

Supporting information

Contents

1. Conformational analysis of the protonated substrate	S2
2. Effect of explicit solvation of the protonated substrate	S2
3. Binding Gibbs energy calculations with the attach-pull-release approach	S3
4. Classical MD simulation of the protonated substrate encapsulated	S4
5. pKa calculation of the protonated substrate in solution	S4
6. Calculated absolute and relative Gibbs energies	S5
7. Adaptively biased molecular dynamic simulation (AMBER-NFE-ABMD)	S8
8. Computational details	S8
9. Force field parameters for molecular dynamic simulation	S9
10. Cartesian coordinates	S11
11. References	S138

1. Conformational analysis of the protonated substrate.

Table S1. Calculated absolute and relative Gibbs energies of conformers of the protonated substrate.

Conformers	Absolute G_{solv}	Relative G_{solv}
1	-467.29895	0.0
2	-467.29590	1.9
3	-467.29820	0.5
4	-467.29329	3.6
5	-467.29763	0.8
6	-467.29654	1.5

2. Effect of explicit solvation of the protonated substrate.

Table S2. Calculated absolute ΔG between the protonated and unprotonated species as a function of the number of explicit solvent molecules included in the calculation.

Number of explicit solvents	Absolute G_{solv}	Relative G_{solv}
0	-259.73	0.0
1	-267.5	-7.8
2	-272.36	-12.6
3	-274.33	-14.6
4	-274.46	-14.7

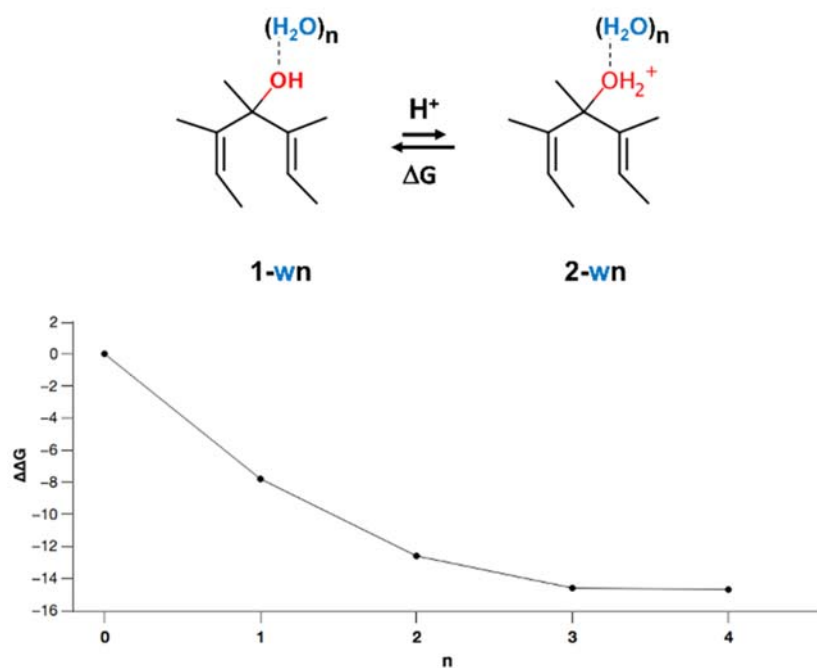


Figure S1. Variation of Gibbs energy difference ($\Delta\Delta G$) for protonated and unprotonated species as a function of the number of explicit water solvent molecules included in the calculation.

3. Binding Gibbs energy calculations with the attach-pull-release approach.

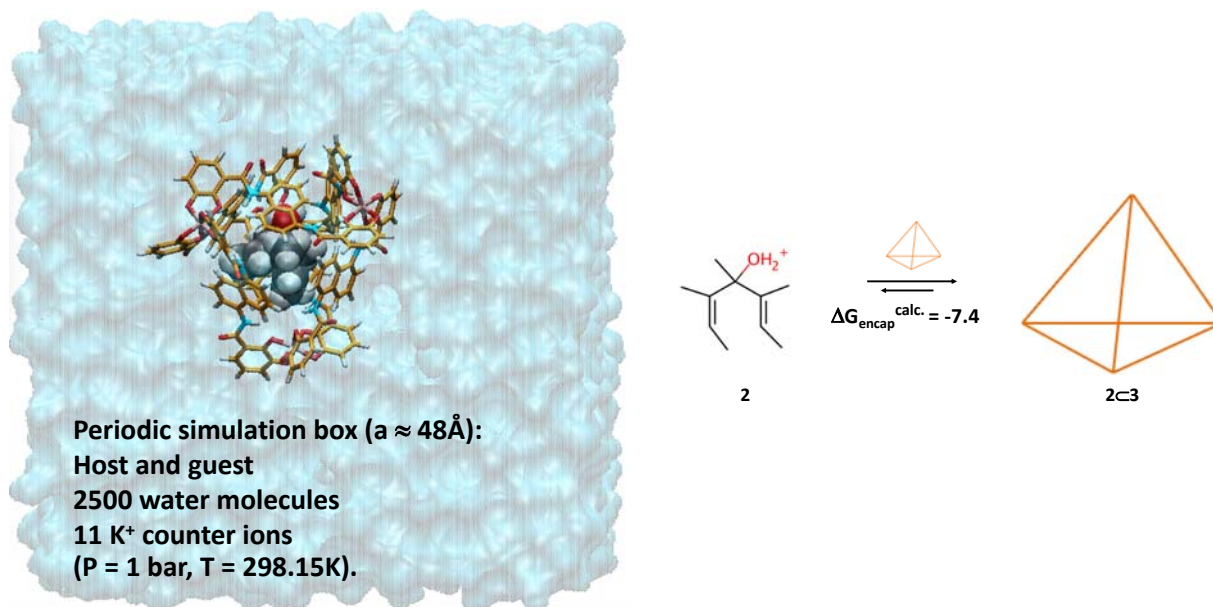


Figure S2. Computation of ΔG_{bind} of the encapsulation of protonated substrate **2** in the metal cage.

4. Classical molecular dynamic simulation of host-guest complex.

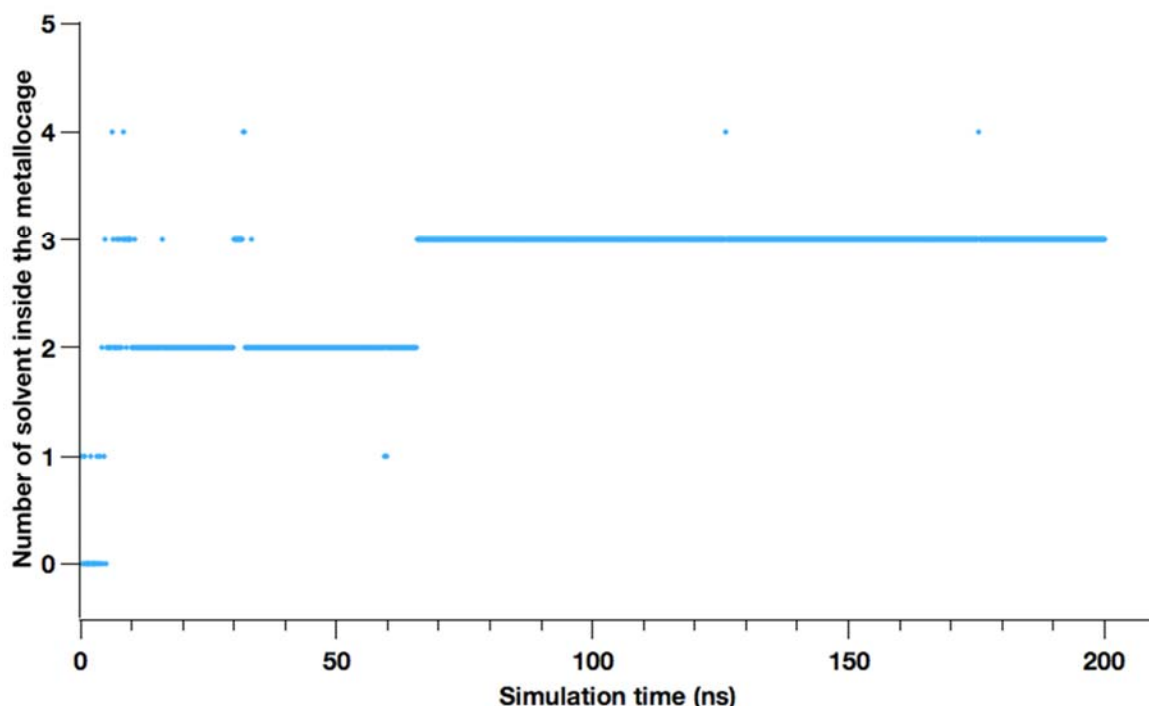
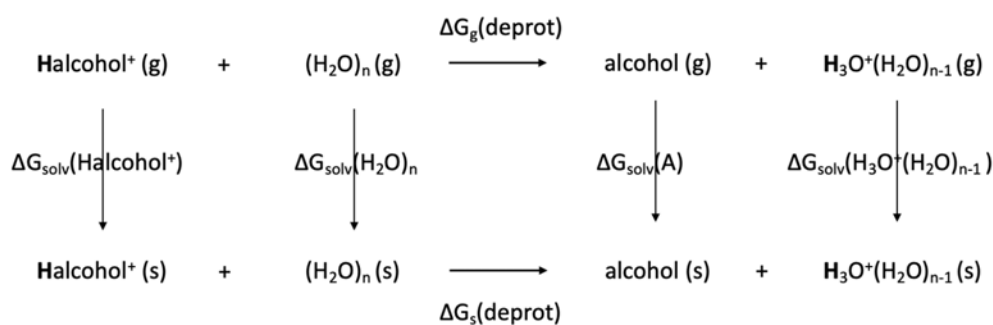


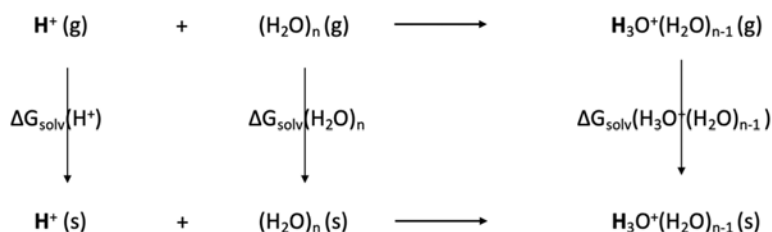
Figure S3. Number of solvent molecules inside the metallocage (along with the protonated substrate).

5. pKa calculation of the protonated substrate in solution.



Scheme S1. The thermodynamic cycle for the pKa calculation (n=4).

The main source of error in these calculations can be the solvation of proton/hydronium and it requires certain number of explicit solvent molecules in the calculations. Here, we considered the explicit solvation of a hydronium ion by three explicit water molecules (n=4 in Scheme S1). In general, when $n \rightarrow \infty$, the actual value of the solvation Gibbs energy of proton is obtained using the thermodynamic cycle in Scheme S2.



Scheme S2. The thermodynamic cycle for the solvation Gibbs energy of proton.

When $n=4$, the calculated standard solvation Gibbs energy of proton is -269.4 kcal/mol in agreement with the experimental value (-265.9 kcal/mol).

Table S3. Calculated absolute energies of the species for the pKa calculation.

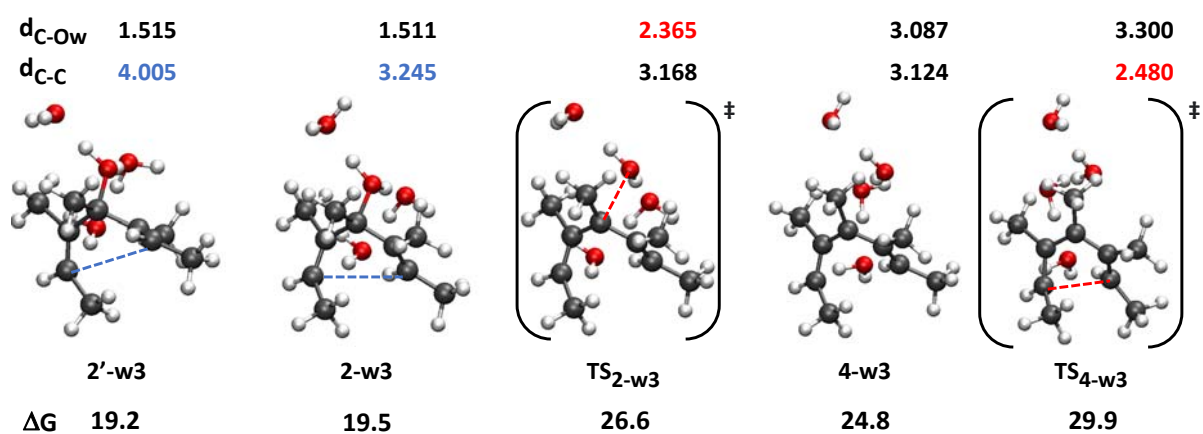
	ROH_2^+	$(\text{H}_2\text{O})_4$	ROH	$\text{H}_3\text{O}^+(\text{H}_2\text{O})_3$
E_{gas}	-467.46361	-305.7011	-467.1013	-306.0617
Thermal	0.227537	0.067586	0.220358	0.074602
G_{gas}	-467.23608	-305.6335	-466.8809	-305.9871
solvation	-45.55464336	-16.6277335	-2.74911693	-65.9273506
E_{solv}	-467.53621	-305.7276	-467.1056	-306.1667
Thermal	0.227537	0.067586	0.220358	0.074602
G_{solv}	-467.308671	-305.660028	-466.885291	-306.092133

6. Calculated absolute and relative Gibbs energies of the species in the reaction in solution and inside the metallocage.

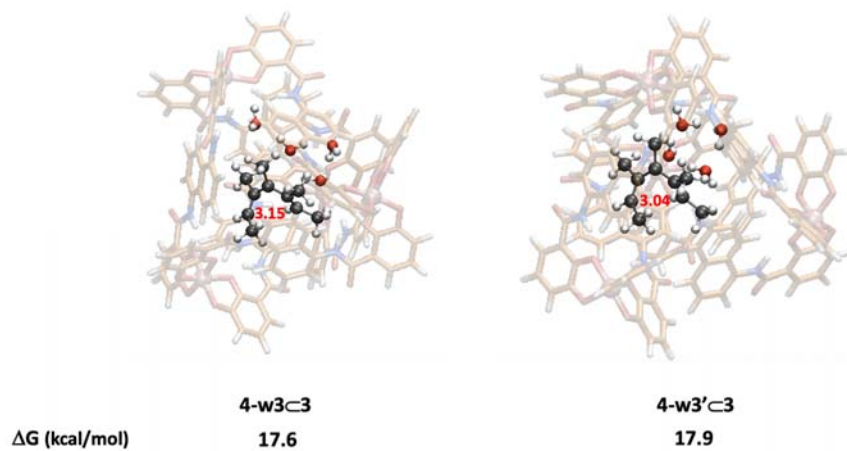
Table S4. Calculated Gibbs energies of the species in the reaction in solution and inside the metallocage.

Species	Absolute G_{solv}	Relative G_{solv}
2'-w3	-696.56344	0.0
2-w3	-696.56303	0.3
TS_{2-w3}	-696.55172	7.4
4-w3	-696.55445	5.6
TS_{4-w3}	-696.54637	10.7
5-w3	-696.598990	-3.1

2-w3 $\subset$ 3	-9609.214665	0.0
TS _{2-w3$\subset$3}	-9609.199253	9.7
4-w3 $\subset$ 3	-9609.205977	5.5
4-w3' $\subset$ 3	-9609.205407	5.8
TS _{4-w3'$\subset$3}	-9609.199172	9.7
5-w3 $\subset$ 3	-9609.239353	-3.4
TS _{4-w3'_a1}	-9609.180677	21.3
TS _{4-w3'_a2}	-9609.187554	17.0
TS _{4-w3'_a3}	-9609.191919	14.3
TS _{4-w3'_a4}	-9609.198015	10.4
2-w3_a1	-9609.207682	4.4
2-w3_a2	-9609.213759	0.6
2-w3_a3	-9609.207931	4.2
2-w3_a4	-9609.206553	5.1



(a)



(b)

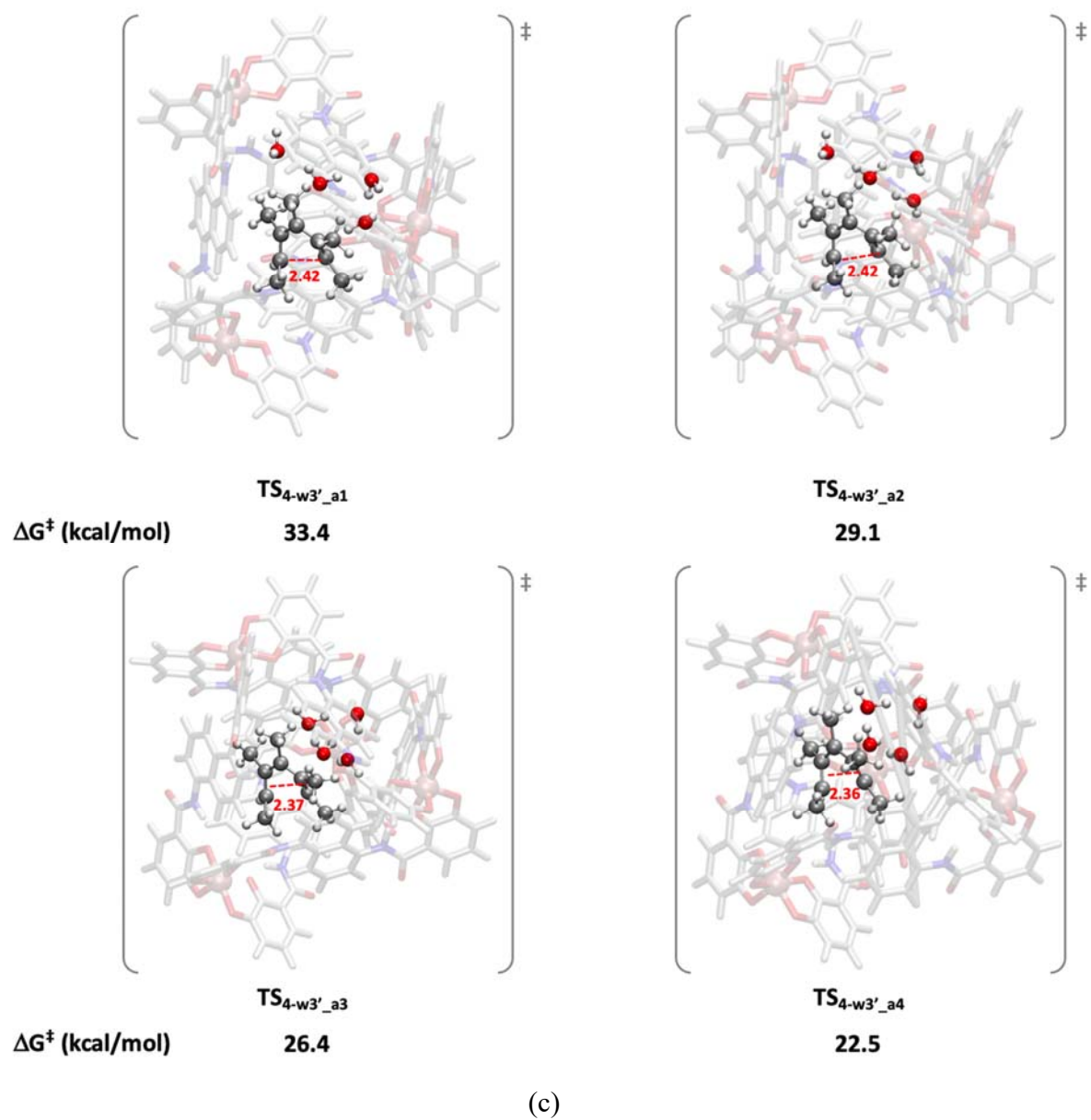


Figure S4. (a) Optimized geometries of TSs and intermediates for the reaction in solution and optimized geometries of (b) the encapsulated intermediate and (c) the encapsulated TS with different rearrangements of water solvent molecules in the metallocage. Distances are in Å; Gibbs energies in kcal/mol.

7. Adaptively biased molecular dynamic simulation (AMBER-NFE-ABMD).

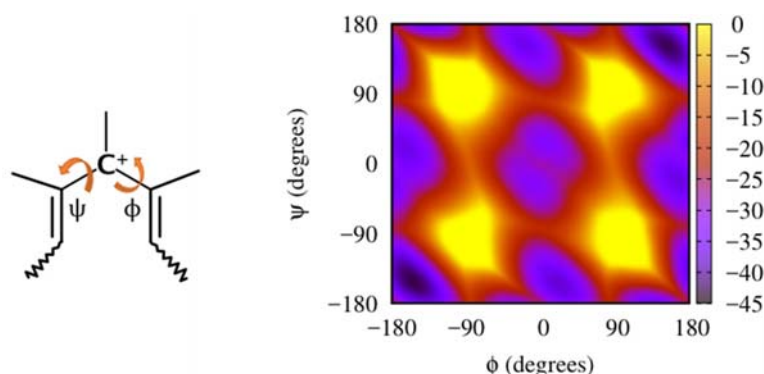


Figure S5. Free energy landscape for the conformational change of **4** inside the metallocage using the ABMD method with AMBER 16 program.^{1,2}

8. Computational details.

All Gibbs energies were calculated at full DFT level except the binding of the neutral and protonated substrate in the metallocage which were computed with molecular dynamics (MD) simulations. DFT calculations for Gibbs energies include three explicit water molecules in the metallocage and in solution. MD simulations for Gibbs energies include 2500 explicit water solvent molecules.

Quantum chemical calculations: all calculations were performed with the Gaussian 09 software³ using the B3LYP-D3 functional as implemented.⁴⁻⁶ The SDD pseudopotential and related basis set complementing with a set of d polarization functions were used for Ga,^{7,8} while the 6-31G(d) basis set was used for all other atoms.⁹ The structures of the reactants, intermediates, transition states and products were optimized in water by using the SMD continuum model.¹⁰ The quasi-rigid-rotor-harmonic-oscillator (quasi-RRHO) approach was used for thermal contributions to the Gibbs energies.¹¹ The standard state correction (1.9 kcal/mol to each of the compounds) was also included.¹² The placement of explicit solvent water molecules was initially determined from the most populated molecular dynamics structure of the protonated substrate in the metallocage. Possible different positions of water molecules are constructed manually and tested to identify the most stable geometry in solution as well as in the metallocage.

Molecular dynamics simulations: simulations were performed at constant temperature (298.15 K, using a Langevin thermostat) and pressure (1 bar, using a Monte Carlo barostat) with the AMBER 16 package¹³ using the CUDA version of the pmemd program. The MD simulation box, of size $46 \times 49 \times 47$ Å and treated under periodic boundary conditions, contains the metallocage, the guest, 11 potassium counterions, and 2500 water molecules (TIP3P).¹⁴ Force field parametrization procedure was described in our previous work (the parameters of the metallocage were directly used).¹⁵ The absolute binding Gibbs energies (ΔG_{bind}) were computed using the attach-pull-release (APR) method¹⁶⁻¹⁸ and the simulation details were described in the previous

work.¹⁵ A cutoff of 9 Å was used for nonbonded interactions, with long range electrostatics interactions accounted by the PME method.¹⁹ A time step of 2 fs was used in plain MD simulations, whereas for Gibbs energy calculations different time steps were used according to recommendations from the literature.^{16–18} The well-tempered adaptively biased molecular dynamics simulations were performed using the non-equilibrium free energy toolkit for AMBER.^{1,2} The resolution of collective variables was 0.1.

9. Force field parameters for molecular dynamic simulation.

Parameters for the protonated 1,4-pentadien-3-ol:

BOND

O-C	7.0	1.6287	Created by Seminario method using MCPB.py
O-H1	506.9	0.9845	Created by Seminario method using MCPB.py
O-H2	503.7	0.9845	Created by Seminario method using MCPB.py
C-c2	326.8	1.5095	SOURCE1_SOURCE5 10204 0.0042
C-c3	300.9	1.5375	SOURCE1_SOURCE5 88072 0.0058

ANGL

H1-O-C	54.31	107.24	Created by Seminario method using MCPB.py
H2-O-C	57.90	112.00	Created by Seminario method using MCPB.py
c3-c3-O	100.33	104.13	Created by Seminario method using MCPB.py
O-C-c2	130.90	102.38	Created by Seminario method using MCPB.py
O-C-c3	100.35	104.13	Created by Seminario method using MCPB.py
H1-O-H2	50.12	106.11	Created by Seminario method using MCPB.py
H1-c2-c2	64.06	123.63	SOURCE3_SOURCE5 4623 2.2803
H1-c2-c3	62.87	115.65	SOURCE3_SOURCE5 1743 1.5647
H1-c3-hc	46.20	110.56	SOURCE3_SOURCE5 1758 0.9658
c2-H1-c2	63.89	112.00	SOURCE4_SOURCE5 453 0.8153
c3-H1-c2	63.41	111.56	SOURCE4_SOURCE5 9345 1.7373

atomic charges for the protonated 1,4-pentadien-3-ol:

1 C1	0.3380	-0.5590	0.3450 C	1 MOL	0.152628
2 C2	-0.9870	-0.2090	-0.2940 c2	1 MOL	0.019381
3 C3	1.5330	0.2620	-0.1280 c2	1 MOL	0.019381
4 C4	2.7610	-0.4820	-0.6000 c3	1 MOL	-0.287611
5 H1	3.1300	-1.1810	0.1640 hc	1 MOL	0.100174
6 H2	2.5620	-1.0670	-1.5060 hc	1 MOL	0.100174
7 H3	3.5680	0.2220	-0.8200 hc	1 MOL	0.100174
8 C5	-0.9300	0.1080	-1.7710 c3	1 MOL	-0.287611
9 H4	-0.1820	-0.5110	-2.2770 hc	1 MOL	0.100174

10 H5	-1.8920	-0.0650	-2.2580 hc	1 MOL	0.100174
11 H6	-0.6490	1.1550	-1.9390 hc	1 MOL	0.100174
12 C6	1.5390	1.6010	-0.0280 c2	1 MOL	-0.059805
13 H7	2.4600	2.0980	-0.3330 hc	1 MOL	0.120745
14 C7	-2.1100	-0.1980	0.4450 c2	1 MOL	-0.059805
15 H8	-2.0420	-0.4310	1.5040 hc	1 MOL	0.120745
16 C8	0.4720	2.5350	0.4640 c3	1 MOL	-0.346876
17 H9	0.8600	3.1360	1.2970 hc	1 MOL	0.124811
18 H10	0.1930	3.2440	-0.3270 hc	1 MOL	0.124811
19 H11	-0.4340	2.0310	0.8040 hc	1 MOL	0.124811
20 C9	-3.4920	0.1510	-0.0120 c3	1 MOL	-0.346876
21 H12	-4.1870	-0.6640	0.2320 hc	1 MOL	0.124811
22 H13	-3.8490	1.0350	0.5340 hc	1 MOL	0.124811
23 H14	-3.5650	0.3600	-1.0820 hc	1 MOL	0.124811
24 O1	0.5820	-2.0390	-0.2890 O	1 MOL	-0.490681
25 H15	-0.2290	-2.5690	-0.1150 H1	1 MOL	0.495304
26 C10	0.3850	-0.7870	1.8470 c3	1 MOL	-0.052165
27 H16	-0.3420	-1.5330	2.1750 hc	1 MOL	0.052679
28 H17	1.3880	-1.1180	2.1350 hc	1 MOL	0.052679
29 H18	0.1830	0.1630	2.3510 hc	1 MOL	0.052679
30 H19	1.3200	-2.5150	0.1580 H2	1 MOL	0.495304

atomic charges (resp) for 1,4-pentadien-3-ol:

1 C1	0.0650	-0.0010	0.0720 c3	1 MOL	0.178211
2 C2	0.5750	1.3750	-0.4030 c2	1 MOL	0.021153
3 C3	-1.3990	-0.2530	-0.3280 c2	1 MOL	0.021153
4 C4	-2.4110	0.3660	0.6150 c3	1 MOL	-0.300415
5 H1	-2.3940	-0.1010	1.6060 hc	1 MOL	0.096844
6 H2	-2.1910	1.4310	0.7690 hc	1 MOL	0.096844
7 H3	-3.4260	0.2820	0.2150 hc	1 MOL	0.096844
8 C5	1.7270	1.9400	0.3960 c3	1 MOL	-0.300415
9 H4	2.2010	2.7890	-0.1030 hc	1 MOL	0.096844
10 H5	1.3890	2.2780	1.3830 hc	1 MOL	0.096844
11 H6	2.5010	1.1840	0.5750 hc	1 MOL	0.096844
12 C6	-1.8350	-0.8990	-1.4230 c2	1 MOL	-0.101241
13 H7	-2.9190	-0.9710	-1.5260 hc	1 MOL	0.091067
14 C7	0.0430	1.9760	-1.4780 c2	1 MOL	-0.101241
15 H8	-0.7960	1.4840	-1.9670 hc	1 MOL	0.091067
16 C8	-1.0700	-1.5090	-2.5720 c3	1 MOL	-0.331165
17 H9	-0.2480	-0.8700	-2.9140 hc	1 MOL	0.110976

18 H10	-0.6410	-2.4880	-2.3210 hc	1 MOL	0.110976
19 H11	-1.7420	-1.6630	-3.4230 hc	1 MOL	0.110976
20 C9	0.4540	3.2700	-2.1220 c3	1 MOL	-0.331165
21 H12	1.3120	3.7510	-1.6440 hc	1 MOL	0.110976
22 H13	0.7050	3.1090	-3.1800 hc	1 MOL	0.110976
23 H14	-0.3790	3.9860	-2.1110 hc	1 MOL	0.110976
24 O1	0.1340	0.0420	1.5240 oh	1 MOL	-0.645917
25 H15	-0.1190	-0.8430	1.8380 ho	1 MOL	0.453815
26 C10	1.0450	-1.1040	-0.3770 c3	1 MOL	-0.205424
27 H16	1.2340	-1.0840	-1.4510 hc	1 MOL	0.071198
28 H17	1.9990	-0.9640	0.1390 hc	1 MOL	0.071198
29 H18	0.6530	-2.0920	-0.1090 hc	1 MOL	0.071198

10. Cartesian coordinates.

2-w3c3

C	119.654999	-15.034000	45.069000
H	118.582001	-14.880000	45.101002
C	122.457001	-15.355000	44.889999
C	120.401001	-14.297000	44.176998
H	119.907997	-13.597000	43.515999
C	121.799004	-14.433000	44.095001
H	122.362000	-13.810000	43.414001
C	120.288002	-15.984000	45.917999
C	121.710999	-16.179001	45.806000
C	119.553001	-16.783001	46.868000
C	122.338997	-17.188999	46.584999
H	123.399002	-17.393999	46.484001
C	120.222000	-17.716000	47.646000
H	119.676003	-18.299000	48.372002
C	121.601997	-17.933001	47.476002
H	122.087997	-18.705000	48.061001
C	117.228996	-17.563999	47.294998
C	115.796997	-17.214001	47.089001
C	115.343002	-16.011999	46.494999
C	114.847000	-18.179001	47.514000
H	115.212997	-19.087000	47.980999
C	113.932999	-15.833000	46.271000
C	113.032997	-16.802000	46.705002
H	111.971001	-16.635000	46.540001

C	113.490997	-17.975000	47.335999
H	112.776001	-18.719999	47.673000
C	124.693001	-15.311000	43.786999
C	126.114998	-15.701000	43.990002
C	127.004997	-15.446000	42.916000
H	126.609001	-14.984000	42.019001
C	126.611000	-16.296000	45.174000
C	128.347000	-15.772000	43.011002
H	129.018997	-15.565000	42.182999
C	128.001007	-16.658001	45.251999
C	128.845001	-16.381001	44.178001
H	129.895004	-16.653000	44.259998
C	118.758003	-7.176000	47.661999
C	117.320999	-9.111000	46.174000
H	116.748001	-9.822000	45.590000
C	116.667999	-8.185000	46.956001
H	115.584000	-8.178000	46.991001
C	117.372002	-7.211000	47.694000
H	116.830002	-6.474000	48.265999
C	118.741997	-9.130000	46.139000
C	119.482002	-8.188000	46.931000
C	119.472000	-10.062000	45.330002
C	120.898003	-8.286000	46.965000
H	121.497002	-7.629000	47.580002
C	120.850998	-10.122000	45.384998
H	121.384003	-10.848000	44.783001
C	121.556999	-9.250000	46.235001
H	122.632004	-9.338000	46.326000
C	119.013000	-11.237000	43.201000
C	118.105003	-12.232000	42.563999
C	117.073997	-12.899000	43.264999
C	116.263000	-13.872000	42.589001
C	116.519997	-14.160000	41.249001
H	115.902000	-14.902000	40.749001
C	117.557999	-13.502000	40.558998
H	117.745003	-13.743000	39.515999
C	118.335999	-12.555000	41.203999
H	119.141998	-12.049000	40.683998
C	119.114998	-5.004000	48.866001
C	120.212997	-4.078000	49.264000

C	119.831001	-2.853000	49.867001
H	118.775002	-2.666000	50.028999
C	120.779999	-1.914000	50.233002
H	120.473000	-0.981000	50.698002
C	122.146004	-2.157000	49.993000
H	122.898003	-1.417000	50.256001
C	122.563004	-3.349000	49.403000
C	121.588997	-4.350000	49.064999
C	126.360001	-12.375000	44.972000
H	126.513000	-13.108000	44.188000
C	125.752998	-11.147000	44.640999
H	125.438004	-10.963000	43.625000
C	126.766998	-12.651000	46.257999
H	127.237000	-13.604000	46.476002
C	125.550003	-10.178000	45.611000
C	126.583000	-11.687000	47.285999
C	125.977997	-10.419000	46.966999
C	126.966003	-11.945000	48.646000
C	125.790001	-9.468000	48.005001
H	125.337997	-8.504000	47.807999
C	126.733002	-11.001000	49.631001
H	126.995003	-11.219000	50.659000
C	126.153000	-9.763000	49.299999
H	125.961998	-9.044000	50.085999
C	128.539993	-13.411000	49.876999
C	128.904007	-14.832000	50.118999
C	129.957001	-15.079000	51.035000
H	130.425003	-14.231000	51.521999
C	130.378998	-16.370001	51.301998
H	131.184998	-16.546000	52.008999
C	129.774994	-17.461000	50.646999
H	130.112000	-18.478001	50.834000
C	128.738007	-17.260000	49.738998
C	128.268005	-15.926000	49.485001
C	124.071999	-8.644000	44.297001
C	123.551003	-7.250000	44.301998
C	123.598000	-6.397000	45.430000
C	123.022003	-6.761000	43.083000
H	122.969002	-7.437000	42.236000
C	122.605003	-5.445000	42.967999

H	122.204002	-5.079000	42.026001
C	123.228996	-5.018000	45.283001
C	122.722000	-4.569000	44.063999
H	122.429001	-3.526000	43.976002
C	120.528000	-6.772000	51.597000
H	120.152000	-6.115000	50.827999
C	119.612999	-7.424000	52.445000
H	118.549004	-7.288000	52.301998
C	121.886002	-6.953000	51.730000
H	122.543999	-6.410000	51.060001
C	120.073997	-8.238000	53.463001
C	122.404999	-7.803000	52.743999
C	121.487000	-8.438000	53.652000
C	123.819000	-8.033000	52.911999
C	121.997002	-9.208000	54.731998
H	121.327003	-9.661000	55.453999
C	124.271004	-8.799000	53.973999
H	125.329002	-8.966000	54.105999
C	123.357002	-9.355000	54.889000
H	123.740997	-9.912000	55.733002
C	126.044998	-7.276000	52.042999
C	126.670998	-6.592000	50.874001
C	125.970001	-6.175000	49.717999
C	128.059998	-6.331000	50.972000
H	128.585007	-6.673000	51.855999
C	128.729004	-5.643000	49.973999
H	129.794998	-5.453000	50.061001
C	128.026001	-5.170000	48.852001
H	128.531006	-4.603000	48.074001
C	126.657997	-5.408000	48.717999
C	118.004997	-8.434000	54.830002
C	117.320000	-9.321000	55.812000
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TS_{2-w3c3}

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O	125.091003	-17.711000	48.682999
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O	113.778999	-12.127000	44.368000
O	116.690002	-12.643000	44.498001
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O	113.446999	-14.693000	45.584000
O	116.049004	-15.029000	46.006001
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O	119.935997	-10.753000	42.577999
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C	120.723000	-13.088000	49.657001
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H	121.246002	-10.369000	50.353001
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H	124.003998	-11.929000	47.062000
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H	122.890999	-12.504000	45.842999
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4-w3c3

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C	122.136002	-17.259001	46.485001
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C	121.406998	-17.974001	47.409000
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4-w3'c3

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H	115.362000	-19.309999	48.345001
C	113.992996	-16.174999	46.478001
C	113.146004	-17.233000	46.793999
H	112.100998	-17.169001	46.500999
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H	112.960999	-19.181000	47.716999
C	124.526001	-15.521000	43.993999
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C	126.867996	-15.285000	43.223000
H	126.454002	-14.746000	42.377998
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H	129.824005	-16.393000	44.508999
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H	116.693001	-6.136000	48.084000
C	118.694000	-9.237000	46.804001
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C	118.734924	-12.737676	47.397789
H	118.996857	-13.744307	47.729511
H	117.670952	-12.729464	47.139565
H	119.289055	-12.552647	46.469135
C	124.058990	-14.444416	48.277271
H	124.054466	-14.132334	47.230186
H	124.788200	-13.796960	48.787067
H	124.405922	-15.471775	48.359585
O	122.122978	-12.503791	51.425079
H	121.653236	-12.237123	52.250496
C	120.152191	-14.033275	50.359676
H	119.340034	-14.442500	49.743439
H	120.806145	-14.852670	50.655224
H	119.687340	-13.604087	51.248833
H	122.760040	-11.779716	51.202240
O	124.107803	-10.727011	50.748466
H	124.679085	-11.318215	50.229252
H	123.817734	-10.036204	50.101109
O	120.584534	-12.134399	53.670273
H	120.934616	-11.985487	54.573513
H	120.137627	-12.993878	53.760490
O	123.311699	-8.798991	48.925209
H	122.396767	-8.534292	49.119579
H	123.833961	-7.976700	49.061565

2'-w3

C	121.274002	-12.635000	50.164001
C	122.206001	-13.162000	49.071999
C	120.309998	-11.507000	49.752998
C	119.876999	-10.570000	50.867001
H	119.412003	-11.122000	51.692001
H	120.713997	-10.006000	51.289001
H	119.143997	-9.850000	50.493999
C	123.083000	-12.131000	48.389999
H	124.042999	-12.023000	48.910999
H	123.300003	-12.404000	47.355000

H	122.612000	-11.146000	48.379002
C	119.751999	-11.368000	48.535000
H	119.040001	-10.547000	48.441002
C	122.272003	-14.471000	48.784000
H	121.616997	-15.163000	49.305000
C	119.917000	-12.158000	47.266998
H	120.383003	-13.131000	47.415001
H	118.934998	-12.310000	46.801998
H	120.523003	-11.598000	46.541000
C	123.158997	-15.128000	47.765999
H	122.554001	-15.589000	46.973000
H	123.872002	-14.445000	47.299000
H	123.727997	-15.942000	48.234001
O	122.244003	-12.087000	51.191002
H	121.843002	-12.000000	52.139000
C	120.487000	-13.717000	50.909000
H	119.807999	-14.217000	50.215000
H	121.160004	-14.455000	51.355000
H	119.887001	-13.273000	51.707001
H	122.697998	-11.145000	50.943001
O	123.330002	-9.884000	50.741001
H	124.139999	-10.082000	50.238998
H	122.747002	-9.392000	50.091999
O	121.375999	-11.888000	53.606998
H	120.871002	-12.707000	53.757000
H	120.695999	-11.191000	53.606998
O	121.686996	-8.638000	48.993000
H	121.167000	-9.426000	48.743999
H	121.089996	-8.159000	49.595001

2-w3

O	122.210999	-12.425000	51.183998
H	121.799004	-12.191000	52.102001
H	122.865997	-11.660000	50.839001
O	123.799004	-10.704000	50.279999
H	124.286003	-11.266000	49.650002
H	123.260002	-10.102000	49.691002
O	121.272003	-11.953000	53.533001
H	121.975998	-12.298000	54.112999

H	120.556999	-12.611000	53.613998
O	122.321999	-9.084000	48.654999
H	121.573997	-9.679000	48.466000
C	119.640999	-11.552000	48.584000
C	120.391998	-11.591000	49.700001
C	121.218002	-12.818000	50.115002
C	122.138000	-13.454000	49.063999
C	122.620003	-12.721000	48.048000
H	119.038002	-10.654000	48.444000
C	122.541000	-14.881000	49.341999
H	121.688004	-15.564000	49.247002
H	123.319000	-15.229000	48.660000
H	122.924004	-14.987000	50.365002
C	120.278000	-13.812000	50.806999
H	119.625999	-14.270000	50.057999
H	120.832001	-14.597000	51.327000
H	119.649002	-13.290000	51.534000
C	120.278000	-10.478000	50.721001
H	119.616997	-9.690000	50.351002
H	119.860001	-10.856000	51.661999
H	121.242996	-10.023000	50.964001
C	119.463997	-12.583000	47.506001
H	118.398003	-12.671000	47.258999
H	119.977997	-12.280000	46.583000
H	119.835999	-13.572000	47.779999
C	123.592003	-13.130000	46.981998
H	124.463997	-12.462000	46.992001
H	123.952003	-14.158000	47.077999
H	123.133003	-13.022000	45.990002
H	122.269997	-11.698000	47.948002
H	121.948997	-8.456000	49.299000

TS_{2-w3}

O	122.736000	-12.486000	51.405998
H	122.342003	-12.147000	52.243999
H	123.108002	-11.695000	50.943001
O	123.900002	-10.371000	50.054001
H	124.372002	-10.879000	49.373001
H	123.210999	-9.878000	49.542999

O	121.524002	-11.711000	53.796001
H	120.771004	-12.320000	53.706001
H	121.142998	-10.850000	53.554001
O	121.959000	-8.974000	48.646000
H	121.462997	-9.686000	48.208000
C	119.703003	-11.568000	48.500000
C	120.327003	-11.820000	49.680000
C	120.997002	-13.106000	49.926998
C	121.917999	-13.675000	48.976002
C	122.598999	-12.808000	48.167999
H	119.151001	-10.628000	48.462002
C	122.183998	-15.161000	49.016998
H	121.249001	-15.728000	49.063000
H	122.737000	-15.494000	48.138000
H	122.772003	-15.424000	49.904999
C	120.420998	-13.978000	50.993999
H	119.642998	-14.588000	50.507000
H	121.157997	-14.660000	51.419998
H	119.943001	-13.406000	51.789001
C	120.202003	-10.827000	50.817001
H	119.556000	-9.995000	50.523998
H	119.777000	-11.282000	51.715000
H	121.183998	-10.428000	51.085999
C	119.540001	-12.405000	47.269001
H	118.476997	-12.437000	46.999001
H	120.060997	-11.937000	46.423000
H	119.906998	-13.427000	47.369999
C	123.660004	-13.119000	47.180000
H	124.584999	-12.604000	47.478001
H	123.869003	-14.183000	47.056999
H	123.380997	-12.691000	46.207001
H	122.389999	-11.750000	48.282001
H	121.373001	-8.717000	49.377998

4-w3

O	123.167999	-12.118000	51.410999
H	122.621002	-12.196000	52.223000
H	123.160004	-11.150000	51.227001
O	123.168999	-9.356000	50.928001

H	124.133003	-9.242000	50.905998
H	122.917000	-9.401000	49.972000
O	121.591003	-12.317000	53.762001
H	122.299004	-12.362000	54.428001
H	121.313004	-13.243000	53.665001
O	122.416000	-9.564000	48.284000
H	121.450996	-9.509000	48.387001
C	119.658997	-11.551000	48.258999
C	120.167999	-11.872000	49.486000
C	120.768997	-13.157000	49.770000
C	121.677002	-13.800000	48.874001
C	122.422997	-12.992000	48.047001
H	119.184998	-10.570000	48.203999
C	121.912003	-15.288000	49.000999
H	120.969002	-15.826000	49.133999
H	122.407997	-15.688000	48.115002
H	122.545998	-15.508000	49.868999
C	120.389999	-13.863000	51.027000
H	119.707001	-14.681000	50.749001
H	121.257004	-14.329000	51.505001
H	119.872002	-13.221000	51.737999
C	119.977997	-10.903000	50.641998
H	119.883003	-9.884000	50.254002
H	119.070999	-11.129000	51.215000
H	120.827003	-10.936000	51.326000
C	119.510002	-12.351000	47.007000
H	118.462997	-12.300000	46.679001
H	120.105003	-11.895000	46.203999
H	119.806999	-13.395000	47.103001
C	123.480003	-13.402000	47.098000
H	124.426003	-12.917000	47.380001
H	123.635002	-14.479000	47.020000
H	123.227997	-12.997000	46.105999
H	122.276001	-11.918000	48.117001
H	122.651001	-8.732000	47.838001

TS_{4-w3}

O	123.120003	-11.795000	51.764000
H	122.515999	-11.963000	52.519001

H	123.057999	-10.821000	51.645000
O	122.925003	-9.011000	51.388000
H	123.857002	-8.792000	51.553001
H	122.891998	-9.164000	50.410999
O	121.399002	-12.230000	53.977001
H	122.081001	-12.248000	54.669998
H	121.196999	-13.170000	53.834000
O	122.787003	-9.669000	48.716999
H	121.846001	-9.502000	48.535000
C	120.091003	-11.745000	48.062000
C	120.306000	-11.996000	49.418999
C	120.886002	-13.230000	49.803001
C	121.737999	-13.799000	48.828999
C	122.258003	-12.934000	47.861000
H	119.982002	-10.693000	47.791000
C	122.055000	-15.271000	48.852001
H	121.142998	-15.871000	48.754002
H	122.754997	-15.557000	48.064999
H	122.508003	-15.529000	49.817001
C	120.620003	-13.895000	51.113998
H	120.079002	-14.833000	50.928001
H	121.552002	-14.158000	51.625000
H	120.007004	-13.275000	51.770000
C	119.992996	-10.934000	50.448002
H	119.986000	-9.943000	49.983002
H	118.997002	-11.101000	50.875999
H	120.722000	-10.943000	51.261002
C	119.549004	-12.669000	47.008999
H	118.498001	-12.386000	46.853001
H	120.053001	-12.522000	46.047001
H	119.593002	-13.723000	47.285999
C	122.814003	-13.367000	46.554001
H	123.898003	-13.532000	46.654999
H	122.361000	-14.287000	46.175999
H	122.692001	-12.566000	45.817001
H	122.454002	-11.902000	48.133999
H	123.250999	-9.022000	48.158001

5-w3

O	121.950614	-9.592046	50.069251
H	121.557195	-10.099768	50.815051
H	122.712884	-9.175776	50.522579
O	124.146955	-9.662977	51.933880
H	123.372480	-10.047617	52.390001
H	124.345790	-10.355366	51.266797
O	121.652497	-11.035969	52.413084
H	120.848832	-11.111009	52.954264
H	121.839966	-11.947397	52.133735
O	123.896103	-11.598517	49.878516
H	123.128639	-10.988581	49.767606
H	124.394352	-11.494324	49.050923
C	120.103019	-11.494795	48.152166
C	120.116528	-12.249722	49.442184
C	121.127612	-13.207665	49.474901
C	121.877874	-13.088422	48.298687
C	121.393638	-11.971771	47.439831
H	120.155209	-10.423461	48.381806
C	123.020603	-13.943388	47.923385
H	122.644284	-14.708935	47.225860
H	123.780817	-13.372455	47.381807
H	123.464186	-14.454232	48.779709
C	121.439029	-14.173283	50.579751
H	121.465672	-15.200479	50.200732
H	122.428389	-13.955245	51.001110
H	120.699973	-14.127530	51.382572
C	119.123084	-11.978237	50.503822
H	118.190035	-12.500717	50.241595
H	119.441878	-12.329485	51.485887
H	118.885815	-10.910406	50.544725
C	118.787501	-11.743556	47.380451
H	117.933346	-11.398193	47.970460
H	118.798678	-11.190328	46.437710
H	118.653532	-12.807618	47.163012
C	121.315345	-12.296915	45.941470
H	120.975522	-11.416055	45.389432
H	122.301242	-12.577199	45.559013
H	120.621604	-13.119532	45.745548
H	122.155370	-11.184162	47.565920

TS4-w3'_a1

C	119.543099	-15.204535	44.728188
H	118.466891	-15.071499	44.755203
C	122.354530	-15.480623	44.587849
C	120.278988	-14.523182	43.784025
H	119.775555	-13.873296	43.078747
C	121.682696	-14.631604	43.724181
H	122.236733	-14.038490	43.011228
C	120.191844	-16.083634	45.639020
C	121.615293	-16.273697	45.535685
C	119.471203	-16.813786	46.649188
C	122.249686	-17.240020	46.362384
H	123.309817	-17.445517	46.266992
C	120.140438	-17.711324	47.465178
H	119.600467	-18.247530	48.232150
C	121.517259	-17.945064	47.289700
H	122.003971	-18.691760	47.904281
C	117.141983	-17.511984	47.165788
C	115.725065	-17.057529	47.147261
C	115.298641	-15.805723	46.645046
C	114.758398	-17.978438	47.626914
H	115.105119	-18.925085	48.026225
C	113.889966	-15.536544	46.536978
C	112.972191	-16.465708	47.021474
H	111.912314	-16.233049	46.949433
C	113.408186	-17.682631	47.579373
H	112.678505	-18.392955	47.959498
C	124.640948	-15.332573	43.590044
C	126.078250	-15.577757	43.892800
C	126.993208	-15.377335	42.827766
H	126.609120	-15.008336	41.883066
C	126.561246	-16.044110	45.139772
C	128.338714	-15.659718	42.981264
H	129.029122	-15.496318	42.157789
C	127.949652	-16.395659	45.268305
C	128.816199	-16.180963	44.198948
H	129.866077	-16.436071	44.322317
C	118.923502	-7.582710	47.425197
C	117.518015	-9.606527	46.039539

H	116.929522	-10.350991	45.517486
C	116.967501	-8.988537	47.139380
H	115.972599	-9.263137	47.469155
C	117.669267	-7.994102	47.847753
H	117.214437	-7.531060	48.710771
C	118.830797	-9.263544	45.612371
C	119.555053	-8.229963	46.304093
C	119.452725	-9.909269	44.486233
C	120.851367	-7.864935	45.843034
H	121.423643	-7.085148	46.333413
C	120.710131	-9.514526	44.062183
H	121.172905	-10.006261	43.218986
C	121.396114	-8.490016	44.743027
H	122.375012	-8.192095	44.387161
C	118.835321	-11.418800	42.591387
C	117.868557	-12.493195	42.228486
C	116.916990	-13.037740	43.124554
C	115.992493	-14.032828	42.655149
C	116.088705	-14.493840	41.343266
H	115.389947	-15.257171	41.009063
C	117.062832	-13.975153	40.468924
H	117.124339	-14.348715	39.450019
C	117.931356	-12.988659	40.901431
H	118.676680	-12.572583	40.232632
C	119.060124	-5.453956	48.711124
C	120.016925	-4.432019	49.212871
C	119.461537	-3.345952	49.936683
H	118.392935	-3.345422	50.120824
C	120.257504	-2.309370	50.389137
H	119.819558	-1.487213	50.949185
C	121.637820	-2.307728	50.111601
H	122.271776	-1.487326	50.439590
C	122.219636	-3.353459	49.399139
C	121.410834	-4.461737	48.971046
C	125.263111	-12.648054	46.103591
H	124.859867	-13.509204	45.585051
C	124.949235	-11.355142	45.639209
H	124.312810	-11.230742	44.772126
C	126.038527	-12.832700	47.226067
H	126.205783	-13.846916	47.568488

C	125.413631	-10.241933	46.312280
C	126.580843	-11.714989	47.920254
C	126.262198	-10.388594	47.461690
C	127.459043	-11.859374	49.054873
C	126.806875	-9.263914	48.138724
H	126.578572	-8.259316	47.799646
C	127.967852	-10.734775	49.684064
H	128.631765	-10.846499	50.528604
C	127.640948	-9.446547	49.217869
H	128.067027	-8.586470	49.720352
C	128.180618	-13.598312	50.700608
C	128.368717	-15.069302	50.827370
C	129.065981	-15.531934	51.970978
H	129.390913	-14.802984	52.705920
C	129.341673	-16.878579	52.135815
H	129.880350	-17.222533	53.015055
C	128.942396	-17.807769	51.156038
H	129.176985	-18.864380	51.262446
C	128.249221	-17.391858	50.019629
C	127.913045	-16.004297	49.868571
C	125.033794	-8.481340	44.614185
C	124.624575	-7.061881	44.421885
C	124.270365	-6.194888	45.481922
C	124.569379	-6.581123	43.089139
H	124.828050	-7.262113	42.285708
C	124.191434	-5.277648	42.818960
H	124.149246	-4.923007	41.792302
C	123.906011	-4.834147	45.195644
C	123.864194	-4.400722	43.872464
H	123.575512	-3.371958	43.670171
C	120.393837	-7.581861	51.228549
H	119.977720	-7.210549	50.302034
C	119.525308	-8.118479	52.198605
H	118.459135	-8.149219	52.016315
C	121.757760	-7.564491	51.418654
H	122.382423	-7.169532	50.628924
C	120.038538	-8.655801	53.362706
C	122.328880	-8.076913	52.615073
C	121.455635	-8.642821	53.609610
C	123.746904	-8.046978	52.875431

C	122.006540	-9.158048	54.813259
H	121.363729	-9.572007	55.581573
C	124.239166	-8.573854	54.060398
H	125.299727	-8.549503	54.258344
C	123.365813	-9.115140	55.021618
H	123.780754	-9.486756	55.950348
C	125.950562	-7.520483	51.818380
C	126.589891	-6.606012	50.830580
C	125.896403	-5.961444	49.785519
C	127.984271	-6.397527	50.972483
H	128.501877	-6.906657	51.778072
C	128.670453	-5.566791	50.102817
H	129.739338	-5.411478	50.224168
C	127.984343	-4.913236	49.064012
H	128.508621	-4.251865	48.378425
C	126.610138	-5.088655	48.896244
C	117.977728	-8.839994	54.747836
C	117.385219	-9.615112	55.875175
C	116.077813	-9.264094	56.295757
H	115.575318	-8.446611	55.789749
C	118.051153	-10.680284	56.524344
C	115.452147	-9.954433	57.320066
H	114.447208	-9.678997	57.629338
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2-w3_a1

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O	125.818512	-16.369795	46.142147
O	128.328766	-17.230659	46.238445
O	127.299721	-15.760345	48.587688
O	128.027374	-18.297956	48.904430
O	126.286362	-19.223633	46.813850
O	125.171974	-17.685934	48.663517
O	114.960983	-12.312115	47.035679
O	113.647507	-11.957072	44.751205
O	116.518135	-12.579286	44.634472
O	114.796211	-14.277354	43.526318
O	113.338715	-14.594999	46.012417
O	115.965904	-14.921241	46.164810
O	120.336349	-11.841126	58.524021
O	121.603951	-12.833433	56.409924
O	119.192299	-11.460409	55.796646
O	117.780258	-12.783308	57.617317
O	119.201988	-14.360141	55.598965
O	120.010307	-14.657843	58.105801
O	125.731728	-12.030060	55.836460
O	126.821625	-7.415743	53.117279
O	129.207932	-12.713259	50.831951

O	124.185547	-15.103078	42.428425
O	124.960609	-9.202306	43.204098
O	119.847977	-11.152281	42.444592
O	117.605736	-18.580183	47.538883
O	114.976051	-9.286664	49.984112
O	117.653046	-7.896838	54.078823
O	122.284035	-19.257837	51.327576
O	118.063545	-5.000729	49.168983
O	117.953171	-17.703749	53.321404
Ga	124.138062	-5.250200	47.931835
Ga	126.845505	-17.448366	47.538155
Ga	114.819855	-13.449810	45.344009
Ga	119.673904	-13.003458	57.046860
C	120.217247	-11.708094	49.879860
C	121.240952	-12.547348	49.093266
C	119.042816	-11.169080	49.037788
C	118.448990	-9.862494	49.517971
H	118.119423	-9.925739	50.563255
H	119.175606	-9.045740	49.460735
H	117.581902	-9.580082	48.917480
C	121.533363	-13.943663	49.575684
H	122.273415	-14.447958	48.952564
H	121.907219	-13.935599	50.605125
H	120.634438	-14.571903	49.587093
C	118.479324	-11.791279	47.988846
H	117.624504	-11.285851	47.540428
C	121.866035	-11.960053	48.062805
H	121.571930	-10.940876	47.820560
C	118.831017	-13.087484	47.313984
H	119.212563	-13.848988	47.996223
H	117.940552	-13.484396	46.821301
H	119.587685	-12.938671	46.534267
C	122.944550	-12.511892	47.179180
H	123.232132	-13.538548	47.417576
H	122.629532	-12.484244	46.127342
H	123.841469	-11.885304	47.251606
O	121.002419	-10.552080	50.357349
H	120.523994	-10.106309	51.081123
C	119.668983	-12.422499	51.120636
H	119.162926	-13.346943	50.842316

H	120.476784	-12.660142	51.819809
H	118.946350	-11.784037	51.637478
H	122.541290	-10.751595	50.661118
O	123.561584	-10.650672	50.675266
H	123.977577	-11.548285	50.393681
H	123.712616	-9.947116	49.932495
O	124.592735	-12.950502	50.040527
H	125.472878	-13.023417	50.451317
H	124.063690	-13.626843	50.498772
O	123.546417	-8.853952	48.838631
H	122.624847	-8.564951	48.966614
H	124.088905	-8.050992	49.030334

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