921
H 4.859201 0.207321 0.933216
O 5.257476 0.548116 0.096711
H 5.897025 -0.135667 -0.151951

s11b
C 1.524083 -1.530147 -0.054044
C 2.877283 -1.333924 -0.443029
C 3.437034 -0.029338 -0.432313
C 2.731913 1.052901 0.020630
C 1.356313 0.899937 0.597004
C 0.779704 -0.486887 0.414456
H 1.074371 -2.513650 -0.176736
H 3.463594 -2.172477 -0.806207
H 4.448191 0.109710 -0.809361
H 3.179129 2.044747 0.016309
C -0.702608 -0.399916 0.676358
C -1.021889 0.981131 0.102859
C -1.625169 -1.463034 0.067392
C -2.205337 1.228911 -0.477568
C -3.079422 -0.973527 0.133572
H -1.349657 -1.632066 -0.980330
H -1.539481 -2.420869 0.594069

H -2.418495 2.178408 -0.965173
H -3.752596 -1.717871 -0.307511
C 0.229319 1.847661 0.055584
N -3.222767 0.275391 -0.612209
H -3.369200 -0.853549 1.192117
H 0.155411 2.760113 0.662099
H -4.159598 0.660267 -0.589999
H 0.464569 2.160385 -0.969745
H 1.417428 1.099139 1.688477
H -0.861630 -0.392619 1.772045

s11b with 1 H_2O
C 1.655119 1.435910 -0.609239
C 2.927925 1.620286 -0.003704
C 3.588789 0.523109 0.608749
C 3.072270 -0.743761 0.566595
C 1.819151 -1.047237 -0.199171
C 1.101268 0.191615 -0.688783
H 1.105879 2.304561 -0.966585
H 3.365271 2.612680 0.045698
H 4.522314 0.703258 1.137677
H 3.593887 -1.569638 1.045614
C -0.299413 -0.216725 -1.069810
C -0.596337 -1.255954 0.010851
C -1.398122 0.850638 -1.122680
C -1.822292 -1.393006 0.529986
C -2.771596 0.167570 -1.105167
H -1.336270 1.511541 -0.251034
H -1.311058 1.471240 -2.021835
H -3.569811 0.915605 -1.142518
C 0.697242 -1.867023 0.532722
N -2.928795 -0.600565 0.140927
H -2.028667 -2.065701 1.359998
H -2.874330 -0.484838 -1.987474
H 0.786797 -2.939802 0.318279
H -3.806512 -1.110806 0.171490
H 0.786443 -1.747019 1.619299
H 2.100713 -1.649522 -1.089282
O -2.912465 1.835669 1.800137
H -2.110508 1.746387 2.335981
H -3.009634 0.950164 1.389070
H -0.257245 -0.722034 -2.054044

s11b with 2 H_2O
C -2.534806 -1.462940 0.108827
C -3.749859 -1.217262 0.804615
C -4.211904 0.113843 0.978355
C -3.559947 1.181033 0.421845
C -2.366122 0.987030 -0.464578
C -1.851395 -0.435644 -0.473589
H -2.131864 -2.473606 0.084433
H -4.291844 -2.042531 1.256160
H -5.099775 0.284783 1.583541
H -3.929746 2.193341 0.570469
C -0.462070 -0.410109 -1.058639
C 0.065588 0.908294 -0.492929
C 0.501569 -1.560208 -0.745296
C 1.352585 1.056080 -0.155188
C 1.932927 -1.126959 -1.090408
H 0.445726 -1.809235 0.321605
H 0.245495 -2.464269 -1.310031
H 1.726761 1.962076 0.317380
H 2.642630 -1.936115 -0.885757
C -1.087508 1.847942 -0.166483
N 2.322962 0.037343 -0.284213
H 1.991515 -0.898602 -2.167041
H -1.081781 2.768309 -0.764632
H 3.255108 0.395618 -0.517690
H -1.071827 2.148851 0.888356
H -2.666406 1.243901 -1.502916
O 3.903390 -0.634808 1.982360
H 3.670313 -0.108228 2.762138
H 3.144405 -0.505462 1.357736
H 4.937384 0.334987 0.822090
O 5.160594 0.814218 -0.010591
H 5.818188 0.247673 -0.440815
H -0.551238 -0.324759 -2.158881

s11c with 1 H_2O
C 2.174581 -1.541860 -0.024150
C 3.524972 -1.305295 -0.400741
C 4.018470 0.024220 -0.471171
C 3.264706 1.095441 -0.072409
C 1.923760 0.900336 0.573757
C 1.386720 -0.510875 0.396184
H 1.757366 -2.540972 -0.134891
H 4.151007 -2.132934 -0.719461
H 5.015279 0.191392 -0.873375
H 3.659504 2.106737 -0.142092
H 2.060543 1.074815 1.661489
C -0.103771 -0.420773 0.531455
C -0.366392 0.848442 -0.308945
C -1.059675 -1.515615 0.077802
H -0.347134 -0.166011 1.579908
C -1.821460 1.230298 -0.233429
C -2.502907 -1.005609 0.292073
H -0.883979 -1.743178 -0.982028
H -0.920032 -2.450396 0.634777
H -2.101555 2.270540 -0.431714
H -3.224537 -1.572556 -0.305773
H -2.806405 -1.164006 1.336044
C 0.734945 1.841818 0.129573
H 1.028608 2.516020 -0.681106
H 0.399725 2.461027 0.969342
N -2.770359 0.415916 0.016723
H -0.160839 0.583903 -1.359474
O -5.599539 -0.079420 -0.284736
H -4.729178 0.336455 -0.108921
H -5.753250 0.109954 -1.221887

s12a
C 1.812543 -1.483241 0.039559
C 3.184449 -1.177051 -0.019604
C 3.617328 0.157359 -0.027845
C 2.704380 1.207493 0.001409
C 1.321364 0.916264 0.030739
C 0.891608 -0.452543 0.070286
H 1.487990 -2.520975 0.068843
H 3.915203 -1.980558 -0.050547
H 4.682195 0.372865 -0.065894
H 3.047489 2.238870 -0.020094
C -0.608207 -0.455883 0.267319
C -1.025017 0.934324 -0.275862
C -1.553784 -1.531535 -0.262997
C -2.425481 1.277351 0.225582
C -2.980713 -1.133326 0.166296
H -1.494279 -1.594072 -1.356394
H -1.318320 -2.523331 0.143813
H -2.772461 2.238945 -0.171656
H -3.713732 -1.821577 -0.270107
C 0.194083 1.774093 -0.010546
N -3.318013 0.223813 -0.284476
H -2.419362 1.354912 1.330503
H -3.047002 -1.243024 1.267664
H -1.126536 0.835304 -1.373330
H 0.232938 2.857280 -0.067933
H -0.762787 -0.414194 1.361521
H -4.280559 0.433030 -0.031068

s12a with 1 H_2O
C -2.119578 -1.482823 -0.000474
C -3.465174 -1.173579 0.268822
C -3.890947 0.161533 0.335303
C -2.993025 1.209858 0.157763
C -1.631726 0.915698 -0.084049
C -1.214240 -0.453867 -0.180617
H -1.803889 -2.521184 -0.070702
H -4.182513 -1.975577 0.419730
H -4.936656 0.379014 0.537735
H -3.327457 2.242028 0.226507
C 0.237073 -0.462713 -0.606928
C 0.732060 0.930441 -0.141327
C 1.251655 -1.535234 -0.213414
C 2.034119 1.272376 -0.861549
C 2.595458 -1.149792 -0.864352
H 1.366167 -1.581109 0.875061
H 0.957308 -2.530533 -0.569701
H 2.440522 2.237887 -0.536767
H 3.387999 -1.830877 -0.536445
C -0.511468 1.772062 -0.222610
N 3.007071 0.220806 -0.489013
H 1.866575 1.328447 -1.952228
H 2.499666 -1.254782 -1.960804
H 1.003294 0.832453 0.926090
H -0.539905 2.855496 -0.163979
H 0.220962 -0.429285 -1.712616
H 3.909151 0.422536 -0.915942
O 2.974999 -0.079644 2.387908
H 3.026588 0.792537 2.805723
H 3.117447 0.100700 1.428764

s12a with 2 H_2O
C -2.348955 0.526782 1.372949
C -3.664986 0.779205 0.945137
C -4.086787 0.383752 -0.333037
C -3.213301 -0.248367 -1.212948
C -1.879680 -0.483852 -0.808054
C -1.468291 -0.099997 0.511513
H -2.037113 0.818302 2.373424
H -4.362524 1.278235 1.612259
H -5.109731 0.582498 -0.642821
H -3.543759 -0.537505 -2.207443
C -0.064786 -0.620996 0.724201
C 0.467871 -0.760068 -0.724306
C 0.993768 0.059234 1.589186
C 1.676738 -1.689834 -0.731095
C 2.251141 -0.830384 1.544494
H 1.215414 1.056186 1.192511
H 0.675060 0.164878 2.633986
H 2.114680 -1.787512 -1.731746
H 3.083385 -0.351262 2.071678
C -0.782279 -1.034486 -1.514909
N 2.703859 -1.084612 0.154171
H 1.383473 -2.698984 -0.393028
H 2.028458 -1.777834 2.066515
H 0.831473 0.239882 -1.023050
H -0.809102 -1.374367 -2.545316
H -0.186525 -1.649294 1.114390

H 3.511213 -1.705607 0.194214
O 3.928819 1.351509 -0.556330
H 4.251262 1.292187 -1.468441
H 3.480108 0.476052 -0.387645
H 2.420530 2.318299 -0.721477
O 1.502717 2.653931 -0.848941
H 1.391681 3.318674 -0.153821

s12b
C 1.853645 -1.436807 0.308051
C 3.180525 -1.117580 0.006034
C 3.536805 0.197226 -0.309357
C 2.570622 1.207300 -0.325570
C 1.246917 0.888708 -0.027185
C 0.888576 -0.430594 0.288619
H 1.581581 -2.460540 0.555703
H 3.939899 -1.895246 0.018119
H 4.571470 0.435789 -0.542053
H 2.852634 2.229172 -0.569818
C -0.596300 -0.539831 0.575445
C -1.071714 0.882303 0.418940
C -1.398972 -1.475509 -0.368738
C -2.537761 1.154163 0.352674
C -2.899331 -1.188058 -0.235054
H -1.093716 -1.291869 -1.405188
H -1.192479 -2.528149 -0.136254
H -2.735656 2.175271 0.005102
H -3.465947 -1.830809 -0.918850
C 0.040203 1.807682 0.012757
N -3.173661 0.207757 -0.589552
H -2.979951 1.069499 1.370484
H -3.224675 -1.440645 0.795701
H 0.184203 2.645903 0.717669
H -4.180658 0.364228 -0.583577
H -0.150559 2.282785 -0.966038
H -0.769819 -0.903701 1.606157

s12b with 1 H_2O
C 2.121186 1.461210 -0.208528
C 3.394548 1.110099 0.248288
C 3.710482 -0.227930 0.503372
C 2.756739 -1.230223 0.304686
C 1.485782 -0.879586 -0.147117
C 1.167923 0.462670 -0.403495
H 1.881054 2.503095 -0.407892
H 4.143842 1.881572 0.405342
H 4.703791 -0.490544 0.857895
H 3.007095 -2.270011 0.503323
C -0.261685 0.603837 -0.891131
C -0.758508 -0.819146 -0.872395
C -1.189675 1.507680 -0.036798
C -2.217100 -1.088222 -1.027115
C -2.655062 1.244817 -0.402739
H -1.059121 1.280527 1.026474
H -0.949028 2.566505 -0.193236
H -2.465653 -2.119224 -0.749802
H -3.312810 1.858738 0.221358
C 0.301248 -1.786231 -0.426801
N -2.987065 -0.169641 -0.150733
H -2.520469 -0.956298 -2.087246
H -2.835699 1.525946 -1.457806
H 0.538810 -2.547963 -1.191121
H -3.983176 -0.315001 -0.312260
H -0.003936 -2.362371 0.464998
H -0.278336 1.011565 -1.920626
O -2.364364 -0.188443 2.691067
H -1.554513 -0.712460 2.777743
H -2.622746 -0.312900 1.748088

s12b with 2 H_2O
C -2.690773 -1.189783 0.334923
C -3.802926 -0.396245 0.631284
C -3.773105 0.980068 0.386877
C -2.632504 1.578713 -0.156552
C -1.520929 0.789716 -0.448465
C -1.551359 -0.592181 -0.201903
H -2.719420 -2.260874 0.523302
H -4.695334 -0.851719 1.052759
H -4.642685 1.588932 0.620838
H -2.614136 2.649609 -0.345722
C -0.239564 -1.244538 -0.598922
C 0.593827 -0.066369 -1.034298
C 0.489275 -2.047917 0.508020
C 2.061802 -0.224226 -1.234463
C 1.948862 -2.290064 0.106963
H 0.464418 -1.482355 1.447877
H -0.011448 -3.007270 0.688792
H 2.558159 0.750866 -1.262412
H 2.476344 -2.833609 0.898746
C -0.188388 1.216018 -1.035330
N 2.636385 -1.003066 -0.098820
H 2.272791 -0.746952 -2.190640
H 1.980208 -2.918176 -0.802763
H -0.313427 1.635860 -2.050816
H 3.622962 -1.177435 -0.289833
H 0.317457 2.009911 -0.464087
H -0.399957 -1.946344 -1.441713
O 2.565090 0.881301 1.990098
H 1.642583 0.901124 2.287526
H 2.593355 0.137037 1.324636
H 2.621782 2.220470 0.794942
O 2.562787 2.836064 0.025777
H 3.203334 3.534304 0.224502

s12c
C -1.716686 -1.518077 0.036128
C -3.064151 -1.249789 -0.176720
C -3.533684 0.069902 -0.263801
C -2.641731 1.150397 -0.142471
C -1.297389 0.902688 0.069554
C -0.810025 -0.437504 0.169448
H -1.364720 -2.543812 0.109356
H -3.766357 -2.074207 -0.273845
H -4.591169 0.257663 -0.427795
H -3.011402 2.170818 -0.219915
C 0.581786 -0.425559 0.400876
C 1.087552 0.993408 0.520112
C 1.566057 -1.546923 0.442901
C 2.312230 1.186186 -0.395873
C 2.772187 -1.203939 -0.459930
H 1.944597 -1.686523 1.468229
H 1.118501 -2.496815 0.127029
H 2.788003 2.155900 -0.205703
H 3.575103 -1.934179 -0.307087
C -0.146076 1.882022 0.191761
N 3.281256 0.125085 -0.113508
H 1.968714 1.182488 -1.449749
H 2.451760 -1.273649 -1.517590
H 1.435579 1.176997 1.549317
H 0.002427 2.427427 -0.751672
H 4.145400 0.303803 -0.619797
H -0.325639 2.641621 0.961873

s12c with 1 H_2O
C -2.058984 -1.543793 0.031321
C -3.428692 -1.306669 0.049635
C -3.936053 0.000171 0.117543
C -3.061219 1.100218 0.163137
C -1.695299 0.883392 0.145547
C -1.167482 -0.443826 0.084975
H -1.676506 -2.560060 -0.013795
H -4.118608 -2.146180 0.014418
H -5.010095 0.162762 0.133240
H -3.461399 2.110973 0.207809
C 0.242313 -0.400866 0.091434
C 0.727346 1.025237 0.206831
C 1.253902 -1.485075 -0.071578
C 1.764123 1.310220 -0.895616
C 2.275122 -1.072477 -1.155225
H 1.814174 -1.626972 0.865036
H 0.793572 -2.442778 -0.340005
H 2.241047 2.285919 -0.743438
H 3.115930 -1.773915 -1.168153
C -0.562820 1.892187 0.149611
N 2.804684 0.270202 -0.851068
H 1.248458 1.336410 -1.873203
H 1.789346 -1.101506 -2.146569
H 1.246031 1.159715 1.170367
H -0.584367 2.509163 -0.760397
H 3.545165 0.498570 -1.511604
H -0.628926 2.587908 0.994448
O 3.847845 -0.368255 1.789651
H 3.572365 0.329064 2.402642
H 3.584719 -0.026748 0.903797

s12c with 2 H_2O
C -2.252185 1.719626 0.034121
C -3.641382 1.728808 -0.017819
C -4.367544 0.537569 -0.171245
C -3.698126 -0.695039 -0.269318
C -2.316065 -0.723243 -0.219176
C -1.566186 0.484706 -0.073354
H -1.699150 2.648413 0.146100
H -4.174463 2.673211 0.058373
H -5.452751 0.567733 -0.211920
H -4.267831 -1.615443 -0.378826
C -0.185052 0.195554 -0.063890
C 0.044856 -1.284566 -0.267172
C 0.990300 1.078053 0.192757
C 1.007279 -1.816310 0.809722
C 1.924284 0.426194 1.233596
H 1.578998 1.227618 -0.726711
H 0.691305 2.073222 0.539774
H 1.310446 -2.846869 0.590413
H 2.870723 0.973479 1.261411
C -1.377827 -1.913829 -0.261339
N 2.212315 -0.969189 0.835876
H 0.489581 -1.816244 1.785517
H 1.447912 0.464853 2.227961
H 0.535210 -1.456124 -1.240715
H -1.520525 -2.554147 0.621120
H 2.886810 -1.365335 1.489028
H -1.551364 -2.551257 -1.136199
O 3.907551 -0.586187 -1.389187
H 3.367153 -0.419805 -2.176110
H 3.252733 -0.823142 -0.676403
H 4.402561 1.036535 -0.726200
O 4.534350 1.878309 -0.232031

H 5.437125 1.805520 0.110703

s12d with 1 H_2O
C -2.050718 -1.502109 -0.217480
C -3.383415 -1.300278 0.162980
C -3.850874 -0.016203 0.450698
C -2.992882 1.087792 0.367977
C -1.666123 0.888472 0.000038
C -1.197171 -0.406499 -0.294267
H -1.692023 -2.503818 -0.442504
H -4.057401 -2.149774 0.237878
H -4.886532 0.127301 0.747912
H -3.361274 2.084648 0.600196
C 0.250860 -0.311875 -0.726514
C 0.696343 0.997540 -0.029767
C 1.278425 -1.410740 -0.458676
C 2.033708 1.424511 -0.536411
C 2.631689 -0.938146 -1.018030
H 1.377443 -1.597096 0.616762
H 1.010125 -2.356812 -0.945064
H 2.424140 2.418798 -0.327927
H 3.426969 -1.635446 -0.736336
C -0.543334 1.905688 -0.149678
N 3.003022 0.396193 -0.489962
H 2.578084 -0.910799 -2.118607
H 0.788425 0.739755 1.044988
H -0.575971 2.702649 0.601889
H 0.256459 -0.117155 -1.814685
H 3.906653 0.693947 -0.846037
O 3.158265 -0.623176 2.295122
H 2.633779 -0.025174 2.847837
H 3.222131 -0.154393 1.436562
H -0.577340 2.386508 -1.139333

s12d with 2 H_2O
C -2.677294 -1.178413 0.560699
C -3.861751 -0.463740 0.779442
C -3.965823 0.870300 0.379925
C -2.887527 1.513687 -0.240575
C -1.705675 0.809942 -0.450894
C -1.604029 -0.537131 -0.049425
H -2.602352 -2.218594 0.870388
H -4.703834 -0.949960 1.265382
H -4.888840 1.416303 0.557745
H -2.972929 2.555151 -0.542325
C -0.242790 -1.063402 -0.455019
C 0.584192 0.241099 -0.521990
C 0.521488 -2.108162 0.358082
C 1.910271 -0.004300 -1.155976
C 1.882801 -2.343009 -0.321604
H 0.667911 -1.753128 1.387273
H -0.010783 -3.065837 0.416086
H 2.534786 0.836758 -1.444065
H 2.516498 -2.991659 0.292700
C -0.403434 1.278804 -1.084253
N 2.616934 -1.074858 -0.541982
H 1.710924 -2.855955 -1.281589
H -0.457330 1.214748 -2.181979
H 3.507994 -1.252907 -0.998669
H -0.122194 2.303656 -0.824070
H -0.327785 -1.453147 -1.485463
O 3.429781 0.554080 1.728939
H 2.749431 0.467993 2.413909
H 3.179650 -0.115876 1.047428
H 2.963389 2.106376 0.821079
O 2.631602 2.844901 0.264677
H 3.382394 3.453690 0.209951

H 0.760896 0.540488 0.530694

s12e with 1 H_2O
C -2.057093 -1.500474 -0.182756
C -3.377902 -1.266930 0.219032
C -3.816434 0.030917 0.491175
C -2.941347 1.117378 0.370616
C -1.626436 0.887002 -0.021484
C -1.186601 -0.421655 -0.298466
H -1.720724 -2.512809 -0.394144
H -4.065404 -2.102262 0.323570
H -4.843116 0.198686 0.806056
H -3.286571 2.124645 0.592561
C 0.257249 -0.364042 -0.753995
C 0.732092 0.947056 -0.092217
C 1.263522 -1.476721 -0.471984
C 2.105498 1.351360 -0.662639
C 2.654024 -0.986278 -0.976429
H 1.327954 -1.674685 0.603742
H 1.013787 -2.414601 -0.983363
H 2.479775 2.276299 -0.210607
H 3.423994 -1.732570 -0.752811
C -0.488816 1.881433 -0.210671
N 3.035510 0.272443 -0.361803
H 2.603091 -0.870992 -2.073794
H -0.536936 2.345762 -1.208442
H -0.491304 2.691261 0.526927
H 0.247340 -0.202495 -1.848565
O 2.970852 -0.302733 2.414588
H 3.550016 -1.052426 2.616631
H 3.278756 0.006067 1.534582
H 0.877401 0.732771 0.975195
H 2.020020 1.507832 -1.752706

s12e with 1 H_2O
C 2.807971 -1.142579 -0.579520
C 3.979993 -0.415545 -0.821000
C 4.066732 0.929109 -0.453240
C 2.983092 1.571233 0.158392
C 1.814262 0.853626 0.393465
C 1.729611 -0.503169 0.023728
H 2.745985 -2.190006 -0.866116
H 4.826356 -0.900147 -1.300842
H 4.980512 1.484048 -0.649482
H 3.054259 2.620855 0.434132
C 0.374887 -1.038907 0.442158
C -0.464141 0.253621 0.478129
C -0.368003 -2.111875 -0.349582
C -1.817160 -0.007083 1.158022
C -1.785282 -2.276007 0.278020
H -0.461081 -1.815074 -1.401690
H 0.137410 -3.085178 -0.325381
H -2.424221 0.900874 1.173173
H -2.382328 -2.984304 -0.306029
C 0.507219 1.318443 1.020858
N -2.509193 -1.022303 0.373618
H -1.659100 -2.699103 1.290620
H 0.566636 1.279956 2.120188
H 0.216127 2.335116 0.739716
H 0.470267 -1.406789 1.480699
O -4.445849 0.382355 -1.119565
H -4.275173 0.154771 -2.046038
H -3.882395 -0.251657 -0.605481
H -3.449530 1.877801 -0.820439
O -2.822595 2.596170 -0.570957
H -3.388160 3.249878 -0.134344
H -0.682954 0.535400 -0.561020

H -1.655796 -0.363726 2.190599

s13
C 1.451837 0.040988 -1.086728
C 2.829707 0.097104 -1.295658
C 3.711147 -0.053999 -0.222853
C 3.202187 -0.258949 1.059459
C 1.822035 -0.313786 1.263639
C 0.925661 -0.166660 0.197800
H 0.778444 0.169273 -1.929848
H 3.215469 0.259260 -2.298878
H 4.784675 -0.011652 -0.386322
H 3.877417 -0.377198 1.902983
H 1.433882 -0.474657 2.267213
C -0.571709 -0.257527 0.441063
C -1.355253 1.031718 0.218653
C -1.229484 -1.391417 -0.385716
H -0.714008 -0.527192 1.500548
C -2.862749 0.862128 0.388266
C -2.750073 -1.462592 -0.128472
H -1.061095 -1.214888 -1.454186
H -0.767179 -2.354219 -0.138104
H -3.379016 1.796979 0.147578
H -3.199373 -2.256363 -0.736029
C -0.828384 2.219140 -0.085412
H 0.241657 2.368377 -0.187558
H -1.461389 3.090343 -0.234868
N -3.404660 -0.207726 -0.431997
H -3.070744 0.633000 1.453081
H -2.915667 -1.723877 0.934136

s13 with 1 H_2O
C 1.818232 -0.572746 0.995390
C 3.145328 -0.904871 1.267033
C 4.168461 -0.460363 0.426666
C 3.852289 0.315811 -0.688192
C 2.522223 0.645197 -0.956707
C 1.486067 0.209726 -0.121540
H 1.032444 -0.934320 1.653261
H 3.380196 -1.512631 2.137015
H 5.202414 -0.718117 0.639714
H 4.639153 0.667330 -1.350487
H 2.284927 1.252158 -1.827911
C 0.049555 0.610719 -0.414441
C -0.893794 -0.529619 -0.780994
C -0.570565 1.418733 0.754144
H 0.070363 1.289924 -1.282641
C -2.340246 -0.083947 -0.978044
C -2.030296 1.820555 0.449561
H -0.553933 0.816678 1.669476
H 0.022531 2.320353 0.946331
H -2.996192 -0.943451 -1.137936
H -2.461706 2.363651 1.297329
C -0.549715 -1.808469 -0.940216
H 0.475577 -2.147995 -0.834113
H -1.293420 -2.560724 -1.189494
N -2.846765 0.663833 0.160195
H -2.391606 0.563914 -1.875516
H -2.034397 2.501016 -0.422028
O -4.923757 -1.273031 0.667743
H -4.298596 -0.524827 0.765039
H -5.705574 -0.859896 0.272688

s13 with 2 H_2O
C 1.690292 1.030008 -0.194184
C 2.968287 1.590468 -0.159994
C 4.100971 0.774682 -0.121199
C 3.948821 -0.611987 -0.114366
C 2.671064 -1.172992 -0.147985

C 1.527430 -0.364943 -0.189062
H 0.820960 1.682529 -0.221548
H 3.076240 2.672009 -0.165848
H 5.093730 1.216480 -0.097541
H 4.822007 -1.258777 -0.085624
H 2.560246 -2.255603 -0.144366
C 0.150794 -1.010611 -0.239236
C -0.656992 -0.922549 1.052220
C -0.713575 -0.478853 -1.410160
H 0.303310 -2.086913 -0.425239
C -2.052435 -1.537796 0.933524
C -2.102506 -1.163835 -1.428957
H -0.860335 0.599773 -1.298654
H -0.209052 -0.660661 -2.365730
H -2.615259 -1.398985 1.861590
H -2.714460 -0.758810 -2.241079
C -0.241947 -0.384297 2.202299
H 0.753904 0.033279 2.310902
H -0.883185 -0.366138 3.080398
N -2.777633 -0.937262 -0.170338
H -1.946916 -2.624674 0.757235
H -1.970874 -2.247091 -1.600421
O -3.976028 1.614331 -0.315603
H -3.742907 0.660096 -0.203480
H -4.562371 1.819021 0.427928
H -2.293196 2.328249 -0.014430
O -1.362545 2.494597 0.259274
H -1.221058 1.851850 0.971511

s14
C -1.474516 -0.333150 1.098636
C -2.856820 -0.337725 1.282931
C -3.711616 -0.124763 0.199092
C -3.170845 0.092931 -1.068004
C -1.786013 0.096344 -1.246929
C -0.915012 -0.116494 -0.170210
H -0.825216 -0.502304 1.954586
H -3.267443 -0.508491 2.274811
H -4.788796 -0.128626 0.342501
H -3.825007 0.260272 -1.919828
H -1.372600 0.264758 -2.239029
C 0.588472 -0.127806 -0.387266
C 1.328144 0.994635 0.392116
C 1.239876 -1.476090 -0.023854
H 0.771984 0.052966 -1.455407
C 2.838293 0.768812 0.371987
C 2.732603 -1.467489 -0.371944
H 1.114773 -1.663677 1.051165
H 0.735542 -2.296878 -0.547654
H 3.438279 1.634926 0.676673
H 3.234296 -2.333542 0.077341
H 2.874973 -1.571309 -1.457547
C 0.994737 2.368877 -0.090280
H -0.007714 2.603008 -0.431433
H 1.700862 3.185432 0.026595
N 3.478477 -0.276582 0.039019
H 1.022904 0.911054 1.456447

s14 with 1 H_2O
C -2.037811 -0.206860 1.135152
C -3.409718 -0.100056 1.361689
C -4.285281 0.101865 0.292472
C -3.776060 0.195452 -1.002623
C -2.401559 0.088037 -1.223998
C -1.510321 -0.113947 -0.161974
H -1.372417 -0.365466 1.980748
H -3.795554 -0.174831 2.375070
H -5.354260 0.185512 0.468709
H -4.446803 0.352513 -1.843373
H -2.013159 0.160829 -2.237622
C -0.019341 -0.243084 -0.422921
C 0.818024 0.867067 0.270603
C 0.549770 -1.612961 -0.004815
H 0.140459 -0.133518 -1.504508
C 2.303775 0.538330 0.239254
C 2.026039 -1.728851 -0.396477
H 0.448166 -1.735974 1.081724
H -0.025317 -2.422547 -0.469170
H 2.987930 1.355123 0.489332
H 2.483213 -2.603763 0.080889
H 2.127085 -1.889497 -1.479578
C 0.573430 2.231092 -0.290189
H -0.413376 2.507255 -0.645015
H 1.327300 3.008006 -0.208709
N 2.854775 -0.569844 -0.058499
H 0.536015 0.871460 1.344559
O 5.488657 0.515876 0.324109
H 4.743357 -0.106724 0.183561
H 5.749001 0.757014 -0.577047

s14 with 2 H_2O
C -2.487587 0.004359 1.161104
C -3.839199 0.266292 1.383238
C -4.718001 0.390481 0.304898
C -4.232507 0.250371 -0.995129
C -2.878393 -0.012362 -1.212053
C -1.984053 -0.139401 -0.141030
H -1.819402 -0.089427 2.014137
H -4.206853 0.373571 2.400484
H -5.771083 0.595029 0.478010
H -4.905855 0.345453 -1.843031
H -2.508278 -0.121145 -2.229242
C -0.516064 -0.434953 -0.395879
C 0.425435 0.704706 0.083403
C -0.044238 -1.753666 0.246232
H -0.378409 -0.525827 -1.482173
C 1.881453 0.264183 0.081993
C 1.406248 -2.056114 -0.140834
H -0.123602 -1.678815 1.338956
H -0.692824 -2.582301 -0.061176
H 2.630023 1.059911 0.172172
H 1.808129 -2.867214 0.478120
H 1.461890 -2.412923 -1.179488
C 0.269810 1.972607 -0.694176
H -0.710244 2.280643 -1.041596
H 1.099522 2.664475 -0.797180
N 2.331451 -0.924948 -0.025749
H 0.177571 0.909826 1.146412
O 5.144531 -0.720400 -0.004145
H 4.176624 -0.944977 0.009308
H 5.401440 -0.845058 -0.930388
H 4.962160 1.073131 0.169726
O 4.670998 2.009431 0.282911
H 4.857376 2.189017 1.216457

s15
C -1.449926 -0.252164 1.094907
C -2.829741 -0.243152 1.295589
C -3.697513 -0.111403 0.208912
C -3.171945 0.013156 -1.076920
C -1.789094 0.005052 -1.271926
C -0.905858 -0.128495 -0.192942
H -0.789143 -0.352200 1.953069
H -3.228366 -0.337852 2.302422
H -4.772943 -0.104698 0.364797
H -3.836309 0.117509 -1.930902
H -1.387778 0.102917 -2.278431
C 0.596524 -0.153335 -0.423546
C 1.378466 0.946842 0.338811
C 1.208451 -1.523777 -0.066549
H 0.769908 0.019873 -1.494861
C 2.879060 0.851237 -0.031812
C 2.719803 -1.498045 -0.012000
H 0.832549 -1.870927 0.907857
H 0.888077 -2.287524 -0.787907
H 3.463410 1.490104 0.642557
H 3.211947 -2.476911 0.019666
C 0.864204 2.326876 0.103547
H -0.131807 2.504581 -0.286219
H 1.447949 3.186114 0.421700
N 3.481549 -0.479530 -0.001151
H 1.309334 0.710911 1.418732
H 3.037741 1.258067 -1.040865

s15 with 1 H_2O
C -1.978283 -0.210304 1.132700
C -3.342946 -0.143682 1.411424
C -4.265920 0.005759 0.373757
C -3.811067 0.089951 -0.941954
C -2.443098 0.024605 -1.215405
C -1.505376 -0.127230 -0.186041
H -1.274373 -0.322976 1.954270
H -3.686261 -0.207120 2.440769
H -5.329443 0.057393 0.590589
H -4.518924 0.207600 -1.758321
H -2.096648 0.092625 -2.244478
C -0.020643 -0.211069 -0.501602
C 0.842641 0.878180 0.189961
C 0.558814 -1.597772 -0.150110
H 0.096712 -0.065326 -1.584117
C 2.310339 0.720514 -0.258165
C 2.067875 -1.630743 -0.149525
H 0.211364 -1.921905 0.842566
H 0.185106 -2.359672 -0.847271
H 2.972785 1.351307 0.344900
H 2.528431 -2.622902 -0.095966
C 0.365117 2.270065 -0.055923
H -0.676605 2.479481 -0.271419
H 1.031725 3.111149 0.111124
N 2.859523 -0.635946 -0.200151
H 0.819585 0.671171 1.278355
H 2.425729 1.072001 -1.293204
O 5.524936 0.332915 0.341589
H 5.667083 0.046498 1.255682
H 4.762845 -0.210667 0.050161

s15 with 2 H_2O
C -2.381232 -0.461828 1.095496
C -3.714737 -0.806483 1.312959
C -4.609129 -0.865879 0.241722
C -4.157899 -0.575548 -1.045609
C -2.821722 -0.229135 -1.257597
C -1.912223 -0.167558 -0.194146
H -1.699659 -0.419568 1.942165
H -4.056118 -1.029248 2.320545
H -5.648029 -1.135893 0.410688
H -4.843943 -0.617960 -1.887577
H -2.478159 -0.003956 -2.264985
C -0.457399 0.196165 -0.443037
C 0.023157 1.458937 0.320858
C 0.491776 -0.971451 -0.102775
H -0.348830 0.414669 -1.514354
C 1.489219 1.756446 -0.063498

C 1.945016 -0.573135 -0.047225
H 0.227794 -1.415344 0.868844
H 0.377002 -1.787648 -0.828256
H 1.896380 2.525584 0.604704
H 2.685067 -1.380585 -0.015304
C -0.831614 2.661465 0.099649
H -1.882225 2.567715 -0.150990
H -0.448114 3.652229 0.326675
N 2.406940 0.617660 -0.031494
H 0.024273 1.205510 1.399422
H 1.528640 2.184329 -1.075278
O 5.220803 0.436539 0.035132
H 5.038736 -1.364690 0.044591
H 4.251454 0.646873 -0.025375
H 5.452199 0.655800 0.950466
O 4.746551 -2.307231 0.026186
H 4.956837 -2.587890 -0.876840

s16
C -1.459472 1.189954 0.102923
C -2.833179 1.414398 0.197617
C -3.723430 0.339497 0.151812
C -3.229777 -0.958497 0.010586
C -1.854657 -1.178397 -0.083934
C -0.950761 -0.108582 -0.041311
H -0.769685 2.030292 0.134832
H -3.208798 2.428976 0.303607
H -4.793988 0.512862 0.222297
H -3.915486 -1.801134 -0.028388
H -1.473939 -2.190698 -0.197321
C 0.534580 -0.350670 -0.091440
C 1.364461 0.303552 -1.179098
C 1.200810 -0.440458 1.280728
C 2.742085 0.877594 -0.846874
C 2.742282 -0.421491 1.212247
H 0.870668 0.412254 1.887819
H 0.872423 -1.346945 1.806215
H 2.742616 1.957924 -1.050564
H 3.154028 -0.407818 2.228103
C 1.100429 -1.186691 -1.217115
H 0.407758 -1.549904 -1.971489
H 1.921655 -1.868857 -1.010629
N 3.282403 0.706905 0.487313
H 3.497721 0.462855 -1.542350
H 3.102030 -1.357014 0.745559
H 0.815949 0.887616 -1.915733

s16 with 1 H_2O
C -1.597050 1.285521 -0.067985
C -2.870713 1.850175 0.005849
C -3.995026 1.030237 0.122981
C -3.836275 -0.355904 0.165309
C -2.560398 -0.917103 0.090911
C -1.424904 -0.105282 -0.028739
H -0.724519 1.927732 -0.163728
H -2.985112 2.930433 -0.031589
H -4.987919 1.468675 0.177571
H -4.706145 -1.001782 0.253789
H -2.440398 -1.997520 0.120218
C -0.045089 -0.708442 -0.057890
C 0.870795 -0.421965 -1.233052
C 0.632265 -0.781488 1.310241
C 2.357678 -0.159407 -0.998267
C 2.133863 -1.132638 1.227237
H 0.531912 0.191707 1.806443
H 0.127418 -1.517072 1.949864
H 2.632796 0.837831 -1.363102
H 2.579811 -1.091977 2.226764
C 0.257104 -1.795473 -1.064435
H -0.532964 -2.076409 -1.755452
H 0.900263 -2.622896 -0.773952
N 2.863847 -0.240223 0.358035
H 2.964090 -0.865859 -1.599070
H 2.251341 -2.170045 0.866894
H 0.448414 0.179092 -2.035494
O 4.388193 2.186956 0.095635
H 3.996162 1.356817 0.440291
H 5.258871 1.907792 -0.223722

s16 with 2 H_2O
C 1.527095 1.132772 0.061122
C 2.729747 1.829098 -0.073038
C 3.927909 1.139909 -0.272878
C 3.919881 -0.254585 -0.337837
C 2.718348 -0.952077 -0.203922
C 1.512034 -0.268893 -0.001476
H 0.596820 1.673676 0.226974
H 2.730140 2.914843 -0.016350
H 4.862794 1.685504 -0.373069
H 4.848351 -0.799694 -0.488981
H 2.714074 -2.039028 -0.248343
C 0.210386 -1.021596 0.094695
C -0.685822 -0.789667 1.293914
C -0.494919 -1.215367 -1.248025
C -2.201139 -0.666332 1.108166
C -1.974432 -1.642441 -1.095485
H -0.465513 -0.267773 -1.799514
H 0.031163 -1.958225 -1.861835
H -2.529618 0.282639 1.540141
H -2.452757 -1.681561 -2.080174
C 0.056658 -2.099617 1.144903
H 0.896760 -2.276948 1.811029
H -0.508186 -2.997617 0.903276
N -2.686358 -0.705419 -0.258961
H -2.723111 -1.473840 1.656804
H -2.026928 -2.656052 -0.664142
H -0.298708 -0.110000 2.047873
O -3.750318 1.819665 -0.865764
H -3.556642 0.855233 -0.734722
H -3.491625 1.991576 -1.783891
H -2.383891 2.399249 0.172819
O -1.623624 2.552594 0.781482
H -1.921562 3.270658 1.358256

s17
C -1.33552 0.06807 -0.38417
C -1.90779 -1.33772 -0.17548
C -3.2613 -1.47002 0.13627
C -4.06106 -0.32264 0.25067
C -3.51547 0.962 0.05486
C -2.15502 1.13846 -0.26096
H -1.28197 -2.20079 -0.26698
H -3.68676 -2.44013 0.28715
H -5.09903 -0.42443 0.48976
H -4.1478 1.82012 0.1481
H -1.76624 2.12494 -0.40453
C 0.15278 0.26093 -0.72966
H 0.28186 0.23255 -1.79147
C 1.03658 -0.88376 -0.11895
H 0.52484 -1.81632 -0.2345
C 2.46248 -0.45215 -0.26538
H 2.36759 -1.51565 -0.19564
C 1.36445 -0.40766 1.28052
H 0.52716 -0.01671 1.81997
H 1.80547 -1.16953 1.88875
C 0.57328 1.65248 -0.10625
H 0.16457 2.45029 -0.6905
H 0.20992 1.72719 0.89739
C 2.0755 1.69769 -0.04141
H 2.46407 2.61757 0.34295
H 2.46626 1.54801 -1.0262
O 3.91496 -1.05191 -0.19838
H 4.62442 -0.81843 -0.8015
N 2.40438 0.57669 0.83835
H 3.64573 -0.05469 0.76213

s18
C -1.329676 0.147439 1.076672
C -2.691651 0.200584 1.370038
C -3.635305 -0.084259 0.379861
C -3.204063 -0.419923 -0.903317
C -1.838622 -0.468867 -1.193042
C -0.882311 -0.187718 -0.210620
H -0.603076 0.372747 1.854353
H -3.017120 0.464356 2.373062
H -4.696950 -0.043731 0.608127
H -3.928817 -0.642909 -1.682082
H -1.510997 -0.731251 -2.196882
C 0.606059 -0.283542 -0.522678
C 1.390844 0.977446 -0.215522
C 1.256771 -1.483117 0.202559
H 0.694520 -0.461429 -1.609303
C 2.716530 0.867085 0.247964
C 2.777794 -1.479656 0.024984
H 1.023826 -1.420423 1.273102
H 0.825271 -2.422211 -0.162999
H 3.236463 1.798230 0.491525
H 3.233740 -2.286185 0.612008
H 3.036353 -1.689678 -1.026810
C 0.796368 2.321409 -0.506540
H 0.499231 2.399768 -1.563379
H -0.115134 2.503780 0.076697
H 1.507980 3.126448 -0.296351
N 3.434040 -0.229829 0.392397

s18 with 1 H_2O
C 1.790487 -0.347525 1.081774
C 3.114765 -0.570687 1.456645
C 4.156064 -0.252010 0.581353
C 3.860850 0.288396 -0.670007
C 2.532694 0.507137 -1.042467
C 1.480028 0.194395 -0.174857
H 0.987488 -0.600477 1.770684
H 3.334310 -0.993341 2.433631
H 5.188221 -0.424914 0.873707
H 4.662612 0.539500 -1.359505
H 2.310865 0.928913 -2.020621
C 0.036557 0.476069 -0.573088
C -0.878433 -0.731721 -0.508350
C -0.565395 1.624686 0.267641
H 0.054432 0.806212 -1.626984
C -2.226655 -0.554322 -0.143974
C -2.056147 1.807975 -0.027264
H -0.439863 1.390381 1.332051
H -0.017930 2.555009 0.078516
H -2.864359 -1.437350 -0.069172
H -2.491588 2.561457 0.639257
H -2.196748 2.190485 -1.052143

C -0.379335 -2.080327 -0.926074
H 0.015111 -2.052157 -1.953011
H 0.449849 -2.423453 -0.294558
H -1.176090 -2.829634 -0.889248
N -2.844134 0.587106 0.096274
O -5.336553 -0.723112 0.646090
H -4.620937 -0.054614 0.575260
H -5.786903 -0.653262 -0.208508

s18 with 2 H_2O
C 2.490080 0.539120 -0.875842
C 3.873617 0.478869 -1.038354
C 4.634879 -0.396691 -0.259975
C 4.000908 -1.207843 0.680800
C 2.615237 -1.141712 0.842234
C 1.840133 -0.270477 0.068269
H 1.906982 1.224006 -1.487767
H 4.358133 1.115172 -1.774411
H 5.712935 -0.444892 -0.387234
H 4.582635 -1.893170 1.291685
H 2.128399 -1.778938 1.577507
C 0.325243 -0.233611 0.224706
C -0.235264 1.133781 0.564181
C -0.389700 -0.784837 -1.029370
H 0.073269 -0.896511 1.070968
C -1.521140 1.477844 0.109056
C -1.907309 -0.629989 -0.926616
H -0.029149 -0.238288 -1.910169
H -0.124955 -1.837555 -1.177298
H -1.900903 2.467136 0.376922
H -2.384048 -0.893960 -1.878411
H -2.345797 -1.313216 -0.181355
C 0.516067 2.054566 1.475459
H 0.744512 1.560220 2.431373
H 1.484171 2.348346 1.050833
H -0.056565 2.962230 1.691543
N -2.354792 0.715071 -0.572199
O -4.388761 -1.928634 0.896513
H -4.329344 -1.543119 1.782926
H -4.779040 -1.201560 0.358933
H -4.203185 0.671229 -0.645108
O -5.143293 0.370938 -0.548666
H -5.554579 1.034819 0.024390

s2 with 1 H_2O
C 0.537052 -2.302366 0.121674
C 2.041326 -2.566897 -0.017320
C 2.644661 -0.302116 -0.413017
C 1.224794 0.231546 -0.076016
C 0.158914 -0.841265 0.039273
C 1.281745 1.074133 1.219497
C -1.231389 -0.478449 0.008696
C -2.248444 -1.448596 0.248188
C -1.675249 0.848467 -0.274519
C -3.596201 -1.117184 0.219066
C -3.027272 1.165214 -0.305276
C -4.002155 0.192941 -0.056084
H 2.538447 -2.471953 0.969561
H 2.204269 -3.593488 -0.361655
H 0.017966 -2.837914 -0.686801
H 0.176167 -2.756925 1.058169
H 0.293474 1.463221 1.467984
H 1.620309 0.449206 2.058844
H -1.971265 -2.473465 0.469743
H -0.959680 1.633281 -0.501019
H -4.339287 -1.887059 0.412653
H -3.326756 2.184750 -0.535994
H -5.057516 0.449789 -0.081111
H 3.032329 1.932561 0.947902
H 3.129947 0.375979 -1.123407
H 3.261656 -0.298670 0.514789
H 0.933906 0.919227 -0.879180
N 2.593670 -1.634839 -0.995593
O 2.122846 2.232542 1.102835
H 3.530691 -1.923099 -1.268410
H 1.311037 3.234706 -0.261752
O 0.709027 3.532062 -0.974140
H 0.146935 4.194326 -0.545705

s3 with 1 H_2O
C 0.703901 -1.988554 -0.763813
C 2.138399 -2.470053 -0.546038
C 2.712610 -0.231517 0.264836
C 1.286341 0.256545 0.230392
C 0.299272 -0.939190 0.298228
C 1.021287 1.267515 1.354913
C -1.169148 -0.562371 0.155406
C -2.122307 -1.181727 0.976869
C -1.622714 0.349588 -0.811772
C -3.484485 -0.912125 0.838929
C -2.985146 0.623234 -0.949032
C -3.922178 -0.007245 -0.128751
H 2.190566 -3.035125 0.402048
H 2.442905 -3.147159 -1.352003
H 0.612734 -1.545232 -1.763603
H 0.020713 -2.844838 -0.722713
H 3.508336 0.512006 0.321033
H 1.103715 0.792028 -0.715839
H 0.425594 -1.415226 1.282986
H -0.040032 1.522596 1.391120
H 1.305679 0.840999 2.327728
H -1.790324 -1.887202 1.736269
H -0.914336 0.874120 -1.447056
H -4.201277 -1.406183 1.490054
H -3.314178 1.334092 -1.703107
H -4.981713 0.207916 -0.239663
H 2.648753 2.358709 1.167401
H 4.024490 -1.592421 -0.472960
N 3.048209 -1.325753 -0.537365
O 1.693086 2.522052 1.154326
H 1.022991 3.115396 -0.540062
O 0.530672 3.204504 -1.381458
H -0.327143 3.558732 -1.104021

s4 **with 1 H_2O**
C 1.502028 -0.273538 -0.194893
C 2.287990 0.261202 -1.223802
C 3.681813 0.204588 -1.171889
C 4.318722 -0.389899 -0.082212
C 3.549367 -0.925023 0.952997
C 2.156929 -0.867162 0.894616
H 1.798636 0.733034 -2.072556
H 4.269229 0.626096 -1.983848
H 5.403709 -0.436261 -0.038768
H 4.034343 -1.389884 1.807834
H 1.574948 -1.289991 1.710528
C -0.015463 -0.218974 -0.278628
H -0.275115 0.262510 -1.230469
C -0.650821 0.651716 0.845157
H -0.379977 0.214980 1.818676
C -0.135169 2.053941 0.840912
H -0.210264 2.667327 1.740147
C -2.203466 0.615329 0.724621
H -2.655064 1.159925 1.561401
H -2.501824 1.132702 -0.194773
C -0.649372 -1.627493 -0.286388
H -0.252085 -2.205748 -1.130602
H -0.360553 -2.169867 0.625642
C -2.179229 -1.561602 -0.368965
H -2.613198 -2.566818 -0.307541
H -2.495402 -1.134819 -1.329386
O -0.278290 2.710598 -0.362951
H 0.046004 3.618217 -0.266348
N -2.790819 -0.731790 0.681636
H -2.664644 -1.185703 1.586741
H -4.481317 -0.372536 -0.147750
O -5.108987 -0.105211 -0.857161
H -5.583454 -0.922243 -1.068638

s5 with 1 H_2O
C -0.765220 -1.576251 0.940604
C -2.245970 -1.943096 0.753652
C -2.513673 -0.392620 -1.067282
C -1.061447 0.006610 -1.002681
C -0.132374 -1.009591 -0.369337
C -0.642174 1.324312 -1.561176
C 1.292634 -0.533946 -0.128085
C 2.364394 -1.123028 -0.809838
C 1.571202 0.485807 0.797250
C 3.679835 -0.714836 -0.577279
C 2.883584 0.897408 1.028981
C 3.943805 0.297736 0.344657
H -2.343981 -2.794152 0.062915
H -2.674271 -2.261627 1.711647
H -0.692965 -0.816221 1.725613
H -0.185723 -2.449493 1.268531
H -0.074308 -1.866868 -1.067348
H 0.437582 1.464968 -1.511542
H -0.950277 1.431514 -2.613737
H 2.166928 -1.914513 -1.530073
H 0.752443 0.959778 1.333347
H 4.495793 -1.189475 -1.116472
H 3.079539 1.688619 1.748423
H 4.965814 0.618292 0.529092
H -2.139075 2.526077 -1.072098
H -2.988867 -0.061248 0.880232
H -3.137601 0.432651 -1.437608
H -2.655483 -1.223436 -1.781242
N -3.060426 -0.844155 0.224856
O -1.201991 2.462138 -0.827178
O -1.752419 1.622601 1.807242
H -1.788074 2.379306 2.411101
H -1.456792 1.995970 0.947922

s6 with 1 H_2O
C 0.560613 -1.688793 -0.406565
C 2.091443 -1.740249 -0.306615
C 2.223992 0.692046 -0.246745
C 0.691954 0.837512 -0.338099
C -0.007637 -0.411067 0.255059
C 0.248992 2.137282 0.355571
C -1.525662 -0.355709 0.171323
C -2.305697 -0.455841 1.331747
C -2.188281 -0.224597 -1.059785
C -3.700125 -0.427184 1.270307
C -3.581197 -0.193842 -1.126229
C -4.343424 -0.295453 0.039487
H -0.854864 2.243419 0.264778

H -1.812947 -0.560927 2.296079
H -1.612244 -0.147666 -1.978834
H -4.281824 -0.507149 2.184938
H -4.072020 -0.090870 -2.090557
H -5.428528 -0.271839 -0.012348
H 2.653262 -0.510263 -1.849761
H 2.700218 1.550400 -0.733646
H 2.539508 0.702105 0.805869
H 0.420879 0.930829 -1.400031
H 0.261182 -0.454479 1.322073
H 0.123007 -2.576734 0.066927
H 0.259348 -1.716231 -1.463531
H 2.398070 -1.838261 0.742738
H 2.485734 -2.614746 -0.835892
H 0.432619 2.103037 1.448681
N 2.761743 -0.540861 -0.836115
O 0.752183 3.282421 -0.194321
H 4.409074 -0.651465 0.162556
O 4.943641 -0.678270 0.987620
H 5.490906 0.119020 0.939642

s7 with 1 H_2O
C 1.174332 -0.432899 -0.720767
C 1.810212 0.803149 -0.108216
C 2.981716 0.481789 0.773749
C 3.573615 -0.751385 0.740023
C 3.043291 -1.811570 -0.042902
C 1.800346 -1.646739 -0.708983
H 2.172161 1.453356 -0.932345
H 3.398863 1.277537 1.387964
H 4.461398 -0.936824 1.340668
H 3.540793 -2.776367 -0.054773
H 1.318289 -2.513090 -1.157655
C -0.259674 -0.096711 -1.009888
H -0.302985 0.626016 -1.843951
C -0.608889 0.688946 0.285139
H -0.622167 -0.039659 1.107920
C 0.599598 1.613474 0.507567
H 0.759004 1.824919 1.574078
C -2.007235 1.297926 0.198484
H -2.285839 1.787467 1.136473
H -2.047586 2.052951 -0.601496
C -1.295359 -1.192744 -1.264291
H -1.115385 -1.714038 -2.212821
H -1.250918 -1.937781 -0.459410
C -2.693697 -0.561560 -1.286837
H -3.459847 -1.342375 -1.376108
H -2.790415 0.091512 -2.173915
O 0.359984 2.836164 -0.195539
H 1.151775 3.389488 -0.108682
N -2.934749 0.174039 -0.035118
H -3.893467 0.519790 -0.046593
O -3.007654 -1.571868 2.323047
H -3.035380 -2.459267 1.935754
H -2.983204 -0.986331 1.532173

s8 with 1 H_2O
C 1.336880 -0.500597 -0.022980
C 2.000021 0.828328 0.261736
C 3.471618 0.845756 -0.011193
C 4.171850 -0.312578 -0.190429
C 3.511863 -1.568722 -0.237736
C 2.095951 -1.627183 -0.202537
H 3.958862 1.816408 0.001673
H 5.250679 -0.275991 -0.322147
H 4.086265 -2.479126 -0.378423
H 1.612653 -2.585799 -0.378095
C -0.169420 -0.421870 -0.175180
H -0.386677 -0.318101 -1.253552
C -0.701814 0.857441 0.509870
H -0.492621 0.762365 1.587028
C 0.017471 2.114605 -0.025472
H 0.032485 2.894045 0.754548
C -2.227009 0.968923 0.345538
H -2.613185 1.844181 0.881518
H -2.476107 1.109262 -0.714787
C -0.942474 -1.653359 0.334153
H -0.644515 -2.553799 -0.216998
H -0.687376 -1.829328 1.389212
C -2.459154 -1.454108 0.192652
H -2.999219 -2.299291 0.635190
H -2.741920 -1.413541 -0.867085
O 1.342758 1.862040 -0.491346
N -2.967195 -0.215740 0.807441
H -0.520108 2.521101 -0.890549
H 1.864135 1.072285 1.340439
H -2.894940 -0.285334 1.822487
O -5.085750 0.101694 -1.063064
H -4.572388 0.010604 -0.228988
H -5.696419 -0.649442 -1.048811

s9
C -1.357240 0.360979 1.016149
C -2.716504 0.411071 1.320401
C -3.661613 -0.051251 0.400501
C -3.233889 -0.561168 -0.824742
C -1.870086 -0.610485 -1.124195
C -0.912614 -0.153545 -0.211272
H -0.629593 0.739004 1.729460
H -3.040266 0.816075 2.275946
H -4.721656 -0.009256 0.636792
H -3.959202 -0.918755 -1.551312
C 0.572016 -0.269033 -0.526622
C 1.362495 1.039305 -0.352844
C 1.206898 -1.411720 0.303035
C 2.683379 0.956225 0.098014
C 2.717983 -1.485598 0.088953
H 1.008147 -1.247162 1.368846
H 0.743933 -2.366437 0.029466
H 3.273378 1.859036 0.225371
H 3.155601 -2.284656 0.697979
C 0.791475 2.256945 -0.689658
N 3.312198 -0.216572 0.489204
H 2.931472 -1.718397 -0.969463
H 1.358957 3.180070 -0.611437
H 4.323712 -0.187647 0.463271
H -0.231815 2.329669 -1.037336
H -1.544425 -1.008347 -2.083309
H 0.652559 -0.557542 -1.585032

s9 with 1 H_2O
C 1.378596 0.987725 0.072173
C 2.679762 1.480084 0.154482
C 3.771117 0.628291 -0.038769
C 3.549390 -0.719626 -0.316912
C 2.243535 -1.210330 -0.400704
C 1.143264 -0.367674 -0.207904
H 0.535734 1.659171 0.217685
H 2.843340 2.533101 0.369234
H 4.784940 1.014587 0.026297
H 4.389613 -1.392254 -0.469812
C -0.276350 -0.906920 -0.321875
C -1.069624 -0.820767 0.996638
C -1.030043 -0.223713 -1.488880
C -2.428819 -0.503870 0.946357
C -2.515841 -0.576438 -1.487328
H -0.933230 0.863731 -1.409828
H -0.576861 -0.524801 -2.439799
H -3.014141 -0.443554 1.859452
H -3.035267 -0.069439 -2.307107
C -0.451266 -1.109609 2.203450
N -3.103695 -0.125630 -0.220011
H -2.651587 -1.662930 -1.619412
H -1.010778 -1.099954 3.134780
H -4.107176 -0.266628 -0.165950
H 0.603428 -1.350753 2.258263
H 2.077434 -2.263381 -0.619188
H -0.196572 -1.975877 -0.566673
O -1.973040 2.688495 0.190860
H -1.653791 2.512684 1.088593
H -2.507220 1.894838 -0.007708

s9 with 1 H_2O
C 1.405730 0.486608 -0.729880
C 2.718042 0.917646 -0.925585
C 3.790765 0.177314 -0.420370
C 3.539757 -1.002385 0.278494
C 2.224880 -1.435796 0.470092
C 1.142007 -0.700550 -0.025507
H 0.579615 1.068309 -1.131755
H 2.905097 1.831741 -1.484360
H 4.811735 0.515748 -0.575977
H 4.364363 -1.590457 0.673235
C -0.285147 -1.190871 0.187412
C -1.084339 -0.338252 1.192800
C -1.036890 -1.333303 -1.157880
C -2.452864 -0.154583 0.973200
C -2.513799 -1.661346 -0.946776
H -0.971072 -0.399251 -1.723706
H -0.564590 -2.119893 -1.756440
H -3.044662 0.436371 1.666254
H -3.035822 -1.723082 -1.907084
C -0.466619 0.196043 2.317326
N -3.125309 -0.590907 -0.157536
H -2.623110 -2.634476 -0.439050
H -1.047492 0.705144 3.082485
H -4.130935 -0.656039 -0.053448
H 0.584591 0.027332 2.520494
H 2.038846 -2.360782 1.012205
H -0.214184 -2.195381 0.630043
O -1.674164 2.051391 -1.579265
H -1.310901 2.497637 -0.784257
H -2.335365 1.439626 -1.216529
O -0.353431 2.989990 0.777093
H 0.562449 3.060723 0.466176
H -0.359770 2.138872 1.261888

TS_1a_s13
C 0.944676 -0.691662 -0.306529
C 1.779806 -0.100227 -1.269537
C 3.159617 -0.014620 -1.085041
C 3.742802 -0.524078 0.077532
C 2.932015 -1.124663 1.040621
C 1.549678 -1.209276 0.848891
H 1.336344 0.281158 -2.187715
H 3.780250 0.441220 -1.852322
H 4.817506 -0.462832 0.225034
H 3.374028 -1.537372 1.943891

H 0.943747 -1.698490 1.606157
C -0.559603 -0.705790 -0.538675
C -1.287242 -1.965257 -0.022342
C -1.268898 0.561557 0.003903
C -2.805000 -1.848360 -0.311246
H -1.154031 -2.064801 1.061893
H -0.891359 -2.878041 -0.487137
C -2.774729 0.529351 -0.339909
H -0.809125 1.677961 -0.730659
H -3.328648 -2.722071 0.094111
H -2.949074 -1.848354 -1.408751
H -3.273988 1.428284 0.038971
C -0.963128 0.983976 1.335715
H -0.299855 0.405057 1.973689
H -1.737110 1.504491 1.891669
O 0.180921 2.440215 1.316943
H 1.065724 2.036463 1.361400
N -3.354770 -0.645978 0.279575
O -0.308168 2.746850 -1.029237
H 0.467960 2.538821 -1.576123
H 0.062555 2.760874 0.255392
H -0.703555 -0.692778 -1.630302
H -2.899963 0.510030 -1.438167

TS_1a_s14
C -0.995735 -0.179207 -0.042937
C -2.341952 0.428977 -0.530696
C -1.655571 2.439623 0.399191
C -0.148042 2.217465 0.087776
C 0.142750 0.808688 -0.496919
H -3.325852 -0.369081 0.519834
H -1.847390 2.086516 1.431982
H 0.198084 2.965399 -0.633618
H 0.437352 2.367693 1.002904
C 1.541283 0.308334 -0.170656
C 2.453720 0.026366 -1.196996
C 1.959131 0.106946 1.155453
C 3.738380 -0.442124 -0.915159
H 2.153759 0.182567 -2.231224
C 3.239029 -0.368298 1.441762
H 1.278611 0.328519 1.974468
C 4.135708 -0.644684 0.407151
H 4.428468 -0.646251 -1.729963
H 3.539131 -0.516990 2.476115
H 5.134708 -1.009425 0.630507
C -0.710453 -1.517751 -0.607128
H -0.690633 -1.586730 -1.691662
H 0.039482 -2.131439 -0.114863
O -2.116552 -2.579811 -0.316044
H -1.793577 -3.292742 0.263329
N -2.517831 1.765534 -0.545140
O -3.760652 -1.239606 0.992503
H -4.663101 -1.280295 0.633169
H -2.882733 -2.066942 0.247102
H -0.953957 -0.241702 1.055365
H -2.743831 -0.083977 -1.421291
H -1.870661 3.514758 0.394986
H 0.055105 0.870701 -1.587881

TS_1a_s15
C -0.597438 -0.618060 1.530240
C -2.095403 -0.899846 1.351160
C -1.923098 -1.422812 -0.959316
C -0.652313 -0.498081 -0.999090
C 0.201650 -0.898807 0.240018
H -2.630176 -1.090022 2.288391
H -3.065000 0.589978 1.116837
H -0.444713 0.419954 1.863893
H -0.174568 -1.230621 2.343200
H -1.535072 -2.427221 -1.202103
H -2.602906 -1.161595 -1.786102
N -2.656944 -1.470079 0.270098
C -0.892347 0.992058 -1.040433
H -0.813890 1.513144 -0.089685
O -2.494249 1.325806 -1.469907
H -2.518549 2.197457 -1.919195
H -0.101455 -0.765926 -1.909356
C 1.619271 -0.337632 0.197876
C 1.991576 0.881859 0.781627
C 2.607519 -1.056379 -0.493867
C 3.296839 1.367634 0.672119
H 1.262798 1.460985 1.340982
C 3.912289 -0.576567 -0.608507
H 2.346288 -2.011113 -0.946387
C 4.263041 0.642299 -0.025702
H 3.558321 2.314166 1.138865
H 4.655890 -1.158474 -1.147313
O -3.580201 1.426492 0.743250
H -3.277055 2.186076 1.271648
H -3.050629 1.426286 -0.528160
H 5.279160 1.018805 -0.108386
H -0.383522 1.527020 -1.839941
H 0.299775 -1.990730 0.158634

TS_1a_s17
C 0.126737 -2.101010 0.271270
C 1.608261 -2.507124 0.042440
C 1.553307 -0.643842 -1.497527
C 1.083829 0.174224 -0.278765
C -0.022030 -0.568785 0.512917
C 2.438319 -0.025391 0.447232
C -1.440398 -0.106369 0.214069
C -2.403721 -0.137011 1.232121
C -1.838069 0.318680 -1.061375
C -3.724695 0.238478 0.987061
C -3.158144 0.698330 -1.310173
C -4.107201 0.657728 -0.288060
H 2.550074 -0.498652 1.414824
H -2.112745 -0.455575 2.231269
H -1.113534 0.367637 -1.869455
H -4.452376 0.209606 1.793917
H -3.442383 1.031331 -2.304962
H -5.133929 0.955987 -0.481836
H 1.315900 1.604170 1.905022
H 0.810089 -1.193106 -2.083203
H 2.185377 -0.042021 -2.156257
H 0.856557 1.223385 -0.477239
H 0.162406 -0.371093 1.577267
H -0.297443 -2.671322 1.104236
H -0.463276 -2.368104 -0.611564
H 2.110739 -2.768356 0.980522
H 1.646566 -3.399343 -0.600993
N 2.405297 -1.467539 -0.611634
O 2.271215 1.580254 1.712337
H 3.301724 0.490306 0.053146
H 2.495018 2.574786 0.275669
O 2.584620 2.912225 -0.651524
H 3.200309 3.655867 -0.582685

TS_1a_s2
C 0.697963 -1.591593 -1.065506
C 2.194254 -1.960974 -0.826953
C 2.591845 0.419081 -0.759604
C 1.116470 0.829331 -0.440978
C 0.265863 -0.429425 -0.155615
C 1.024371 1.837233 0.716565
C -1.235292 -0.212347 -0.125519
C -1.996240 -0.709264 0.942920
C -1.906045 0.439475 -1.172114
C -3.382981 -0.557941 0.969720
C -3.292699 0.591308 -1.147601
C -4.037012 0.094647 -0.076156
H 2.265254 -2.828227 -0.163229
H 2.654626 -2.247350 -1.781874
H 0.544656 -1.283745 -2.109871
H 0.051836 -2.460071 -0.898997
H 0.704283 1.337603 -1.323916
H 0.549019 -0.775551 0.891454
H -0.025072 2.021090 0.966183
H 1.509411 1.408736 1.611569
H -1.487588 -1.219498 1.757772
H -1.343497 0.827808 -2.017062
H -3.951264 -0.948377 1.810026
H -3.791593 1.100207 -1.968371
H -5.116646 0.216352 -0.056841
H 2.528555 3.016545 0.317698
N 2.986782 -0.881992 -0.227330
O 1.567943 3.112229 0.404987
O 1.185509 -1.205283 2.346816
H 2.836777 -0.894402 0.781222
H 0.857979 -0.418417 2.831156
H 2.745072 0.391081 -1.845577
H 3.290109 1.177408 -0.379406

TS_1a_s3
C 0.019366 2.188481 0.031858
C -1.381010 2.716087 0.352454
C -2.267332 0.576742 -0.469325
C -0.912726 -0.098034 -0.464804
C 0.129476 0.686990 0.368780
C -1.011660 -1.580948 -0.048128
C 1.549770 0.167603 0.201917
C 2.269575 -0.298765 1.309821
C 2.188210 0.168036 -1.047862
C 3.583859 -0.751451 1.179644
C 3.500630 -0.284221 -1.183441
C 4.204795 -0.745701 -0.069366
H -1.537033 2.672505 1.444496
H -1.475227 3.771652 0.074785
H 0.240030 2.346424 -1.032070
H 0.764257 2.758849 0.599685
H -0.575627 -0.094785 -1.516063
H -0.139593 0.572159 1.430582
H -0.026504 -2.045078 -0.168427
H -1.272292 -1.641219 1.020699
H 1.793248 -0.307395 2.288025
H 1.657523 0.524719 -1.927202
H 4.120024 -1.109272 2.054849
H 3.974125 -0.275720 -2.161830
H 5.227297 -1.097999 -0.175345
H -2.775382 -2.337953 -0.346768
H -2.966395 1.185773 0.447402
H -3.007515 0.133110 -1.134148
N -2.468926 2.007156 -0.338792
O -1.933608 -2.305257 -0.842983
O -4.201862 -1.809721 0.776975
H -3.867935 -0.894279 0.797393
H -5.004471 -1.760668 0.234257

H -1.640086 2.467785 0.767373

TS_1a_s4
C -1.170482 0.045457 0.974389
C -2.494070 0.308316 0.413766
C -2.505432 -2.004657 -0.480790
C -1.038112 -1.726369 -0.825809
C -0.330520 -1.094183 0.393729
H -2.181263 1.112761 -0.427296
H -3.014746 -2.510643 -1.306907
H -0.524620 -2.656216 -1.102658
H -0.983460 -1.053378 -1.690123
C 1.109932 -0.701461 0.090507
C 2.166195 -1.259128 0.822790
C 1.411343 0.219480 -0.928647
C 3.493008 -0.907850 0.555848
H 1.949800 -1.976929 1.612991
C 2.735453 0.565898 -1.200252
H 0.606913 0.681360 -1.498662
C 3.781741 0.006064 -0.457378
H 4.296875 -1.348792 1.142230
H 2.950861 1.277576 -1.994627
H 4.811223 0.283472 -0.668566
C -0.628330 0.984122 1.826314
H -1.262132 1.688684 2.341501
H 0.371773 0.851680 2.234939
O -0.024418 2.666226 0.642983
H 0.858344 2.396804 0.349023
N -3.255647 -0.787075 -0.153853
O -1.440622 2.192632 -1.271259
H -2.080699 2.908634 -1.391478
H -0.712694 2.503560 -0.308075
H -3.122484 0.905660 1.092265
H -2.542534 -2.689400 0.381920
H -0.289674 -1.880296 1.167647
H -3.805990 -0.470002 -0.937751

TS_1a_s5
C -0.553053 -1.825481 0.947140
C -2.090873 -1.995388 1.017274
C -2.506394 -0.759000 -0.990699
C -1.174502 -0.084591 -0.741613
C -0.086912 -1.101532 -0.354264
C -0.857779 1.208626 -1.459350
C 1.305776 -0.519985 -0.156043
C 2.398595 -1.064326 -0.840593
C 1.533660 0.538831 0.739701
C 3.690868 -0.573745 -0.639307
C 2.823135 1.033670 0.935677
C 3.906787 0.477895 0.250706
H -2.413288 -2.886471 0.459714
H -2.392557 -2.133137 2.061820
H -0.245566 -1.203856 1.795200
H -0.044850 -2.790481 1.059486
H -0.021489 -1.850640 -1.159427
H 0.116782 1.591852 -1.158493
H -0.831715 1.051274 -2.551475
H 2.237751 -1.884818 -1.537213
H 0.697829 0.993103 1.269501
H 4.525412 -1.013624 -1.179405
H 2.980008 1.858083 1.626360
H 4.910277 0.864355 0.408356
H -2.663389 2.002218 -1.471965
H -1.845570 0.098883 0.501712
H -3.249183 -0.127890 -1.494150
H -2.486694 -1.739123 -1.481312
N -2.799417 -0.822017 0.477331
O -1.784594 2.267491 -1.158278
O -1.480514 2.313829 1.720332
H -2.252750 1.796199 1.994399

TS_1a_s6
C -1.316121 0.449451 -0.822182
C -0.664828 -0.950842 -0.723584
C -1.847119 -1.953039 -0.653924
H -0.086469 -1.159791 -1.632058
H -1.951764 0.538917 -1.707770
H -0.539835 1.225973 -0.869404
H -2.322428 -1.992336 -1.649940
H -1.450956 -2.957754 -0.430424
H -2.795511 -0.353184 0.391451
O -2.765102 -1.612046 0.345168
N -2.146783 0.653048 0.362100
C 0.289846 -1.004899 0.507052
C -0.427633 -0.507441 1.786506
H -1.076097 -1.312951 2.138588
H 0.299903 -0.300721 2.580154
C -1.329621 0.732935 1.575033
H -0.727609 1.648196 1.491322
H -1.995828 0.858994 2.434486
H 0.522305 -2.066359 0.672467
C 1.626098 -0.329230 0.190290
C 2.047148 0.877315 0.763445
C 2.492797 -0.954474 -0.722188
C 3.280193 1.445786 0.429226
H 1.421882 1.383996 1.491191
C 3.722824 -0.394111 -1.058705
H 2.200692 -1.903471 -1.167973
C 4.121904 0.815520 -0.484709
H 3.579942 2.383124 0.890802
H 4.373553 -0.905011 -1.763639
H 5.080948 1.255928 -0.743233
O -4.013067 2.214572 -1.292957
H -3.605269 1.791584 -0.512495
H -3.647560 3.111494 -1.283457

TS_s10_s11a
C 1.718605 -1.291844 -0.129372
C 3.090170 -1.513359 -0.248740
C 3.990547 -0.460190 -0.079362
C 3.505074 0.814932 0.214379
C 2.132744 1.036418 0.327479
C 1.211811 -0.009100 0.145537
H 1.032090 -2.122319 -0.267827
H 3.455207 -2.512073 -0.474328
H 5.059780 -0.633098 -0.167970
H 4.196350 1.640189 0.365462
C -0.257201 0.203836 0.270019
C -0.903412 1.238174 -0.314163
C -1.020131 -0.839094 1.072994
C -2.415391 1.397274 -0.199343
C -2.405876 -0.344585 1.481936
H -1.147113 -1.751075 0.475258
H -0.442068 -1.110551 1.964879
H -2.825716 1.643336 -1.187468
H -3.002424 -1.171836 1.879525
C -0.262141 2.284842 -1.132819
N -3.074944 0.180852 0.284959
H -2.623959 2.271929 0.447540
H -2.317678 0.420175 2.274736
H 0.075860 3.225029 -0.704604
H -4.051609 0.385823 0.487926
H -0.280830 2.222756 -2.219070
H 1.770048 2.026341 0.583476
O -2.814919 -2.200034 -1.368102
H -2.173895 -1.957357 -2.052612
H -2.988886 -1.346782 -0.906093

TS_s10_s11a with 1 H_2O
C -2.470677 -1.486463 0.073912
C -3.812866 -1.443535 0.487695
C -4.501923 -0.222220 0.505180
C -3.893112 0.944869 0.058080
C -2.536646 0.928129 -0.374809
C -1.823270 -0.327827 -0.335722
H -1.919020 -2.422136 0.127879
H -4.308920 -2.353679 0.812582
H -5.539910 -0.197104 0.828549
H -4.463290 1.868045 -0.005075
C -0.371043 -0.165388 -0.480221
C 0.069778 1.002036 0.049166
C 0.555408 -1.183791 -1.093956
C 1.525727 1.401291 0.000057
C 1.890994 -0.525047 -1.458359
H 0.732933 -2.011747 -0.391852
H 0.098382 -1.625421 -1.988751
H 1.836685 1.811194 0.970285
H 2.643285 -1.280723 -1.704666
C -0.944041 1.867598 0.694312
N 2.381673 0.250685 -0.312324
H 1.645054 2.224185 -0.732743
H 1.751611 0.108845 -2.352131
H -0.904253 2.942018 0.507021
H 3.347425 0.553912 -0.473176
H -1.231791 1.616513 1.715545
H -2.251142 1.647217 -1.140229
O 3.709084 -1.293424 1.592412
H 3.550943 -0.963995 2.489785
H 3.022094 -0.838583 1.030312
H 4.987297 -0.372680 0.633641
O 5.345067 0.274200 -0.019509
H 5.767728 0.955228 0.524066

TS_s11_s12b
C -1.726914 1.559625 -0.299862
C -3.083315 1.265571 -0.339143
C -3.557500 -0.072814 -0.340227
C -2.655516 -1.125696 -0.303093
C -1.268980 -0.868740 -0.194474
C -0.787397 0.508941 -0.265644
H -1.392426 2.594734 -0.330643
H -3.801888 2.080509 -0.389833
H -4.625309 -0.266525 -0.383769
H -3.014724 -2.153356 -0.331566
C 0.641035 0.478261 -0.092434
C 1.088142 -0.866616 -0.252816
C 1.627920 1.618969 -0.188850
C 2.532955 -1.239604 -0.267182
C 3.024960 1.110889 0.200777
H 1.673470 1.998242 -1.219613
H 1.346538 2.466477 0.452092
H 2.719282 -2.019890 -1.021662
H 3.775142 1.884275 0.000488
C -0.080365 -1.811121 -0.430183
N 3.358019 -0.067355 -0.602058
H 2.831653 -1.691049 0.708708
H 3.046656 0.909512 1.292645
H -0.066485 -2.682237 0.247932
H 4.338999 -0.302685 -0.467812
H -0.095459 -2.249331 -1.453142
H -1.021159 -0.768708 1.429152
H 0.258693 0.108565 1.484490
O -0.386789 -0.389186 2.271259

H -0.914964 0.330458 2.665648

TS_s11_s12b with 1 H_2O
C -1.540581 -1.314038 -1.082761
C -2.879864 -1.645073 -0.750389
C -3.633264 -0.916324 0.230638
C -3.113792 0.156049 0.918127
C -1.681799 0.582005 0.614261
C -0.980041 -0.276632 -0.451167
H -0.997642 -1.874741 -1.815144
H -3.345519 -2.467352 -1.249504
H -4.639285 -1.220385 0.435372
H -3.698367 0.683051 1.649148
C 0.292877 0.352604 -0.498960
C 0.658354 0.451715 0.828179
C 1.398619 -0.165636 -1.422276
C 2.105775 0.720565 1.276956
C 2.733684 0.520526 -1.073775
H 1.530814 -1.214917 -1.265502
H 1.122461 0.010690 -2.440068
H 2.279494 0.315429 2.251844
H 3.495012 0.164280 -1.738053
C -0.643708 0.344925 1.719930
N 3.068385 0.131078 0.321211
H 2.247106 1.781010 1.297540
H 2.659973 1.582622 -1.164748
H -0.699242 1.034337 2.537461
H 3.984745 0.451406 0.559198
H -0.732409 -0.644181 2.120639
H -1.621382 2.155124 0.067431
O 3.047825 -2.321119 0.473357
H 2.181384 -2.685444 0.281234
H 3.017677 -1.367220 0.404641
H -0.305195 1.724674 -0.699655
O -0.913481 2.901759 -0.921102
H -1.330618 3.144846 -1.750918

TS_s11_s12c with 1 H_2O
C 1.712461 -1.473687 1.026739
C 2.988456 -1.695980 0.587959
C 3.588965 -0.884007 -0.449140
C 2.944610 0.188662 -0.971586
C 1.631647 0.613819 -0.430782
C 0.958698 -0.400575 0.460304
H 1.252099 -2.143339 1.748950
H 3.560523 -2.528584 0.989112
H 4.576309 -1.159723 -0.810974
H 3.412587 0.796518 -1.742840
C -0.381295 -0.108078 0.545841
C -0.662421 1.090785 -0.290556
C -1.452542 -0.798869 1.338185
C -2.114085 1.287394 -0.759389
C -2.796539 -0.080689 1.150955
H -1.558742 -1.826323 0.965475
H -1.197468 -0.859094 2.405778
H -2.155962 1.297689 -1.855020
H -3.615126 -0.721844 1.493496
C 0.471122 1.073295 -1.341492
N -2.984212 0.191405 -0.284276
H -2.483275 2.266435 -0.411786
H -2.827990 0.845751 1.751797
H 0.642294 2.054038 -1.795071
H -3.953982 0.451004 -0.456490
H 0.265961 0.328712 -2.122025
H 1.789729 1.558119 0.188315
H -0.339393 2.001318 0.341073
O 0.866937 3.139660 0.863330
H 0.928469 2.798874 1.777678
H -2.651921 -1.554055 -1.086895
O -2.461065 -2.502301 -1.274783
H -3.336068 -2.916611 -1.301251

TS_s12a_s12b
C -1.872556 -1.650255 0.424826
C -3.229234 -1.302964 0.420586
C -3.640794 -0.064817 -0.078542
C -2.701560 0.849024 -0.572801
C -1.350908 0.512318 -0.556015
C -0.938752 -0.740066 -0.061259
H -1.557589 -2.618686 0.807025
H -3.966620 -2.001886 0.807378
H -4.696854 0.193362 -0.078955
H -3.027707 1.814003 -0.955466
C 0.558274 -0.870586 -0.251429
C 1.009041 0.602991 -0.301712
C 1.457564 -1.664243 0.696038
C 2.436183 0.680993 -0.831630
C 2.905372 -1.517420 0.189890
H 1.380409 -1.268917 1.716508
H 1.186908 -2.727803 0.725870
H 2.805136 1.713580 -0.836045
H 3.601704 -1.997828 0.887283
C -0.148999 1.331933 -1.009388
N 3.283233 -0.103198 0.079975
H 2.463347 0.312567 -1.877666
H 2.987399 -2.057855 -0.775288
H 1.045987 0.982875 0.729490
H -0.041719 1.307354 -2.105408
H 0.715127 -1.294944 -1.261401
H 4.256899 -0.033245 -0.205890
O 0.435597 3.209222 1.499300
H -0.223821 2.379175 -0.683162
H -0.297791 3.345423 2.140123

TS_s11_s12c
C 1.708838 -1.650461 0.455818
C 3.022523 -1.496634 0.113286
C 3.510197 -0.280062 -0.505347
C 2.705314 0.794859 -0.685679
C 1.309416 0.787495 -0.178219
C 0.793446 -0.577556 0.214522
H 1.348229 -2.598083 0.848871
H 3.720885 -2.315930 0.263930
H 4.547083 -0.249211 -0.830826
H 3.089380 1.706044 -1.139423
C -0.578263 -0.557396 0.227614
C -1.045233 0.801731 -0.173198
C -1.532582 -1.661887 0.583716
C -2.470359 0.881673 -0.751454
C -2.984733 -1.222186 0.331489
H -1.309856 -2.539519 -0.037975
H -1.408961 -1.981581 1.629335
H -2.445019 1.368014 -1.734282
H -3.630024 -2.102076 0.240300
C 0.134452 1.352378 -1.007080
N -3.033053 -0.463970 -0.919152
H -3.096314 1.514387 -0.095226
H -3.353242 -0.636248 1.196615
H 0.134862 2.444792 -1.067238
H -3.996349 -0.384715 -1.237397
H 0.126051 0.922833 -2.017748
H 1.262653 1.449646 0.741446
H -0.974621 1.461692 0.762346
O -0.031492 2.533882 1.825478
H 0.030456 1.884967 2.554706

TS_s11c_s14
C 2.033894 -1.457044 -0.274827
C 3.373349 -1.313500 -0.685180
C 4.069829 -0.128464 -0.409271
C 3.464991 0.891137 0.314292
C 2.105835 0.774938 0.731879
C 1.403409 -0.450617 0.433261
H 1.485662 -2.357028 -0.543556
H 3.860534 -2.118054 -1.228796
H 5.102090 -0.022644 -0.733427
H 4.031868 1.778509 0.584384
H 1.824511 1.312343 1.636599
C -0.083521 -0.282123 0.592040
C -0.379174 0.858335 -0.426732
C -1.059573 -1.424369 0.333534
H -0.286897 0.120076 1.598500
C -1.854204 1.209299 -0.387428
C -2.492048 -0.897181 0.545107
H -0.943770 -1.791219 -0.694900
H -0.881316 -2.276250 1.001392
H -2.152439 2.190489 -0.770145
H -3.237566 -1.562072 0.096100
H -2.726773 -0.869085 1.619023
C 0.613776 1.979976 -0.207202
H 1.081238 2.423153 -1.082795
H 0.380880 2.701452 0.575619
N -2.786887 0.448637 0.031827
H -0.185047 0.440664 -1.427341
O -5.540098 -0.229298 -0.517640
H -4.694747 0.250008 -0.387358
H -6.008614 -0.088742 0.318190

TS_s12a_s12b
C -2.479452 -1.358211 0.467593
C -3.716860 -0.742475 0.691072
C -3.917587 0.593594 0.336362
C -2.882344 1.337066 -0.242699
C -1.648220 0.729966 -0.456080
C -1.448170 -0.618286 -0.102392
H -2.329192 -2.399127 0.744272
H -4.525837 -1.307420 1.147094
H -4.881712 1.061605 0.517879
H -3.041980 2.379608 -0.509467
C -0.047695 -1.032680 -0.504569
C 0.683685 0.326655 -0.534073
C 0.781208 -2.035713 0.301140
C 2.034906 0.183815 -1.223407
C 2.171136 -2.131400 -0.355216
H 0.889790 -1.691436 1.336154
H 0.322063 -3.032359 0.317842
H 2.586538 1.129920 -1.213851
H 2.828595 -2.777791 0.236372
C -0.376800 1.318337 -1.049489
N 2.811655 -0.803870 -0.444300
H 1.897095 -0.124429 -2.277245
H 2.061267 -2.596114 -1.353304
H 0.890183 0.586077 0.511967
H -0.423431 1.330447 -2.150201
H -0.103780 -1.413105 -1.542232
H 3.740396 -0.907604 -0.848223
O 2.696716 0.342519 2.241903
H 2.546984 1.282475 2.058476
H 2.878473 -0.038600 1.352490
O 2.071915 3.203255 0.462961
H -0.185490 2.351026 -0.720432

H 2.096558 4.003708 -0.105859

TS_s12a_s12b
C -2.231451 -1.432224 0.687798
C -3.554180 -1.000912 0.840735
C -3.972785 0.209453 0.275504
C -3.076109 1.016311 -0.425207
C -1.745832 0.599636 -0.571795
C -1.333664 -0.642059 -0.021739
H -1.915590 -2.383326 1.110306
H -4.261607 -1.612398 1.394239
H -5.005365 0.528537 0.391284
H -3.403515 1.964954 -0.843946
C 0.089415 -0.947778 -0.433752
C 0.624195 0.370598 -0.949867
C 1.115079 -1.603795 0.503851
C 1.942404 0.282949 -1.669369
C 2.460608 -1.675282 -0.244879
H 1.246661 -1.009109 1.414988
H 0.810524 -2.616136 0.797277
H 2.328942 1.270851 -1.941712
H 3.241480 -2.046269 0.426197
C -0.613742 1.317739 -1.174666
N 2.881458 -0.342648 -0.716173
H 1.840667 -0.306400 -2.603961
H 2.365095 -2.394138 -1.080814
H 0.994514 1.245664 0.284732
H -0.699831 2.005877 -2.012822
H 0.011818 -1.617998 -1.315957
H 3.811534 -0.405421 -1.125117
O 3.457690 0.678242 1.941664
H 3.137559 1.550674 2.218417
H 3.080400 0.580295 1.041881
O 0.787241 2.362123 1.067412
H -0.242597 2.360366 0.053709
H 0.306042 1.991776 1.832208

TS_s12a_s12c
C -1.683120 1.623337 0.324349
C -3.043459 1.459694 0.032925
C -3.511952 0.266793 -0.522666
C -2.625896 -0.781167 -0.805104
C -1.269540 -0.615076 -0.531925
C -0.799955 0.586047 0.040363
H -1.325849 2.552281 0.762208
H -3.740052 2.267569 0.241301
H -4.569641 0.152630 -0.744760
H -2.993827 -1.704342 -1.247264
C 0.687850 0.455052 0.292339
C 1.090329 -0.613142 -0.748990
C 1.646968 1.643604 0.229968
C 2.502596 -1.112628 -0.466799
C 3.072678 1.103220 0.449282
H 1.583512 2.135772 -0.748498
H 1.418868 2.392837 0.999033
H 2.832120 -1.833396 -1.225022
H 3.805727 1.909424 0.330845
C -0.111026 -1.577852 -0.756296
N 3.392653 0.056309 -0.529166
H 2.523469 -1.627983 0.514120
H 3.147211 0.744421 1.495445
H 1.117076 -0.113093 -1.728019
H -0.044380 -2.303177 0.077281
H 0.795478 -0.007255 1.286504
H 4.358186 -0.238753 -0.404784
H -0.203172 -2.158381 -1.681252
O -0.845709 -1.968455 2.350441
H -1.420464 -1.442378 1.748818

TS_s12a_s12c with 1 H_2O
C -2.213528 -0.129320 1.547729
C -3.512390 0.261684 1.258458
C -3.856856 0.761700 -0.020887
C -2.908609 0.877029 -1.026414
C -1.580779 0.497759 -0.752999
C -1.232445 -0.007742 0.545712
H -1.956381 -0.509434 2.533080
H -4.280209 0.193733 2.024569
H -4.882915 1.065884 -0.210467
H -3.181260 1.263479 -2.005135
C 0.160417 -0.362702 0.494143
C 0.781101 0.374817 -0.659628
C 1.069249 -0.633538 1.676488
C 2.118695 -0.230006 -1.087918
C 2.412723 -1.185063 1.165181
H 1.256492 0.296558 2.236893
H 0.623190 -1.346483 2.381094
H 2.622022 0.422354 -1.808316
H 3.138869 -1.238353 1.983731
C -0.401524 0.438961 -1.578515
N 2.960820 -0.298247 0.125923
H 1.968140 -1.217016 -1.549578
H 2.256965 -2.210861 0.786578
H 1.013085 1.403464 -0.317821
H -0.452402 -1.124108 -1.901858
H -0.007337 -1.762676 -0.250346
H 3.896504 -0.607768 -0.129137
H -0.358247 0.992666 -2.516153
O -0.150657 -2.422065 -1.473872
H -1.047424 -2.795713 -1.374638
H 3.266699 1.593410 0.336960
O 3.545114 2.498829 0.067799
H 3.226485 3.073006 0.779567

TS_s12a_s12b with 1 H_2O
C -2.348509 -1.487505 0.518045
C -3.619160 -0.915862 0.655738
C -3.866579 0.389168 0.216804
C -2.844069 1.148954 -0.357226
C -1.571023 0.589884 -0.479562
C -1.324959 -0.733661 -0.046286
H -2.170049 -2.507783 0.848746
H -4.422755 -1.493276 1.105252
H -4.859175 0.816719 0.329368
H -3.035647 2.166805 -0.688356
C 0.098835 -1.114074 -0.399389
C 0.773351 0.275185 -0.492080
C 0.955639 -2.030538 0.477066
C 2.139131 0.158297 -1.152400
C 2.373427 -2.077403 -0.126571
H 1.001717 -1.639876 1.500767
H 0.553826 -3.050722 0.524638
H 2.638695 1.131234 -1.208097
H 3.043317 -2.648620 0.525271
C -0.314475 1.193486 -1.032585
N 2.942077 -0.725470 -0.282310
H 2.039388 -0.232422 -2.182660
H 2.322281 -2.611678 -1.094427
H 0.961180 0.584215 0.539819
H -0.316189 1.363097 -2.118948
H 0.074716 -1.555266 -1.412564
H 3.888743 -0.802116 -0.648832
O 2.767568 1.381924 1.885133
H 2.464287 2.032704 1.228870
H 2.986668 0.602378 1.333142
O 0.875756 3.038740 0.151694
H -0.061719 2.267348 -0.610352
H 0.439933 2.914647 1.020596

TS_s12a_s12c with 1 H_2O
C -1.897868 -1.230976 -1.134923
C -3.198216 -1.475767 -0.674632
C -3.662049 -0.877649 0.499842
C -2.830423 -0.028032 1.238485
C -1.530630 0.204737 0.791300
C -1.065433 -0.393476 -0.398180
H -1.545209 -1.697967 -2.051179
H -3.852077 -2.137599 -1.236499
H -4.672857 -1.077153 0.845250
H -3.191898 0.431757 2.155370
C 0.343384 0.096765 -0.675232
C 0.823473 0.482344 0.741887
C 1.391937 -0.773334 -1.368891
C 2.109246 1.296127 0.644235
C 2.707057 0.026923 -1.400304
H 1.541413 -1.709498 -0.819529
H 1.101485 -1.021805 -2.397469
H 2.505875 1.554141 1.633835
H 3.517994 -0.584596 -1.809794
C -0.438118 1.062110 1.410079
N 3.108965 0.446373 -0.039231
H 1.920877 2.241404 0.103467
H 2.577130 0.899847 -2.065422
H 1.075915 -0.450464 1.264949
H -0.580714 2.135045 1.144014
H 0.249987 1.028625 -1.253206
H 3.996137 0.943042 -0.095849
H -0.417014 1.010738 2.504720
O -1.546806 2.889621 -0.969621
H -1.945180 2.009379 -0.782313
H 3.261268 -1.198219 0.871072
O 3.165577 -2.117564 1.224132
H 3.229787 -2.016375 2.185111

TS_s12a_s12c with 1 H_2O
C -2.091336 -1.123986 -1.150138
C -3.415180 -1.225093 -0.708224
C -3.842210 -0.521632 0.422323
C -2.951583 0.291203 1.132032
C -1.629666 0.384672 0.703001
C -1.200901 -0.322813 -0.440359
H -1.765526 -1.672276 -2.030998
H -4.116292 -1.858674 -1.245336
H -4.872300 -0.613257 0.756821
H -3.287356 0.829708 2.015399
C 0.247352 0.015243 -0.706024
C 0.733474 0.448587 0.691898
C 1.229883 -0.976332 -1.330432
C 2.109851 1.098243 0.614788
C 2.617632 -0.310298 -1.359845
H 1.275506 -1.889095 -0.724263
H 0.940022 -1.256678 -2.351071
H 2.497124 1.329126 1.614038
H 3.371382 -1.014218 -1.731802
C -0.479049 1.177946 1.291965
N 3.026447 0.110444 -0.004991
H 2.060588 2.035876 0.040432
H 2.590358 0.542541 -2.061555
H 0.861640 -0.477241 1.271592
H -0.500677 2.226276 0.937491
H 0.258548 0.926907 -1.338249
H 3.964310 0.504935 -0.047894
H -0.480949 1.210579 2.387709
O 0.148832 3.020495 -0.856392
H -0.788820 2.898095 -1.120772
H 2.953228 -1.443258 1.118621
O 2.708039 -2.230886 1.660814

H 3.029514 -2.983759 1.143486

TS_s12b_s12c
C 1.959353 -0.898287 1.113644
C 3.286873 -0.840386 0.682283
C 3.626201 -0.115659 -0.465613
C 2.640430 0.559618 -1.189426
C 1.315800 0.508315 -0.752839
C 0.974273 -0.218698 0.394520
H 1.700194 -1.467438 2.003731
H 4.060120 -1.362987 1.239661
H 4.660944 -0.079805 -0.796649
H 2.906274 1.119111 -2.083812
C -0.518829 -0.194187 0.656285
C -1.057232 0.853210 -0.379298
C -1.144662 -1.605446 0.556190
C -2.438860 0.554115 -1.014650
C -2.623842 -1.539823 0.186723
H -0.639373 -2.171151 -0.235084
H -0.995728 -2.149369 1.497406
H -2.462889 0.970806 -2.029282
H -3.034475 -2.552182 0.098367
C 0.094846 1.132873 -1.384973
N -2.727810 -0.878272 -1.114823
H -3.212461 1.088724 -0.431597
H -3.196561 -1.017483 0.979438
H 0.226656 2.210549 -1.547117
H -0.716329 0.227201 1.649531
H -3.668854 -0.994099 -1.485220
H -0.116389 0.697291 -2.372325
O -1.385141 2.222388 2.256099
H -0.798128 2.909295 2.641898
H -1.223316 1.766472 0.208942

TS_s12b_s12c with 1 H_2O
C -2.110666 -0.464177 -1.470862
C -3.433444 -0.789212 -1.171494
C -3.894462 -0.756981 0.150611
C -3.028772 -0.412576 1.194717
C -1.702343 -0.107485 0.906070
C -1.239459 -0.119556 -0.428494
H -1.761974 -0.478254 -2.500683
H -4.114785 -1.065228 -1.972156
H -4.929357 -1.007841 0.367488
H -3.388551 -0.402694 2.221293
C 0.166272 0.308546 -0.478986
C 0.597231 0.589571 0.940833
C 1.237323 -0.232144 -1.409353
C 2.005780 0.209643 1.348604
C 2.551369 0.498705 -1.118141
H 1.390391 -1.306851 -1.225062
H 0.971993 -0.110678 -2.466250
H 1.966466 -0.814649 1.756635
H 3.334126 0.151805 -1.803856
C -0.572762 0.226855 1.859068
N 3.014029 0.215703 0.255580
H 2.363296 0.845004 2.168925
H 2.410033 1.576330 -1.297750
H -0.841407 1.012913 2.577218
H 0.053772 1.781020 -1.067653
H 3.765689 0.857117 0.488262
H -0.315023 -0.657266 2.466841
O 0.201415 3.038323 -0.503964
H -0.726869 3.313252 -0.380581
H 3.369162 -1.631749 0.165577
O 3.233323 -2.606931 0.086451
H 3.959616 -2.906190 -0.479657
H 0.460906 2.175786 0.597014

TS_s13_s18
C -1.786369 0.231505 -1.066268
C -3.156956 0.076031 -1.265869
C -3.998510 -0.202508 -0.185572
C -3.456172 -0.325225 1.093108
C -2.081728 -0.168811 1.288227
C -1.227984 0.112143 0.215437
H -1.138941 0.438123 -1.914797
H -3.569288 0.170476 -2.267154
H -5.067000 -0.324669 -0.341662
H -4.099914 -0.544293 1.941158
H -1.667377 -0.264578 2.289943
C 0.258936 0.337141 0.447145
C 1.160925 -0.526036 -0.439279
C 0.640569 1.825410 0.288798
H 0.467530 0.062011 1.493435
C 2.458986 0.012035 -0.791757
C 2.155418 2.019036 0.436993
H 0.330570 2.176965 -0.703460
H 0.094679 2.426232 1.025813
H 2.953991 -0.475315 -1.641961
H 2.416200 3.079825 0.334910
H 2.456203 1.733402 1.464673
C 0.882245 -1.881221 -0.641498
H -0.093156 -2.274557 -0.372259
H 1.378988 -2.402514 -1.463195
H 2.128816 -2.247628 0.332942
N 2.943156 1.262504 -0.520089
H 3.076412 -0.983095 0.148769
O 3.186041 -2.069399 0.675226
H 3.145699 -1.909720 1.634872

TS_s12b_s12c with 1 H_2O
C 2.200968 0.560085 1.291153
C 3.456595 0.013986 1.009577
C 3.654579 -0.734232 -0.155350
C 2.601268 -0.941613 -1.050615
C 1.350818 -0.388635 -0.775031
C 1.152177 0.359176 0.393221
H 2.048958 1.139546 2.199665
H 4.282502 0.171183 1.698809
H 4.633555 -1.157620 -0.365667
H 2.758424 -1.528783 -1.952647
C -0.290485 0.810726 0.521354
C -0.862138 0.553181 -0.914213
C -1.030045 0.038535 1.637935
C -2.372536 0.249627 -0.986242
C -2.543367 0.073282 1.437307
H -0.714064 -1.011348 1.619968
H -0.763169 0.450987 2.618795
H -2.588331 -0.306220 -1.906259
H -3.049646 -0.490537 2.229320
C 0.070864 -0.499650 -1.571732
N -2.850083 -0.563130 0.146801
H -2.925332 1.203501 -1.042642
H -2.914913 1.114139 1.479051
H 0.222357 -0.283749 -2.637145
H -0.341516 1.890466 0.720410
H -3.857793 -0.682691 0.055923
H -0.343677 -1.513925 -1.499769
O -0.590041 3.666967 -0.759673
H 0.281559 4.026099 -1.038742
H -2.024957 -2.256616 -0.009845
O -1.483974 -3.070065 -0.156281
H -1.743180 -3.669121 0.558566
H -0.750254 1.504579 -1.451950

TS_s12b_s12c with 1 H_2O
C -2.141548 -0.400895 -1.472367
C -3.434942 -0.812762 -1.146402
C -3.863468 -0.811169 0.186306
C -3.000040 -0.403152 1.205280
C -1.704994 0.000500 0.878827
C -1.276009 0.005189 -0.453702
H -1.815971 -0.395714 -2.510172
H -4.114893 -1.132858 -1.931658
H -4.872851 -1.132842 0.429397
H -3.334356 -0.409038 2.240410
C 0.132693 0.529377 -0.580012
C 0.585509 0.822021 0.867091
C 1.146150 -0.352634 -1.343978
C 1.891919 0.104384 1.263501
C 2.536625 0.249542 -1.152992
H 1.149770 -1.386455 -0.977124
H 0.896270 -0.378267 -2.410970
H 1.636691 -0.934771 1.515478
H 3.275253 -0.244170 -1.797985
C -0.597429 0.444673 1.803516
N 2.960757 0.072580 0.248123
H 2.303789 0.549013 2.176245
H 2.504536 1.311956 -1.444154
H -0.903219 1.280700 2.446141
H 0.129384 1.495111 -1.117028
H 3.700037 0.730139 0.476024
H -0.310302 -0.370147 2.483827
O 0.650418 3.209123 -0.513324
H -0.158378 3.744046 -0.372931
H 3.276679 -1.805003 0.268269
O 3.090683 -2.773314 0.271041
H 3.588135 -3.115260 -0.485874
H 0.748523 1.948589 0.883099

TS_s13_s18 with 1 H_2O
C -2.101553 -0.618639 1.039069
C -3.456557 -0.819844 1.295948
C -4.404176 -0.594174 0.294018
C -3.984221 -0.164685 -0.964261
C -2.625006 0.035828 -1.217175
C -1.665490 -0.188548 -0.223319
H -1.373589 -0.787349 1.828739
H -3.774314 -1.151760 2.280975
H -5.460568 -0.750391 0.495210
H -4.711800 0.016667 -1.751123
H -2.305667 0.368975 -2.202756
C -0.184038 -0.021634 -0.527329
C 0.547318 0.907143 0.448138
C 0.541221 -1.384608 -0.600550
H -0.109826 0.433117 -1.527870
C 1.953461 0.650568 0.686261
C 2.042963 -1.187785 -0.829717
H 0.387697 -1.930293 0.339046
H 0.100933 -1.992245 -1.399414
H 2.378353 1.120248 1.581850
H 2.571988 -2.144872 -0.888774
H 2.199275 -0.694643 -1.808661
C -0.029493 2.107075 0.863704
H -1.084508 2.289343 0.686646
H 0.396366 2.630394 1.722676
H 1.053804 2.908963 -0.113529
N 2.682723 -0.400293 0.211080
H 2.275217 1.907536 -0.131978
O 2.088705 3.023176 -0.491093
H 2.045508 2.999105 -1.464099
H 4.396767 -1.218749 0.335487
O 5.091894 -1.907834 0.231586

H 4.983925 -2.448925 1.027356
H 5.236335 -1.104019 1.658556
H 3.340341 0.797276 -0.297886

TS_s14_s18
C -1.599010 -1.285676 0.514780
C -2.985452 -1.270810 0.684718
C -3.761088 -0.293169 0.061664
C -3.138945 0.670105 -0.735313
C -1.754392 0.650745 -0.905631
C -0.960199 -0.325135 -0.281090
H -1.015589 -2.059018 1.005842
H -3.458507 -2.028417 1.304284
H -4.839954 -0.284293 0.191336
H -3.732982 1.431796 -1.234101
H -1.273665 1.404008 -1.525403
C 0.546830 -0.296031 -0.485508
C 1.284863 0.689527 0.456079
C 1.254078 -1.661156 -0.395288
H 0.721000 0.080302 -1.503275
C 2.786223 0.561690 0.309383
C 2.718242 -1.509967 -0.828199
H 1.221500 -2.043714 0.633206
H 0.747260 -2.401190 -1.026245
H 3.371109 1.379768 0.743668
H 3.285616 -2.417672 -0.588833
H 2.783269 -1.395225 -1.920176
C 0.876097 0.662915 1.934923
H 1.050581 -0.326214 2.375633
H 1.464819 1.387899 2.507784
H -0.183613 0.902900 2.060670
N 3.440475 -0.382376 -0.240201
H 1.053085 1.751037 0.078950
O 0.443221 3.092815 -0.427330
H -0.426520 2.993913 0.013611

TS_s2_s10 with 1 H_2O
C 2.321441 -2.267490 0.456081
C 0.839108 -2.146320 0.061540
C 0.308371 -0.724477 0.025879
C 1.279949 0.381689 -0.175901
C 2.767974 0.049642 0.103486
H 0.720096 -2.598282 -0.942038
H 2.434698 -2.095516 1.535146
H 2.995332 0.185906 1.169867
C -1.116252 -0.526496 0.029488
C -2.022513 -1.610030 -0.179186
C -1.722354 0.746095 0.252177
C -3.398598 -1.427045 -0.179338
H -1.632330 -2.604121 -0.367492
C -3.100311 0.919607 0.259044
H -1.088833 1.595471 0.471867
C -3.958840 -0.162353 0.036475
H -4.047037 -2.282499 -0.354162
H -3.512922 1.907776 0.452087
H -5.036214 -0.025143 0.038031
C 1.048852 1.278065 -1.293927
H 1.921171 1.587689 -1.866246
H 0.177368 1.093299 -1.918834
O 0.648839 2.925682 -0.811709
H -0.304770 3.024850 -0.976078
N 3.195830 -1.312893 -0.223482
O 1.082765 2.387455 1.474747
H 0.315205 2.368502 2.071295
H 0.797936 2.875610 0.339597
H 2.675060 -3.286323 0.257243
H 1.121438 1.339346 0.905288
H 0.238264 -2.770130 0.736693
H 3.112119 -1.455034 -1.231865
H 3.408817 0.758441 -0.435231

TS_s4_s7 with 1 H_2O
C 1.399772 -0.563033 -0.491680
C 1.925662 0.775128 -0.647747
C 3.303625 0.992033 -0.333539
C 4.085606 -0.038335 0.168993
C 3.556652 -1.329792 0.314265
C 2.206003 -1.574109 -0.001541
H 1.511170 1.398291 -1.443625
H 3.738571 1.973628 -0.504949
H 5.127445 0.147372 0.419459
H 4.181891 -2.139109 0.680666
H 1.791923 -2.565809 0.166642
C -0.106561 -0.563075 -0.501387
H -0.460437 -0.104203 -1.442445
C -0.440144 0.430078 0.661464
H -0.118209 -0.070424 1.586340
C 0.430317 1.669748 0.520294
H 0.932910 2.036863 1.411508
C -1.958444 0.668716 0.755690
H -2.208746 1.291691 1.621017
H -2.325282 1.200606 -0.131321
C -0.876491 -1.869270 -0.307132
H -0.699748 -2.560572 -1.141530
H -0.531837 -2.374694 0.606406
C -2.381679 -1.567640 -0.189579
H -2.944986 -2.485157 0.015866
H -2.760252 -1.165387 -1.137941
O -0.074395 2.749960 -0.177747
H -0.595090 2.431173 -0.932882
N -2.732081 -0.583632 0.851507
H -4.379641 0.078086 0.090918
O -4.902984 0.494820 -0.629908
H -5.598539 -0.150193 -0.823455
H -2.583457 -0.997677 1.771405

TS_s14_s18 with 1 H_2O
C -1.939401 -0.759760 1.026719
C -3.271979 -0.833312 1.428865
C -4.287302 -0.356152 0.595378
C -3.956110 0.194882 -0.641609
C -2.618650 0.266377 -1.039271
C -1.590107 -0.208818 -0.216732
H -1.159170 -1.126755 1.688585
H -3.519240 -1.264083 2.395707
H -5.325888 -0.414302 0.909613
H -4.735917 0.568610 -1.300209
H -2.371079 0.690282 -2.010957
C -0.145371 -0.163497 -0.690681
C 0.824354 0.656322 0.206487
C 0.426231 -1.589475 -0.875570
H -0.164460 0.288781 -1.694149
C 2.185774 0.129694 0.352984
C 1.908055 -1.555353 -1.259492
H 0.319866 -2.146086 0.063859
H -0.156956 -2.124180 -1.634380
H 2.833886 0.644041 1.068718
H 2.298496 -2.575204 -1.354774
H 2.036179 -1.084626 -2.247682
C 0.344096 1.583720 1.216239
H -0.718052 1.621877 1.442749
H 1.006670 1.801401 2.054785
H 0.620785 2.827745 0.290837
N 2.737072 -0.840313 -0.291496
H 1.199617 1.811846 -0.660796
O 1.120888 3.040538 -0.726588
H 0.412881 3.274841 -1.356202
H 4.554070 -0.731037 0.344836
O 5.278480 -0.448628 0.946773

TS_s3_s9 with 1 H_2O
C 2.278102 0.317543 -1.978226
C 0.898924 0.910363 -1.586643
C 0.592789 0.306474 -0.179638
C 2.278034 -0.558007 1.597406
C 1.883185 -0.549559 0.139381
H 0.951792 2.002090 -1.520238
H 2.143063 -0.596672 -2.571836
H 1.672927 -1.580917 -0.184078
C -0.689713 -0.496052 -0.081027
C -0.987094 -1.517034 -1.000613
C -1.599555 -0.265171 0.964041
C -2.147057 -2.279365 -0.879524
H -0.300401 -1.720525 -1.819177
C -2.766981 -1.026486 1.084318
H -1.398168 0.530768 1.676812
C -3.043550 -2.037418 0.165225
H -2.353882 -3.063947 -1.602875
H -3.457858 -0.824963 1.898937
H -3.949898 -2.629614 0.257191
C 3.488444 -0.892377 2.048087
H 3.721480 -0.876130 3.109544
H 4.286958 -1.181478 1.370102
O -2.067517 2.636873 -0.720897
H -1.986352 1.673483 -0.566421
N 2.958172 -0.045434 -0.729429
O -1.206214 3.231410 1.230455
H -1.994903 3.741813 1.493899
H -1.356910 3.099570 0.053483
H 2.896849 1.000519 -2.568079
H 0.528538 1.115644 0.556645
H 1.504351 -0.268571 2.307429
H 0.121547 0.675965 -2.320632

TS_s5_s10 with 1 H_2O
C -1.133178 -0.334211 0.131661
C -1.914512 0.578166 0.852866
C -3.306557 0.580903 0.740330
C -3.943203 -0.331333 -0.101253
C -3.177397 -1.242748 -0.832336
C -1.787685 -1.242325 -0.716176
H -1.418801 1.293482 1.502737
H -3.892292 1.297023 1.311197
H -5.026310 -0.332083 -0.189790
H -3.663224 -1.954356 -1.495172
H -1.199495 -1.952882 -1.292423
C 0.376762 -0.359491 0.279867
C 0.901248 -1.639887 0.966936
C 1.157815 0.102229 -0.876256
C 2.434760 -1.675103 1.011103
H 0.530287 -2.525481 0.428218
H 0.484834 -1.699232 1.980258
C 2.650158 -0.186684 -0.875316
H 2.784096 -2.631423 1.417809
H 2.802716 -0.882950 1.675599
H 3.050460 -0.105335 -1.892443
C 0.660784 1.048945 -1.749415
H -0.402992 1.245611 -1.810903
H 1.276706 1.433058 -2.554951
O 0.978295 2.921309 -0.582278
H 0.086086 3.304371 -0.643715
N 3.052703 -1.470962 -0.302813
H 2.753941 -2.221002 -0.926991
O 1.204719 1.873859 1.598014
H 0.619697 2.221003 2.290791
H 1.058335 2.503857 0.473965
H 0.675518 0.542168 1.014516

H 3.133425 0.608790 -0.286965

TS_s6_s8 with 1 H_2O
C -1.125955 0.566934 -0.006226
C -1.523725 -0.647624 0.655635
C -2.911835 -0.829777 0.969723
C -3.853688 0.087238 0.554983
C -3.454930 1.247656 -0.137213
C -2.101218 1.467215 -0.418015
H -3.206800 -1.717683 1.520891
H -4.905470 -0.072225 0.777684
H -4.199443 1.968993 -0.462441
H -1.805535 2.352466 -0.977740
C 0.321501 0.714342 -0.412989
H 0.327941 1.230595 -1.387538
C 0.964531 -0.675478 -0.625598
H 1.113931 -1.149090 0.351695
C 0.001468 -1.564037 -1.429497
H 0.506939 -2.512631 -1.683989
C 2.361533 -0.496377 -1.224363
H 2.848403 -1.468962 -1.365890
H 2.294093 -0.012432 -2.216809
C 1.210881 1.546730 0.538113
H 0.800891 2.556490 0.661065
H 1.245906 1.074979 1.526239
C 2.629127 1.638146 -0.040661
H 3.294593 2.154614 0.659713
H 2.600596 2.232884 -0.972903
O -1.147457 -1.909989 -0.698926
N 3.177031 0.289846 -0.278332
H -0.247526 -1.062149 -2.384668
H -0.809543 -1.126120 1.316324
H 4.128254 0.371889 -0.633224
O 2.726998 -0.933189 2.315074
H 3.035842 -0.571208 1.451261
H 2.995233 -1.863709 2.296112

TS_s7_s12a with 1 H_2O
C -0.715408 -0.863101 0.213303
C -1.263077 0.402108 -0.326480
C -2.619507 0.343413 -0.880277
C -3.387675 -0.781980 -0.667141
C -2.878267 -1.924394 -0.005716
C -1.510636 -1.960175 0.392387
H -1.507310 1.138174 0.955211
H -3.024567 1.198483 -1.419197
H -4.410088 -0.802902 -1.040379
H -3.509516 -2.795227 0.140605
H -1.096428 -2.876240 0.809968
C 0.758441 -0.640552 0.432801
H 0.884027 -0.071744 1.374084
C 1.093857 0.334313 -0.725600
H 1.079109 -0.268795 -1.652275
C -0.148827 1.205557 -0.850843
H -0.284154 1.723317 -1.802280
C 2.510115 0.899828 -0.572685
H 2.785080 1.550288 -1.412076
H 2.570134 1.506989 0.337973
C 1.765487 -1.788608 0.458973
H 1.593208 -2.456466 1.313799
H 1.663583 -2.396881 -0.451143
C 3.189152 -1.186917 0.541420
H 3.946122 -1.977205 0.479556
H 3.312541 -0.707532 1.522992
O 0.166263 2.602930 0.114716
H -0.059063 3.376625 -0.430623
N 3.508607 -0.178380 -0.480169
H 3.571713 -0.642111 -1.386494
O -1.411004 1.968250 1.775935

H -2.254573 2.454062 1.776156
H -0.624056 2.489419 1.059256

TS_s9_s11b with 1 H_2O
C 1.448124 0.742231 0.379380
C 2.727566 1.370455 0.515211
C 3.869328 0.782380 -0.010683
C 3.784158 -0.409069 -0.746188
C 2.533681 -1.037788 -0.914685
C 1.382533 -0.481236 -0.394062
H 0.578115 1.399616 0.373803
H 2.794000 2.325148 1.030773
H 4.835617 1.264333 0.120503
H 4.679101 -0.859325 -1.166456
C 0.073149 -1.235377 -0.241690
C -0.423500 -0.825257 1.152648
C -1.026366 -0.926134 -1.277128
C -1.740831 -0.725458 1.418251
C -2.348046 -1.548027 -0.819022
H -1.140579 0.160069 -1.369398
H -0.759403 -1.324240 -2.262833
H -2.102369 -0.361054 2.376908
H -3.142613 -1.362936 -1.550221
C 0.635989 -0.265576 1.990602
N -2.769187 -0.952628 0.464797
H -2.227121 -2.638614 -0.721971
H 0.347741 0.398586 2.805641
H -3.555848 -1.457817 0.866838
H 1.496430 -0.892181 2.219379
H 2.481872 -1.998193 -1.425482
H 0.283937 -2.314981 -0.279420
O -3.768673 1.552957 -0.461837
H -4.185238 2.033225 0.269858
H -3.462497 0.698262 -0.061025
O -1.212900 2.666533 -0.617713
H -1.038119 2.858722 -1.550323
H -2.140836 2.336987 -0.609555

TS_s9_s18
C 1.848115 0.113034 1.078120
C 3.221331 -0.009176 1.286704
C 4.085374 -0.170014 0.201021
C 3.564932 -0.209385 -1.092676
C 2.189069 -0.088602 -1.297971
C 1.314347 0.076356 -0.217980
H 1.180389 0.227918 1.928573
H 3.616952 0.017904 2.298671
H 5.155431 -0.266982 0.363415
H 4.227830 -0.337591 -1.944427
H 1.790104 -0.122576 -2.309559
C -0.183063 0.248000 -0.455175
C -1.011217 -0.663956 0.426648
C -0.649673 1.705328 -0.255742
H -0.384988 -0.035752 -1.498619
C -2.049021 -0.105780 1.191358
C -2.173412 1.770647 -0.343378
H -0.323103 2.061610 0.729310
H -0.190265 2.361362 -1.002853
H -2.605246 -0.763051 1.856785
H -2.533476 2.787933 -0.146001
H -2.508855 1.502650 -1.355863
C -1.223743 -2.040647 0.079698
H -0.466629 -2.517024 -0.546979
H -1.591225 -2.691752 0.877761
H -2.368476 -1.779560 -0.515831
N -2.825011 0.860176 0.610488
H -3.552975 0.162041 0.061211
O -3.669731 -1.155234 -0.637042
H -3.910761 -1.141316 -1.576437

TS_s9_s18 with 1 H_2O
C 2.072522 -1.092488 -0.504984
C 3.396793 -1.426801 -0.784118
C 4.435267 -0.583032 -0.382154
C 4.137503 0.596891 0.299244
C 2.809467 0.929003 0.576276
C 1.761023 0.090675 0.180714
H 1.269405 -1.749224 -0.830570
H 3.618397 -2.346574 -1.319211
H 5.467346 -0.843116 -0.601441
H 4.936937 1.262625 0.614277
H 2.585225 1.851863 1.107544
C 0.316551 0.442119 0.519709
C -0.596469 0.363196 -0.697346
C -0.258322 -0.453286 1.637939
H 0.312394 1.481401 0.882186
C -1.778727 -0.406977 -0.586673
C -1.754880 -0.185057 1.808033
H -0.109806 -1.506872 1.371171
H 0.278492 -0.280353 2.577549
H -2.366074 -0.606563 -1.483330
H -2.182813 -0.853117 2.565317
H -1.901990 0.839307 2.192473
C -0.582442 1.364436 -1.688451
H 0.299327 1.994930 -1.800666
H -1.141682 1.188359 -2.609353
H -1.829564 1.985929 -0.906242
N -2.523018 -0.361939 0.557348
O -4.665799 -1.860861 -0.640198
H -4.017890 -1.478229 -0.009030
H -5.343963 -1.172532 -0.705475
H -2.945332 0.964637 0.174781
O -2.859578 2.017427 -0.326993
H -2.813979 2.716502 0.346978

Table S3. Gibbs energies (ΔG_r, in kJ/mol)) for reactions X + *n* H_2O -> $X(H_2O)_n$ where n = 1 – 3, calculated at CPCM/UAKS/B3LYP/6-31G(d) level of theory. Sequential solvation have been calculated for species involved in **1b** -> **TS_1b_2** -> **2** and **1b** -> **TS_1b_5** -> **5** reactions.

Explicit water molecules (n)	Structure (X)	ΔG_r CPCM/UAKS/ B3LYP/6-31G(d)
1	**1b**	-6.6
	2	-67.9
	5	-3.8
	TS_1b_2	-32.9
	TS_1b_5	6.3
2	**1b**	7.7
	2	20.4
	5	13.9
	TS_1b_2	14.8
	TS_1b_5	36.6
3	**1b**	20.0
	2	29.4
	5	31.9
	TS_1b_2	13.2
	TS_1b_5	37.5

B3LYP/6-31G(d) Cartesian coordinates for structures presented in Table S3

One explicit water 1b
C -1.109772 0.722087 -0.598977
C -2.628979 0.879069 -0.223626
C -2.450175 -0.845183 1.539005
C -0.951637 -1.104034 1.171224
C -0.304670 0.174575 0.605281
H -2.684547 1.713256 0.491961
H -3.236620 1.110546 -1.100649
H -1.038733 0.023728 -1.441718
H -2.482707 -0.097279 2.343187
H -2.954499 -1.756262 1.866100
H -0.439281 -1.435282 2.080436
H -0.898731 -1.925165 0.447639
H -0.337345 0.943612 1.386508
N -3.120428 -0.317097 0.386359
H -3.832793 -0.891566 -0.108133
C -0.605557 2.087417 -1.068250
H -1.144879 2.400654 -1.974639
H 0.459551 1.980405 -1.326124
O -0.794423 3.004409 -0.003401
H -0.582548 3.899529 -0.310103
C 1.161921 -0.091425 0.283358
C 2.164976 0.515807 1.054874
C 1.546193 -0.963375 -0.749840
C 3.513916 0.277505 0.801477
H 1.889049 1.192111 1.859637
C 2.889046 -1.214613 -1.017184
H 0.795407 -1.456887 -1.362314
C 3.855475 -0.587968 -0.233361
H 4.295653 0.749301 1.387047
H 3.197040 -1.881618 -1.815225
F 5.149318 -0.824636 -0.486256
O -5.077464 -1.733960 -0.977120
H -6.022854 -1.654186 -0.777341
H -4.991358 -2.536267 -1.514192

One explicit water 2
C 2.551600 -0.301364 1.241989
C 1.624077 -0.225372 0.195084
C 2.095224 0.050480 -1.097602
C 3.452224 0.248188 -1.342898
C 4.343045 0.165812 -0.276737
C 3.913899 -0.107140 1.016853
H 2.210384 -0.516262 2.251781
H 1.404161 0.111854 -1.935707
H 3.826250 0.461136 -2.338578
H 4.637900 -0.163941 1.822562
C 0.145643 -0.450055 0.466089
C -0.700912 0.818329 0.164051
C -0.435605 -1.660110 -0.293043
H 0.033103 -0.659544 1.538808
C -2.164498 0.527116 -0.010874
C -1.884889 -1.911124 0.113635
H -0.381675 -1.496116 -1.376278
H 0.153859 -2.555958 -0.076826
H -2.886346 1.338305 -0.143067
H -2.376575 -2.635832 -0.541961
H -1.960618 -2.287176 1.141016
H -3.700006 -0.749228 -0.025798
C -0.634979 1.847893 1.258731
H -0.595764 1.532604 2.295929
H -0.716380 2.906234 1.038682
N -2.671535 -0.660965 0.032929
F 5.651321 0.355370 -0.505934
H -0.366835 1.280642 -0.777814
O -5.563774 -0.774288 -0.124361
H -6.113442 -1.204953 0.550749
H -5.961199 -1.023901 -0.974884
O -4.764017 1.902811 -0.602815
H -5.404002 1.274026 -0.271349
H -5.170605 2.772437 -0.648622

One explicit water 5
C -0.828276 -1.210113 0.887605
C -2.214196 -1.563657 0.340734
C -2.291464 0.536161 -0.985264
C -0.925294 0.990194 -0.446372
C -0.094698 -0.175496 0.062882
H -2.147367 -2.123283 -0.596847
H -2.794962 -2.149177 1.057740
H -0.943844 -0.859638 1.925636
H -0.273456 -2.150165 0.940238
H -2.185016 -0.069154 -1.889198
H -2.945290 1.384315 -1.205508
N -2.996963 -0.317102 0.034788
H -3.064288 0.262941 0.888831
H -3.954273 -0.556039 -0.302094
C -1.101143 2.111314 0.602210
H -1.546795 2.997584 0.126719
H -0.122614 2.387370 1.011093
O -1.965133 1.621616 1.642059
H -2.043496 2.290882 2.339579
H -0.426724 1.459599 -1.300259
C 1.333882 -0.172875 -0.039104
C 2.044372 0.818564 -0.783134
C 2.134998 -1.164457 0.606090
C 3.425960 0.814330 -0.886361
H 1.510103 1.607884 -1.299682
C 3.516609 -1.174347 0.508829
H 1.669827 -1.935192 1.209199
C 4.152385 -0.184910 -0.240187
H 3.951494 1.570875 -1.459440
H 4.111692 -1.932309 1.007171
F 5.487876 -0.191054 -0.336467
O -5.533650 -0.857846 -1.027421
H -6.385088 -0.584851 -0.652465
H -5.750594 -1.520845 -1.700688

One explicit water TS_1b_2
C 1.157843 -1.988684 -0.571994
C 2.667660 -1.989923 -0.831739
C 2.902296 -0.068851 0.728906
C 1.399362 -0.006777 0.948557
C 0.655059 -0.554004 -0.306497
C 0.896418 1.364622 1.417993
H 0.645102 -2.410586 -1.442216
H 0.926026 -2.631058 0.286004
H 3.054065 -3.012640 -0.858421
H 2.873770 -1.534255 -1.813988
H 3.530964 0.348455 1.516805
H 1.147896 -0.677150 1.790878
H 0.982999 0.052719 -1.163775
H -0.045384 1.289591 1.959009
H 1.621633 1.907210 2.025909
N 3.378492 -1.262743 0.221514
H 3.135980 1.458358 -0.546962
H 1.464115 2.432640 -0.325235
O 2.713261 2.305024 -0.872515
O 0.588635 2.312625 0.301436
C -0.855839 -0.420007 -0.214311
C -1.599879 -1.036932 0.805892
C -1.544355 0.368244 -1.154517
C -2.980226 -0.871799 0.889480
H -1.102534 -1.663381 1.542003
C -2.929226 0.549316 -1.082171
H -1.004453 0.797662 -1.999085
C -3.625638 -0.074447 -0.054660
H -3.562821 -1.349740 1.670043
H -3.466006 1.144712 -1.813005
F -4.951254 0.088815 0.030118
H 4.383579 -1.390053 0.238410
H 3.228570 2.756292 -1.558706
H -0.177678 1.955352 -0.210321

One explicit water TS_1b_5
H -1.147089 -1.460457 -2.260377
C -1.159540 -1.571494 -1.164704
C -1.732712 0.747952 -0.421535
N -2.770766 -1.223566 0.643619
C -2.889870 0.244010 0.489025
C -2.603654 -1.861034 -0.682824
C -0.633257 -0.310223 -0.490765
H -0.773644 -1.178603 1.118469
H -3.855346 0.539922 0.062206
H -3.347837 -1.480279 -1.397365
H -0.519060 -2.429958 -0.935293
H -2.134989 0.778487 -1.448111
H -2.817091 0.705265 1.482292
H -2.766994 -2.937382 -0.585283
H -3.616775 -1.581828 1.086903
O -0.424306 -1.643155 2.025158
H 0.262968 -1.088868 2.455351
H -1.228580 -1.726296 2.582626
C 0.791275 -0.101781 -0.345076
C 1.340782 0.889349 0.523200
C 1.724020 -0.946609 -1.016543
C 2.709330 1.032362 0.699936
H 0.683620 1.551720 1.074181
C 3.093099 -0.800666 -0.856489
H 1.366447 -1.702560 -1.705985
C 3.574407 0.187264 0.003026
H 3.119643 1.788589 1.361030
H 3.795184 -1.431898 -1.390935
F 4.891703 0.326001 0.167497
C -1.412055 2.215169 -0.122709
H -1.131944 2.356437 0.934687
H -0.575378 2.560395 -0.746302
O -2.612300 2.913061 -0.412193
H -2.461219 3.863226 -0.291870

Two explicit waters 1b
C 1.108022 0.410997 -0.542484
C 2.579192 0.075343 -0.976643
C 2.267981 -2.302710 -0.433930
C 0.779598 -2.054177 -0.009579
C 0.199452 -0.820111 -0.738698
H 2.579742 -0.151450 -2.050956
H 3.230979 0.926420 -0.777448
H 1.132189 0.698717 0.516566
H 2.291726 -2.577778 -1.495828
H 2.723607 -3.093884 0.164773
H 0.205819 -2.958109 -0.240432
H 0.739988 -1.909845 1.075739
H 0.187302 -1.046786 -1.814896
N 2.999108 -1.081920 -0.248580
H 3.572369 -0.984228 0.611140
C 0.653462 1.642677 -1.368777
H -0.371132 1.878892 -1.041729
H 0.613917 1.365019 -2.429636
O 1.517993 2.735086 -1.246385
C -1.247205 -0.616265 -0.299840
C -2.292381 -0.940488 -1.178408
C -1.572046 -0.157119 0.987774
C -3.625440 -0.798331 -0.799506
H -2.063606 -1.303823 -2.177181
C -2.898491 -0.008565 1.384038

H -0.787526 0.095359 1.696686
C -3.907973 -0.333471 0.480961
H -4.438611 -1.038694 -1.475931
H -3.161079 0.349789 2.373672
F -5.186197 -0.191593 0.857480
O 4.564252 -1.201507 2.051919
H 5.520995 -1.350802 2.000991
H 4.402724 -0.871086 2.948697
H 1.284403 3.225434 -0.424673
O 0.721811 4.002314 1.088567
H -0.063843 4.552770 0.941004
H 1.384594 4.618051 1.439929

Two explicit waters 2
C 3.139738 0.237094 -1.172007
C 2.145048 0.214045 -0.186079
C 2.527422 -0.022639 1.143110
C 3.861873 -0.233500 1.483301
C 4.820838 -0.204472 0.475224
C 4.480991 0.028847 -0.852060
H 2.868183 0.421295 -2.208604
H 1.782273 -0.040809 1.935699
H 4.167001 -0.415834 2.508171
H 5.256447 0.045292 -1.610368
C 0.690774 0.450306 -0.558817
C -0.187897 -0.805138 -0.290564
C 0.074653 1.680572 0.137810
H 0.651731 0.639931 -1.640426
C -1.658963 -0.491015 -0.236329
C -1.342979 1.935420 -0.365566
H 0.057696 1.536635 1.225245
H 0.687623 2.565867 -0.055913
H -2.396450 -1.292933 -0.154985
H -1.876386 2.671981 0.242054
H -1.348196 2.298627 -1.400489
H -3.190972 0.824970 -0.323716
C -0.020664 -1.872615 -1.336290
H 0.067751 -1.595919 -2.381550
H -0.067736 -2.924577 -1.079353
N -2.147565 0.697748 -0.323541
F 6.108617 -0.407043 0.795744
H 0.064861 -1.233154 0.692115
O -4.795853 1.379890 -0.213699
H -5.365412 0.811147 0.348008
H -5.237687 1.400513 -1.076692
O -4.387769 -1.842511 -0.234548
H -5.078696 -1.616525 0.415745
H -4.655418 -2.694862 -0.608842
O -6.315963 -0.446077 1.363292
H -6.252693 -0.331644 2.325762
H -7.266843 -0.522699 1.180467

Two explicit waters 5
C -0.694490 -0.594795 1.309774
C -2.016778 -1.304622 1.014444
C -2.113198 -0.269652 -1.240976
C -0.716936 0.364918 -1.080563
C 0.083238 -0.230671 0.064964
H -1.849079 -2.284658 0.557136
H -2.610802 -1.433238 1.922329
H -0.919154 0.298297 1.915336
H -0.122956 -1.264990 1.956212
H -2.023686 -1.251672 -1.713642
H -2.760725 0.348110 -1.869730
N -2.842674 -0.507214 0.049576
H -3.132281 0.397327 0.508222
H -3.712152 -1.034585 -0.173030
C -0.725700 1.920856 -1.042484
H -1.460499 2.313371 -1.753571
H 0.261238 2.282797 -1.348861
O -1.060390 2.489750 0.228032
H -0.264120 2.504536 0.781145
H -0.226992 0.125817 -2.032732
C 1.515283 -0.259513 0.032439
C 2.254119 0.061805 -1.148072
C 2.290524 -0.605613 1.181891
C 3.638698 0.031944 -1.182967
H 1.736923 0.324350 -2.064281
C 3.675215 -0.635659 1.154813
H 1.801935 -0.841653 2.120077
C 4.339636 -0.317869 -0.029334
H 4.186058 0.270539 -2.088771
H 4.250966 -0.897203 2.036363
F 5.677705 -0.345406 -0.058578
O -3.378796 1.792233 1.425891
H -2.628486 2.332199 1.092437
H -4.157253 2.368636 1.454094
O -5.022049 -2.052221 -0.848048
H -5.887912 -1.715094 -1.125333
H -5.169443 -2.988602 -0.643803

Two explicit waters TS_1b_2
C 2.459084 -1.428739 -1.280906
C 0.989549 -1.634843 -0.906176
C 0.347976 -0.328675 -0.382429
C 1.148813 0.148487 0.862782
C 2.626354 0.153192 0.602803
H 0.442311 -1.987728 -1.785816
H 2.530347 -0.824764 -2.199138
H 2.946158 -2.386753 -1.484443
H 0.490311 0.440893 -1.153914
H 1.024659 -0.604257 1.676091
H 1.837508 2.567787 -0.046796
H 3.299487 0.630355 1.310492
H 0.902850 -2.417031 -0.141217
C -1.147847 -0.470763 -0.154689
C -2.045072 0.099340 -1.073122
C -1.678122 -1.199726 0.920986
C -3.426521 -0.035489 -0.923311
H -1.656653 0.634825 -1.937246
C -3.055150 -1.343686 1.089676
H -1.018689 -1.673770 1.643869
C -3.911097 -0.754992 0.164456
H -4.123398 0.389286 -1.638541
H -3.469692 -1.905597 1.919897
C 0.599776 1.315558 1.582778
H -0.472901 1.467654 1.571441
H 1.115647 1.660040 2.472836
O 1.120732 2.897870 0.523331
H 0.334620 3.064709 -0.074104
N 3.190049 -0.764821 -0.203314
H 4.212689 -0.839476 -0.183580
F -5.235721 -0.886277 0.323080
O 6.018323 -0.725632 0.177052
H 6.676986 -0.357414 -0.431294
H 6.489418 -1.416156 0.667856
O -1.021479 3.205873 -1.039217
H -1.377583 4.098701 -1.174464
H -1.779995 2.646057 -0.802872

Two explicit waters TS_1b_5
H -0.965673 -1.264210 -2.258672
C -0.816001 -1.544174 -1.204013
C -1.481477 0.529697 0.006382
N -2.153814 -1.691678 0.841729
C -2.391078 -0.234657 1.009418
C -2.156104 -2.039269 -0.603840
C -0.308134 -0.355958 -0.397131
H -0.128514 -1.559543 1.036329
H -3.436639 0.031125 0.827373
H -3.014557 -1.579674 -1.110222
H -0.085154 -2.360989 -1.201561
H -2.073024 0.615020 -0.918235
H -2.137509 0.041344 2.042242
H -2.244185 -3.123965 -0.707531
H -2.908890 -2.198863 1.303967
O 0.363689 -2.147559 1.777064
H 1.026206 -1.608942 2.262900
H -0.380846 -2.428691 2.355858
C 1.098097 -0.037869 -0.339177
C 1.645906 0.850798 0.635428
C 2.027360 -0.667729 -1.220181
C 3.008823 1.096485 0.719754
H 0.991680 1.347121 1.342991
C 3.388793 -0.416301 -1.150350
H 1.665515 -1.334385 -1.994774
C 3.868537 0.462642 -0.178711
H 3.418108 1.772971 1.462903
H 4.085524 -0.881887 -1.839481
F 5.180878 0.700828 -0.101773
C -1.269918 1.984416 0.432157
H -0.888817 2.062894 1.461370
H -0.556562 2.481261 -0.238942
O -2.559375 2.597548 0.357718
H -2.479808 3.530533 0.609227
H -3.974836 1.750935 -0.822344
O -4.321954 0.951326 -1.257861
H -5.010905 1.263225 -1.863322

Three explicit waters 1b
C -0.694851 0.074675 0.742377
C -2.087024 -0.547957 1.134403
C -1.463098 -2.737443 0.186977
C -0.068323 -2.179912 -0.252878
C 0.389342 -1.027995 0.664466
H -2.015824 -0.941115 2.158346
H -2.882350 0.195468 1.066533
H -0.818209 0.546254 -0.239494
H -1.370407 -3.178330 1.188170
H -1.833600 -3.486729 -0.515230
H 0.643962 -3.010834 -0.222372
H -0.135618 -1.841970 -1.292264
H 0.514805 -1.440549 1.676405
N -2.374579 -1.632536 0.239122
H -3.070117 -1.479290 -0.564049
C -0.330414 1.167548 1.747230
H 0.641685 1.591277 1.465140
H -0.241040 0.743803 2.757680
O -1.353390 2.170992 1.724161
H -1.172547 2.818986 2.423239
C 1.751559 -0.511444 0.208525
C 2.886658 -0.742215 0.998201
C 1.909827 0.162952 -1.013180
C 4.148755 -0.309010 0.593761
H 2.788530 -1.269226 1.944265
C 3.162893 0.603722 -1.432678
H 1.052022 0.353055 -1.653661
C 4.266346 0.359210 -0.619807
H 5.031309 -0.482105 1.200202
H 3.296658 1.126471 -2.373750
F 5.474717 0.782019 -1.019078
O -3.964942 -1.077697 -1.813043
H -4.774406 -1.586170 -1.975823
H -4.257722 -0.161131 -1.551113
O -4.396897 1.260457 -0.634127
H -3.655309 1.888193 -0.833701
H -5.211298 1.785099 -0.637633
O -2.111884 2.656712 -0.899731
H -1.820987 2.742934 0.033949
H -1.973047 3.518986 -1.319453

Three explicit waters 2
C -3.639523 0.571137 1.013415
C -2.634390 0.259059 0.089136
C -2.972855 -0.521551 -1.026632
C -4.274043 -0.981365 -1.217670
C -5.244350 -0.651237 -0.276448
C -4.947960 0.120869 0.840395
H -3.401865 1.176386 1.884923
H -2.219029 -0.778723 -1.767745
H -4.545054 -1.584218 -2.077835
H -5.730781 0.358586 1.552667
C -1.217313 0.766894 0.297822
C -0.209939 -0.393706 0.527057
C -0.719222 1.672484 -0.846561
H -1.215499 1.376016 1.212491
C 1.222397 0.010263 0.301446
C 0.657021 2.246987 -0.522498
H -0.668275 1.108847 -1.786343
H -1.422029 2.495543 -1.006709
H 2.034228 -0.696578 0.512056
H 1.115280 2.732448 -1.389260
H 0.606848 2.988957 0.283903
H 2.612438 1.395820 -0.167342
C -0.255624 -0.950609 1.923212
H -0.467425 -0.295418 2.761372
H 0.035477 -1.975249 2.124786
N 1.585776 1.181441 -0.097062
F -6.500547 -1.091243 -0.454045
H -0.410229 -1.210332 -0.184830
O 4.225973 1.844487 -0.419710
H 4.923874 1.237555 -0.075344
H 4.508362 2.734403 -0.161192
O 6.160573 -2.107357 -1.124414
H 6.241785 -2.026058 -2.088375
H 6.668120 -2.902327 -0.893805
O 6.092898 0.065370 0.582317
H 6.360476 -0.610742 -0.080087
H 6.892481 0.315067 1.070396
O 3.789602 -1.569337 0.645846
H 4.243745 -2.007949 -0.093617
H 4.504007 -1.041585 1.047371

Three explicit waters 5
C 0.757996 -0.213764 -1.386752
C 2.114852 -0.920106 -1.415741
C 2.224941 -0.886451 1.067744
C 0.808693 -0.289365 1.182252
C 0.002775 -0.425362 -0.095347
H 1.995202 -2.008131 -1.406188
H 2.691638 -0.635483 -2.298972
H 0.917935 0.860267 -1.569197
H 0.197048 -0.592112 -2.245317
H 2.174920 -1.978242 1.110637
H 2.864761 -0.546155 1.886944
N 2.934835 -0.560389 -0.213706
H 3.202513 0.462228 -0.263662
H 3.819988 -1.106752 -0.232311
C 0.774058 1.170529 1.733813
H 1.461588 1.252732 2.584668
H -0.238164 1.364253 2.108026
O 1.132736 2.175810 0.798452
H 0.331522 2.439925 0.283528
H 0.348798 -0.887530 1.978693
C -1.429315 -0.503834 -0.065616
C -2.153155 -0.765320 1.137720
C -2.219149 -0.308132 -1.241680
C -3.536860 -0.840806 1.166045
H -1.622755 -0.934290 2.068029
C -3.606042 -0.374046 -1.217904
H -1.740294 -0.093404 -2.190412
C -4.254208 -0.644742 -0.013661
H -4.071027 -1.052516 2.086390
H -4.192562 -0.225095 -2.118654
F -5.591596 -0.710881 0.011784
O 3.457711 2.091075 -0.506425
H 2.662106 2.391149 -0.003234
H 4.209936 2.609302 -0.183199
O -1.069226 2.767031 -0.694085
H -1.491482 3.639369 -0.662227
H -1.792216 2.118215 -0.668991
O 5.194270 -2.249513 -0.053283
H 6.073166 -1.987059 0.261114
H 5.346437 -3.036847 -0.598302

Three explicit waters TS_1b_2
C -1.247021 -2.346800 0.685258
C 0.233689 -2.078747 0.412059
C 0.564002 -0.568791 0.418679
C -0.326431 0.140614 -0.643076
C -1.755506 -0.282257 -0.564402
H 0.834791 -2.589985 1.170385
H -1.482389 -2.126605 1.738583
H -1.486768 -3.399868 0.509920
H 0.269775 -0.167069 1.398824
H 0.004238 -0.211197 -1.649532
H -2.046624 2.567051 0.249733
H -2.522267 0.303935 -1.059860
H 0.511829 -2.510035 -0.557411
C 2.048765 -0.303056 0.234524
C 2.783228 0.335290 1.243318
C 2.725783 -0.700791 -0.929886
C 4.151024 0.572794 1.107415
H 2.283888 0.647770 2.157679
C 4.091152 -0.472367 -1.085691
H 2.191422 -1.204343 -1.732436
C 4.784576 0.163458 -0.059957
H 4.724244 1.063825 1.886505
H 4.621412 -0.778778 -1.981068
C -0.062550 1.580470 -0.854703
H 0.919033 1.968324 -0.611957
H -0.590805 2.083600 -1.657520
O -1.077569 2.608623 0.528434
H -1.011126 2.185383 1.399982
N -2.095577 -1.530786 -0.185879
H -3.081860 -1.777353 -0.250410
F 6.099766 0.387717 -0.204280
O -3.503749 2.427336 -0.450328
H -4.239305 1.913286 -0.023698
H -3.901941 3.252798 -0.765933
O -5.509137 0.912725 0.505762
H -5.435214 -0.048370 0.333388
H -5.919181 1.006502 1.377691
O -5.126853 -1.801769 -0.286117
H -5.514521 -1.859354 -1.175559
H -5.563297 -2.507688 0.219124

Three explicit waters TS_1b_5
C -0.341387 1.932560 -0.337293
C -0.667255 0.539931 1.776131
N -2.251408 0.488803 -0.022127
C -2.164666 0.290187 1.434558
C -1.899271 1.857792 -0.445068
C 0.061751 0.645978 0.415847
H -0.286392 -0.263857 2.406477
H -0.900259 -0.014729 -0.201415
H -2.842134 0.978256 1.952811
H -2.394092 2.589047 0.204018
H 0.048979 1.889941 -1.358665
H -0.524613 1.467645 2.341572
H -2.467037 -0.738155 1.647154
H -2.245154 2.023644 -1.465690
H -3.017311 -0.001936 -0.513254
C 1.380822 0.054217 0.229292
C 2.285131 0.536351 -0.758452
C 1.800268 -1.067120 1.000221
C 3.531875 -0.034764 -0.943771
H 2.013915 1.382492 -1.378676
C 3.040060 -1.652801 0.819249
H 1.135740 -1.494580 1.742025
C 3.897358 -1.125329 -0.150089
H 4.226845 0.342578 -1.686085
H 3.358848 -2.507317 1.406204
F 5.093953 -1.682043 -0.327098
C 0.151457 3.252863 0.260643
H 1.250974 3.262578 0.296707
H -0.215842 3.372062 1.292397
O -0.361503 4.265494 -0.589743
H -0.084636 5.131348 -0.252035
O -1.743805 -2.665092 -1.424894
H -2.013442 -3.043203 -0.556704
O -4.041388 -1.347595 -1.218976
H -3.284096 -1.849044 -1.621692
H -1.493179 -3.417330 -1.982419
H -4.740975 -1.282861 -1.886837
O -3.176979 -2.920583 0.884694
H -3.605171 -3.655235 1.350227
H -3.874143 -2.491562 0.346390