Toward Understanding CB[7]-Based Supramolecular Diels-Alder Catalysis

Supporting Information

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CALCULATION OF GIBBS FREE ENERGIES

The reported relative stabilities are obtained from Gibbs free energies defined as

$G = E_0' + (G_0 - E_0) + (G_{sol} - E_0)$

where E_0' and E_0 are electronic energies computed with the 6-311++G(3df,3pd) and the 6-31G* basis sets, G_0 and G_{sol} denote gas-phase and solution-phase Gibbs free energies obtained from B3LYP-D3/6-31G* calculations.

ESTIMATION OF pK_a

We used Epik from the Schrödinger Suite to obtain an empirical estimate for the basicity of the amine moiety of substrates, predicting was 9.4±1. Based on the most stable conformers of **1a** with and without protonation, one can also estimate the pK_a:

$pK_a = \log(\exp(-\Delta G/RT))$

where $\Delta G = G(\mathbf{1a}H^+) - G(\mathbf{1a}) - G(H^+)$ is the reaction change in free energies. The solvated proton's free energy is taken from (D. Tissandier et al., 1998) as a value of -263.98 kcal/mol. Using this approach, the obtained pK_a is 10.8. Considering the experimental pH of 7.4, and assuming that the pK_a of the four substrates are similar, they are protonated under reaction conditions.

TESTING BASIS SETS AND FUNCTIONALS IN DFT CALCULATIONS

For benchmark purposes to evaluate how different functionals perform at different basis sets, we carried out calculations for the following models:

- Substrates **1a-d** in implicit solvent (RS, TS, PS)
- Substrate **1a** with a single explicit water (+implicit solvent) (RS, TS)
- Substrate **1a** complexed with CB[7] in implicit water (RS, TS)
- Substrates **1a-d** complexed with CB[7], with a single explicit water (+implicit solvent) (RS, TS, PS)

Results are reported in Tables S1 and S2.

Basis sets

We tested the variation in electronic energies (E_0') with a series of Pople basis sets using B3LYP hybrid functional. The optimizations, thermochemical and implicit solvent corrections were added in all cases based on the B3LYP-D3/6-31G* calculations. The obtained barriers are summarized in Table S1.

Table S1. Reaction free energy barriers ($\Delta G^‡$) in kcal/mol based on electronic energies (E_0') calculated with different basis sets.

model	**1a**	**1b**	**1c**	**1d**	**1a**+water	**1a**+CB[7]	**1a**+CB[7]	**1b**+CB[7]	**1c**+CB[7]	**1d**+CB[7]
experimental	28.7	28.6	26.8	26.7	28.7	23.6	23.6	23.0	22.5	22.7
6-311++G(3df,3pd)	28.6	29.5	26.9	26.9	28.4	28.6	24.5	26.6	22.2	21.7
6-31G*	26.2	27.2	24.5	23.8	25.9	25.5	22.7	23.5	19.5	19.7
6-31G**	26.3	27.3	24.6	23.8	26.1	25.8	22.9	23.7	19.7	19.9

6-31+G*	26.8	27.7	24.9	24.5	26.5	26.0	22.6	24.4	19.7	20.0
6-31+G**	27.0	27.8	25.0	24.6	26.8	26.4	23.0	24.7	20.0	20.3
6-31++G*	26.8	27.8	24.9	24.7	26.5	26.1	22.7	24.5	19.7	20.0
6-31++G**	27.1	27.9	25.1	24.8	26.8	26.5	22.9	24.8	20.0	20.2

Functionals and semiempiricals

We also tested a few Minnesota functionals (Zhao and Truhlar, 2008; Peverati and Truhlar, 2011a, 2011b, 2012) available in Gaussian 09 to calculate electronic energies, using the 6-31G** basis. They produce slightly lower barriers in general, although the behavior of **1b** with CB[7] is more correctly described (Table S2). In an attempt to speed up calculations, we expanded the benchmark to semiempirical methods am1 and pm6.

Table S2. Reaction free energy barriers ($\Delta G^{\ddagger}$) in kcal/mol based on electronic energies (E_0') calculated with different DFT functionals or semiempirical methods.

model	**1a**	**1b**	**1c**	**1d**	**1a**+water	**1a**+CB[7]	**1a**+CB[7]	**1b**+CB[7]	**1c**+CB[7]	**1d**+CB[7]
experimental	28.7	28.6	26.8	26.7	28.7	23.6	23.6	23.0	22.5	22.7
M06-2X	24.6	25.1	22.9	22.2	24.5	24.8	22.4	21.8	20.0	20.3
M11L	23.0	24.0	21.8	20.9	23.1	23.2	21.9	19.9	18.2	18.1
MN12L	25.4	26.3	24.0	23.2	24.9	26.2	24.7	22.6	21.9	22.2
M11	24.0	24.5	22.3	21.5	23.7	24.6	22.0	21.1	20.2	20.5
MN12SX	24.4	25.6	23.0	22.2	25.4	25.4	24.1	22.4	20.7	20.9
am1	33.7	36.3	34.0	35.1	31.9	28.2	23.1	32.8	25.3	24.9
pm6	30.7	32.4	29.3	29.5	31.0	32.0	23.3	32.2	24.8	25.0

CALCULATIONS WITH 2 WATER MOLECULES

We tested the effect of a few explicit water molecules on the barrier of the cycloaddition of **1a**. The issue with adding a defined number of explicit water molecules is that the number of possible arrangements in geometry is quickly increasing. We have tested several possible conformers and have a standard deviation of 3.1 kcal/mol for the barrier depending on the water placement. The best conformer has a barrier of 26.0 kcal/mol. The ambiguity is similar adding further water molecules to the CB[7] caged system, thus we decided to eliminate the problem using a water box in QM/MM calculations as discussed in the main text.

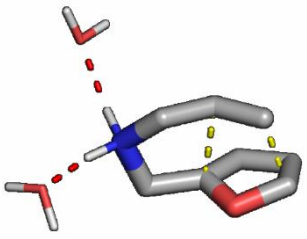

Figure S1. Example TS of **1a** accompanied by two water molecules.

STRUCTURES WITHOUT EXPLICIT WATER

The complexation of the substrates (studied on the example of **1a**) is driven by the H-bonding interaction between the protonated amine and the carbonyl moieties of the CB[7], slightly turning the substrate in the TS as depicted in Figure S1.

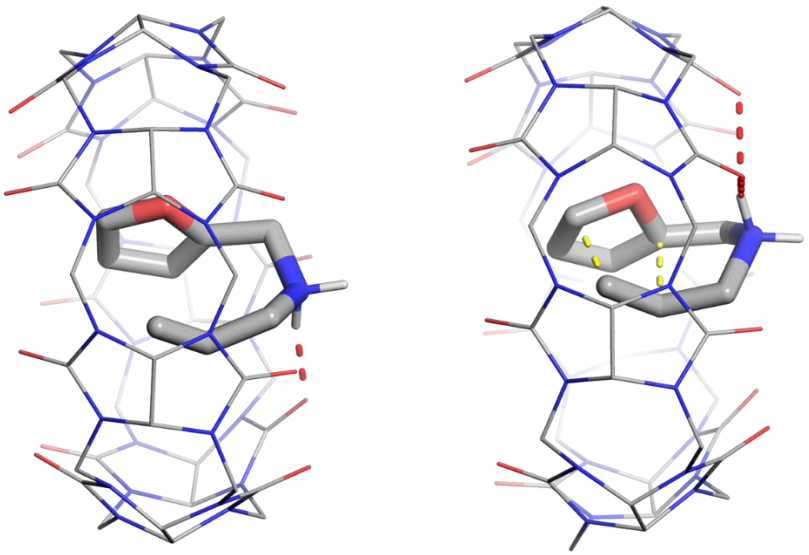

Figure S2. RS (left) and TS (right) of **1a** in complex with CB[7], without explicit water. Non-polar hydrogens are hidden for clarity.

QM/MM RESULTS OF **1b**

The catalytic effect on different substrates are reproduced satisfactorily by DFT as shown in Table 2, apart from **1b**, for which the calculated effect (2.9 kcal/mol) underestimates the experimental value (6.1 kcal/mol). We employed the same QM/MM minimization approach as discussed in the manuscript (Figure 4). The effect of CB[7] is again more precisely reproduced by the QM/MM calculations (6.0 kcal/mol, Figure S3).

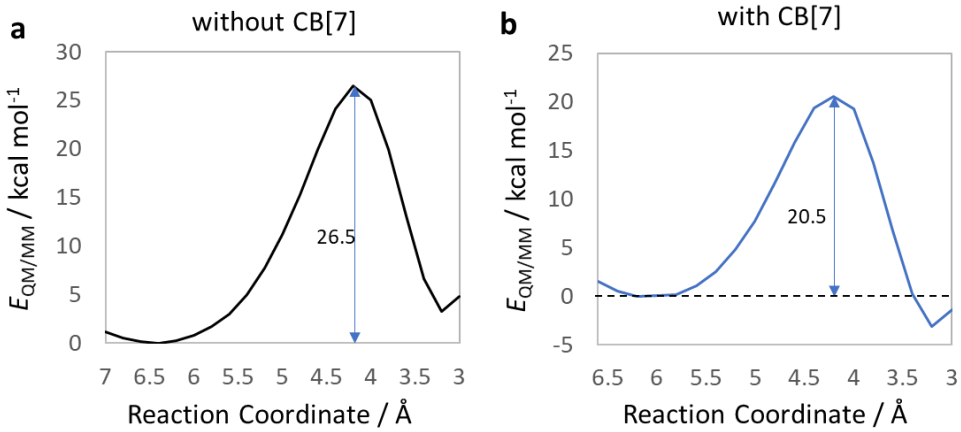

Figure S3. Results of QM/MM potential energy scans **a)** without CB[7] and **b)** with CB[7] for the reaction of **1b**. The reaction coordinate is the sum of the distances of C-C inner and C-C outer bonds. Reaction barriers are shown in kcal/mol, indicated by vertical arrows in the profiles.

RESULTS FOR NITRO-FURILAMINE **1e**

We performed calculations in implicit solvent and QM/MM calculations for an additional substrate **1e** featuring a nitro group in the 5 position of the furan ring.

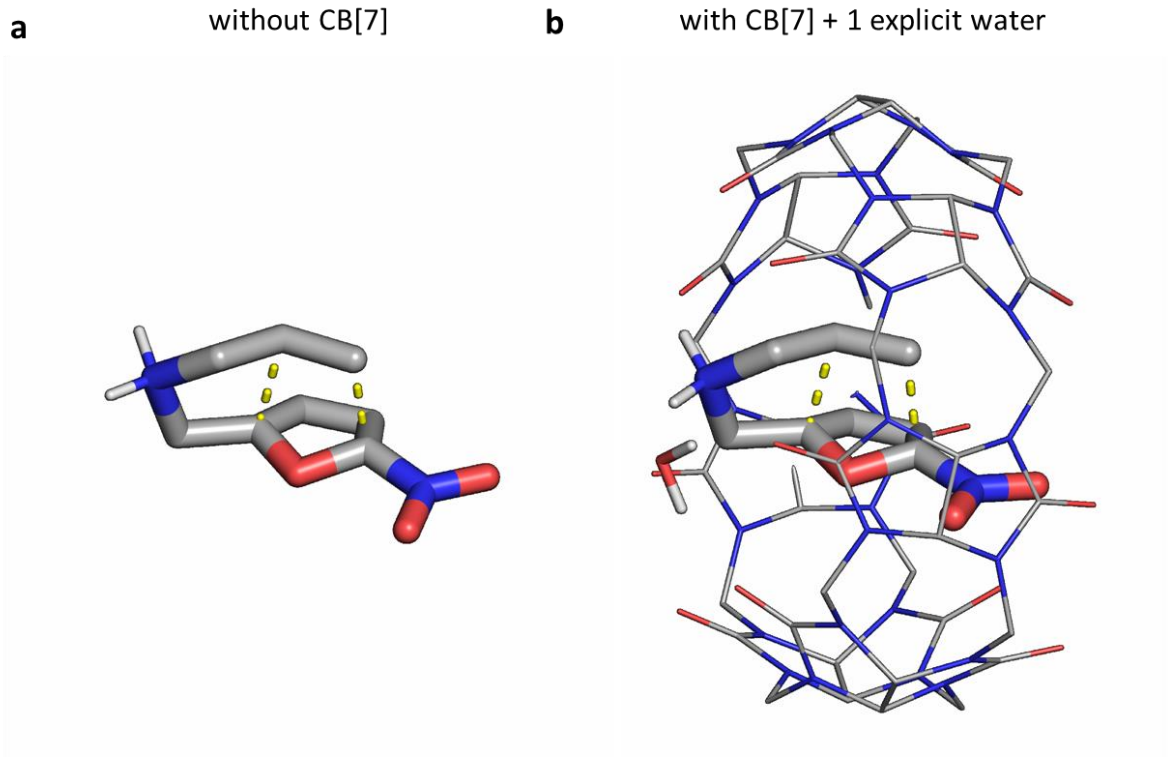

Figure S4. TS geometries of the Diels-Alder reaction of substrate **1e a)** without CB[7] and **b)** with CB[7] and one explicit water molecule. Non-polar hydrogens are hidden for clarity. Forming bonds are depicted with yellow dashes. Barriers are 25.5 and 21.4 kcal/mol, respectively.

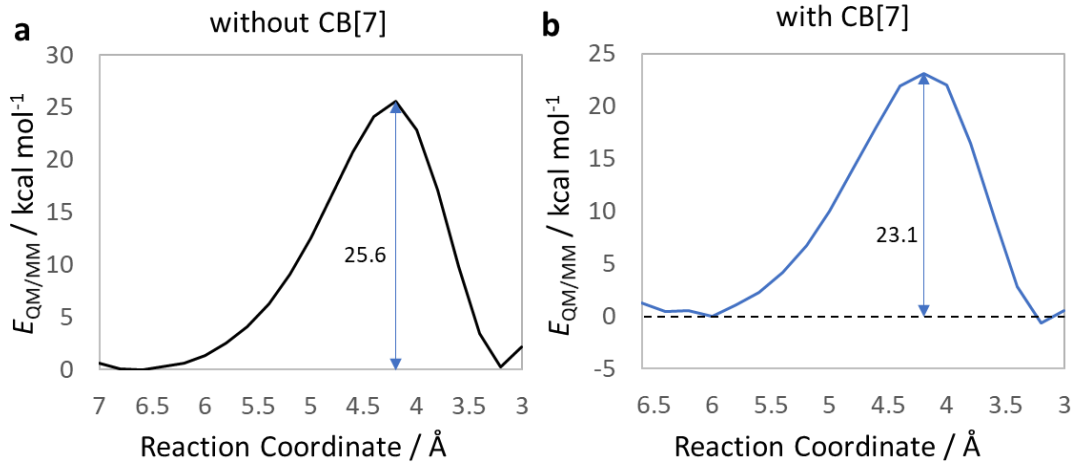

Figure S5. Results of QM/MM potential energy scans **a)** without CB[7] and **b)** with CB[7] for the reaction of **1e**. The reaction coordinate is the sum of the distances of C-C inner and C-C outer bonds. Reaction barriers are shown in kcal/mol, indicated by vertical arrows in the profiles.

POINT CHARGE MAPPING

We carried out the same analysis of the influence of a point charge with a +1 probe. The results are largely complementary as one would expect, however there are regions (i.e. near the furan ring) where both charges are unfavorable, which illustrates the reactions preference for the hydrophobic cavity.

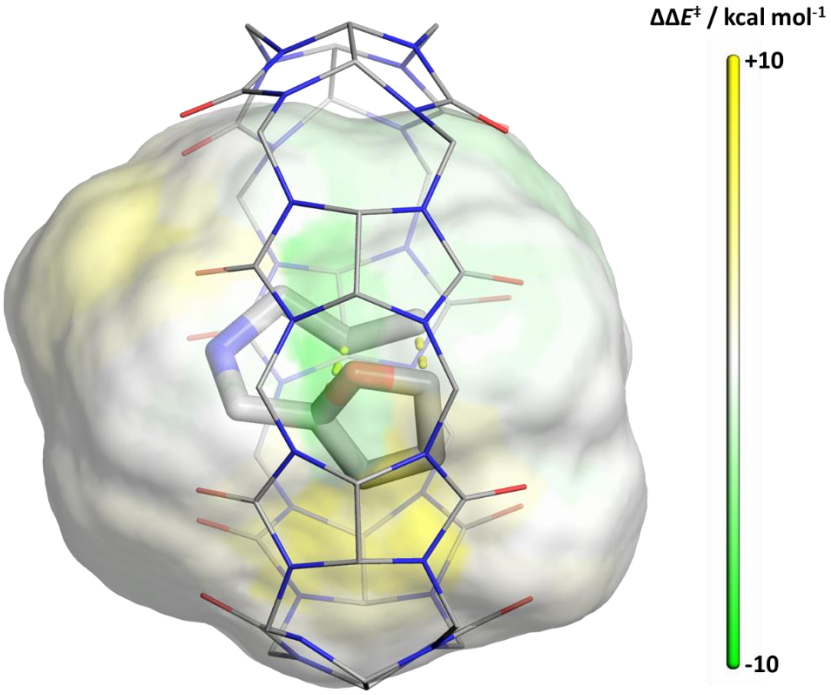

Figure S6. Map of reaction barrier changes upon the addition of a probe +1 point charge (calculated at B3LYP/6-31+G*). CB[7] is overlaid with the results to highlight the area shielded from the polar environment.

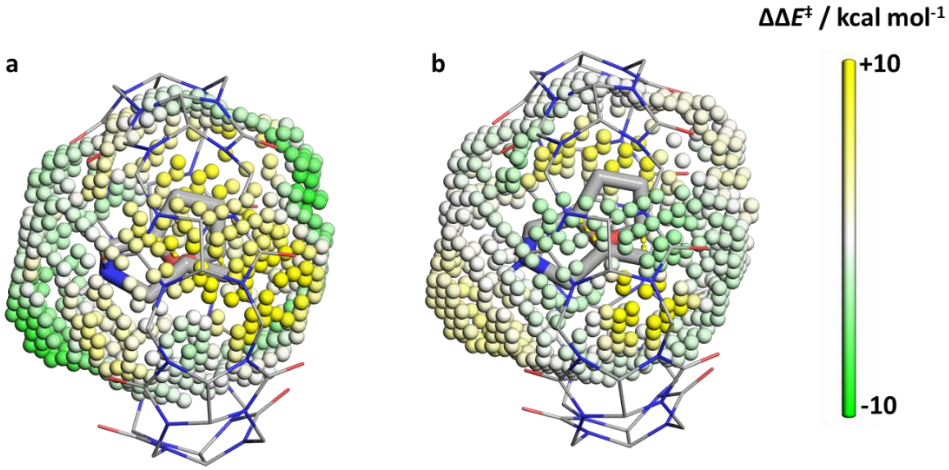

Figure S7. Representation of the point charge analysis by displaying each node as a sphere with a probe charge of **a)** -1 **b)** +1.

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Zhao, Y., and Truhlar, D. G. (2008). The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: Two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.* 120, 215–241. doi:10.1007/s00214-007-0310-x.

DATA

Table S3. Raw energetic data calculated at B3LYP-D3/6-31G*//B3LYP-D3/6-311++G(3df,3pd) level of theory. Values are in Hartree.

	E_0	G_0	G_{sol}	E_0'
w/o CB w/o water				
1a RS	-441.783493	-441.626896	-441.875423	-441.939361
1a TS	-441.742324	-441.580789	-441.838680	-441.894364
1a PS	-441.781740	-441.616551	-441.883425	-441.931282
1b RS	-481.112113	-480.930265	-481.201472	-481.280660
1b TS	-481.069805	-480.882408	-481.163615	-481.234821
1b PS	-481.108329	-480.917288	-481.207634	-481.271060
1c RS	-901.372609	-901.228060	-901.466793	-901.561646
1c TS	-901.332037	-901.182372	-901.432841	-901.517347
1c PS	-901.373995	-901.220892	-901.481829	-901.556389
1d RS	-3012.881598	-3012.738601	-3012.976106	-3015.480004
1d TS	-3012.842072	-3012.694207	-3012.943094	-3015.435526
1d PS	-3012.883935	-3012.732597	-3012.991528	-3015.474631
w/o CB with water				
1a+wat RS	-518.220909	-518.045723	-518.309810	-518.425152
1a+wat TS	-518.183414	-518.003577	-518.273141	-518.383776
with CB w/o water				
1a+CB[7] RS	-4654.400205	-4653.328430	-4654.621921	-4655.962894
1a+CB[7] TS	-4654.359058	-4653.286451	-4654.582168	-4655.916738
with CB with water				
1a+CB[7]+wat RS	-4730.849234	-4729.752425	-4731.065875	-4732.453861
1a+CB[7]+wat TS	-4730.811326	-4729.713778	-4731.030474	-4732.412972
1a+CB[7]+wat PS	-4730.852029	-4729.750588	-4731.073261	-4732.452141
1b+CB[7]+wat RS	-4770.179062	-4769.055765	-4770.399903	-4771.798595
1b+CB[7]+wat TS	-4770.143669	-4769.017200	-4770.365566	-4771.758373
1b+CB[7]+wat PS	-4770.182021	-4769.051748	-4770.407950	-4771.794350
1c+CB[7]+wat RS	-5190.441926	-5189.354741	-5190.661327	-5192.082641
1c+CB[7]+wat TS	-5190.407293	-5189.319482	-5190.630807	-5192.043700
1c+CB[7]+wat PS	-5190.449696	-5189.357676	-5190.678635	-5192.083015
1d+CB[7]+wat RS	-7301.961269	-7300.874265	-7302.176570	-7305.999702
1d+CB[7]+wat TS	-7301.926631	-7300.840650	-7302.144101	-7305.962002
1d+CB[7]+wat PS	-7301.968637	-7300.877411	-7302.190430	-7306.000641

Table S4. Raw energetic data calculated with B3LYP-D3 and the selected basis set. Values are in Hartree.

basis set	6-31G**	6-31+G*	6-31+G**	6-31++G*	6-31++G**
w/o CB w/o water					
1a RS	-441.804121	-441.794630	-441.814837	-441.795061	-441.815239
1a TS	-441.762661	-441.752483	-441.772259	-441.752850	-441.772587
1a PS	-441.801704	-441.792063	-441.811402	-441.792416	-441.811703
1b RS	-481.135326	-481.123894	-481.146550	-481.124330	-481.146959
1b TS	-481.092933	-481.080845	-481.103274	-481.081182	-481.103580
1b PS	-481.131193	-481.119596	-481.141682	-481.119936	-481.141986
1c RS	-901.391590	-901.384053	-901.402606	-901.384461	-901.402993
1c TS	-901.350883	-901.342890	-901.361197	-901.343229	-901.361504
1c PS	-901.392565	-901.385026	-901.403015	-901.385364	-901.403314
1d RS	-3012.900608	-3012.917025	-3012.935594	-3012.918756	-3012.937301

1d TS	-3012.861035	-3012.876379	-3012.894791	-3012.877761	-3012.896140
1d PS	-3012.902629	-3012.918456	-3012.936551	-3012.919781	-3012.937839
w/o CB w/ water					
1a+wat RS	-518.252416	-518.241052	-518.272524	-518.241483	-518.272872
1a+wat TS	-518.214637	-518.202667	-518.233619	-518.203102	-518.233992
w/ CB w/o water					
1a+CB[7] RS	-4654.476145	-4654.520165	-4654.594163	-4654.521838	-4654.595844
1a+CB[7] TS	-4654.434486	-4654.478182	-4654.551516	-4654.479674	-4654.553041
w/ CB w/ water					
1a+CB[7]+wat RS	-4730.935775	-4730.973778	-4731.058035	-4730.975451	-4731.059574
1a+CB[7]+wat TS	-4730.897532	-4730.935926	-4731.019669	-4730.937586	-4731.021331
1a+CB[7]+wat PS	-4730.937823	-4730.977682	-4731.060998	-4730.979251	-4731.062575
1b+CB[7]+wat RS	-4770.268271	-4770.305674	-4770.392271	-4770.307547	-4770.393977
1b+CB[7]+wat TS	-4770.232598	-4770.268943	-4770.354992	-4770.270592	-4770.356650
1b+CB[7]+wat PS	-4770.270569	-4770.307566	-4770.393175	-4770.309207	-4770.394826
1c+CB[7]+wat RS	-5190.526821	-5190.568475	-5190.650855	-5190.570113	-5190.652497
1c+CB[7]+wat TS	-5190.491877	-5190.533640	-5190.615555	-5190.535250	-5190.617169
1c+CB[7]+wat PS	-5190.533895	-5190.576254	-5190.657732	-5190.577833	-5190.659195
1d+CB[7]+wat RS	-7302.046323	-7302.124814	-7302.207416	-7302.127873	-7302.210509
1d+CB[7]+wat TS	-7302.011429	-7302.089710	-7302.171874	-7302.092885	-7302.175061
1d+CB[7]+wat PS	-7302.053021	-7302.132454	-7302.214202	-7302.135512	-7302.217272

Table S5. Raw energetic data calculated with different functionals using the 6-31G** basis set. Values are in Hartree.

method	M06-2X	M11L	MN12L	M11	MN12SX
w/o CB w/o water					
1a RS	-441.583045	-441.648586	-441.411831	-441.523751	-441.339749
1a TS	-441.544391	-441.612513	-441.371881	-441.486043	-441.301311
1a PS	-441.591465	-441.659567	-441.420872	-441.534368	-441.348115
1b RS	-480.889140	-480.968463	-480.700838	-480.822427	-480.618485
1b TS	-480.850246	-480.931322	-480.659976	-480.784495	-480.578815
1b PS	-480.896367	-480.977384	-480.707667	-480.831521	-480.624213
1c RS	-901.143071	-901.194084	-900.946376	-901.082553	-900.852297
1c TS	-901.105122	-901.157826	-900.906690	-901.045510	-900.814198
1c PS	-901.155238	-901.207324	-900.958337	-901.096725	-900.863639
1d RS	-3012.754601	-3012.382400	-3011.879355	-3012.329678	-3011.392511
1d TS	-3012.717634	-3012.347458	-3011.840803	-3012.293753	-3011.355477
1d PS	-3012.767611	-3012.397323	-3011.892433	-3012.345050	-3011.404734
w/o CB w/ water					
1a+wat RS	-517.994796	-518.070073	-517.711185	-517.943454	-517.800865
1a+wat TS	-517.959521	-518.037051	-517.675256	-517.909517	-517.764138
w/ CB w/o water					
1a+CB[7] RS	-4652.598610	-4652.793412	-4650.256256	-4652.139819	-4650.857970
1a+CB[7] TS	-4652.558481	-4652.755804	-4650.213909	-4652.100050	-4650.816919
w/ CB w/ water					
1a+CB[7]+wat RS	-4729.022762	-4729.220336	-4726.638735	-4728.571392	-4727.255970
1a+CB[7]+wat TS	-4728.985341	-4729.183661	-4726.597670	-4728.534499	-4727.215873
1a+CB[7]+wat PS	-4729.032423	-4729.230625	-4726.644459	-4728.581924	-4727.264747
1b+CB[7]+wat RS	-4768.326280	-4768.536731	-4765.909432	-4767.865093	-4766.540408
1b+CB[7]+wat TS	-4768.293718	-4768.507202	-4765.875529	-4767.833595	-4766.506839
1b+CB[7]+wat PS	-4768.338433	-4768.552993	-4765.919390	-4767.878425	-4766.553517
1c+CB[7]+wat RS	-5188.584971	-5188.767645	-5186.150993	-5188.131762	-5186.791922
1c+CB[7]+wat TS	-5188.549583	-5188.735092	-5186.112613	-5188.096111	-5186.755391

1c+CB[7]+wat PS	-5188.598911	-5188.784909	-5186.161033	-5188.145821	-5186.806611
1d+CB[7]+wat RS	-7300.208024	-7299.966910	-7296.704779	-7299.390542	-7297.736514
1d+CB[7]+wat TS	-7300.172458	-7299.934814	-7296.666187	-7299.354699	-7297.700088
1d+CB[7]+wat PS	-7300.221191	-7299.984613	-7296.714266	-7299.404223	-7297.751032

Table S6. Raw energetic data calculated with semiempirical methods am1 and pm6. Values are in Hartree.

method	am1	pm6
w/o CB w/o water		
1a RS	0.281213	0.244996
1a TS	0.334477	0.293473
1a PS	0.278226	0.230915
1b RS	0.269233	0.225270
1b TS	0.326018	0.275743
1b PS	0.271298	0.213612
1c RS	0.282161	0.240963
1c TS	0.337849	0.289150
1c PS	0.282475	0.224287
1d RS	0.300861	0.258740
1d TS	0.358517	0.307464
1d PS	0.304281	0.244212
w/o CB w/ water		
1a+wat RS	0.178317	0.142831
1a+wat TS	0.225392	0.188351
w/ CB w/o water		
1a+CB[7] RS	0.545954	-0.229719
1a+CB[7] TS	0.591509	-0.178085
w/ CB w/ water		
1a+CB[7]+wat RS	0.439981	-0.330705
1a+CB[7]+wat TS	0.478538	-0.291880
1a+CB[7]+wat PS	0.427716	-0.355254
1b+CB[7]+wat RS	0.429918	-0.351822
1b+CB[7]+wat TS	0.480140	-0.302570
1b+CB[7]+wat PS	0.428370	-0.363592
1c+CB[7]+wat RS	0.447677	-0.334771
1c+CB[7]+wat TS	0.491412	-0.291728
1c+CB[7]+wat PS	0.439896	-0.356239
1d+CB[7]+wat RS	0.473699	-0.319112
1d+CB[7]+wat TS	0.516646	-0.276100
1d+CB[7]+wat PS	0.468636	-0.338448

Table S7. QM/MM energetic data calculated in reaction coordinate scans of **1a**, last iteration.

coordinate	w/o CB[7]	w/ CB[7]
7.0	-300246.682	
6.8	-300247.129	
6.6	-300247.433	-300079.834
6.4	-300247.626	-300080.953
6.2	-300247.365	-300081.685
6.0	-300247.006	-300082.013
5.8	-300246.096	-300081.682
5.6	-300244.641	-300080.926
5.4	-300242.688	-300079.426

5.2	-300240.023	-300077.173
5.0	-300236.622	-300074.039
4.8	-300232.378	-300070.206
4.6	-300227.766	-300066.243
4.4	-300223.751	-300062.712
4.2	-300221.743	-300061.197
4.0	-300223.421	-300063.06
3.8	-300228.432	-300068.064
3.6	-300235.282	-300075.065
3.4	-300242.01	-300081.755
3.2	-300245.899	-300085.964
3.0	-300243.856	-300084.384

Table S8. QM/MM energetic data calculated in reaction coordinate scans of **1b**, last iteration.

coordinate	**w/o CB[7]**	**w/ CB[7]**
7.0	-325097.570	
6.8	-325098.259	
6.6	-325098.586	-325033.123
6.4	-325098.734	-325034.083
6.2	-325098.514	-325034.591
6.0	-325097.922	-325034.555
5.8	-325097.005	-325034.413
5.6	-325095.727	-325033.562
5.4	-325093.753	-325032.077
5.2	-325091.056	-325029.781
5.0	-325087.569	-325026.863
4.8	-325083.496	-325022.905
4.6	-325078.784	-325018.756
4.4	-325074.608	-325015.185
4.2	-325072.250	-325014.067
4.0	-325073.690	-325015.283
3.8	-325078.842	-325020.879
3.6	-325085.650	-325027.854
3.4	-325092.113	-325034.362
3.2	-325095.524	-325037.764
3.0	-325093.972	-325035.987

CARTESIAN COORDINATES

```
  22
1a RS
 C 0.936356 -0.140954 0.547934
 C 1.369108 1.152208 0.499375
 C 2.598245 1.136128 -0.235856
 C 2.813779 -0.160141 -0.592888
 O 1.809430 -0.960047 -0.123894
 H 0.885620 2.009191 0.948423
 H 3.234396 1.979769 -0.461773
 H 3.592175 -0.661619 -1.147888
 C -0.238350 -0.817096 1.128347
 H 0.030716 -1.648780 1.787385
 H -0.883319 -0.116592 1.659065
 N -1.086467 -1.445777 0.007838
 H -0.463683 -2.053716 -0.538831
 C -1.758854 -0.438917 -0.932995
 H -0.952917 0.186999 -1.321220
 H -2.177814 -1.035303 -1.749467
 C -2.802035 0.355573 -0.209886
 C -2.678861 1.662636 0.030740
 H -1.800679 2.223472 -0.282103
 H -3.465002 2.223746 0.526796
 H -3.703769 -0.177951 0.089474
 H -1.803076 -2.052726 0.423523
  22
1a TS
 C 0.074208 -0.877904 0.056208
 C 1.104470 -1.224068 -0.858954
 C 2.206352 -0.507936 -0.457515
 C 1.793174 0.260052 0.678262
 O 0.640378 -0.325784 1.174116
 H 0.985084 -1.822206 -1.752849
 H 3.158409 -0.416060 -0.962361
 H 2.442240 0.685129 1.434388
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 H -1.537403 -2.263596 -0.357286
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 N -2.299594 -0.276599 -0.124159
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 H 0.667911 2.345530 0.789007
 H 1.473811 2.235095 -0.837269
 H -0.443539 1.042942 -1.751251
 H -2.540987 -0.380489 -1.115681
  22
1a PS
 C -0.009856 -0.641965 -0.024658
 C 1.185635 -1.310383 -0.675540
 C 2.232895 -0.590170 -0.260751
 C 1.666079 0.498752 0.641080
 O 0.517221 -0.165466 1.218208
 H 1.148539 -2.114365 -1.400105
 H 3.268648 -0.671946 -0.566341
 H 2.308714 0.904746 1.420197
 C -1.345729 -1.319783 0.185975
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 C 0.929742 -0.141172 0.517381
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 H -3.721834 -0.185953 0.103964
 H -1.810011 -2.054740 0.383290
 C 3.904385 -0.804587 -1.402018
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 H 4.421683 -1.549053 -0.785929
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 C -1.300942 -1.391768 0.246942
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 H -3.181081 -0.380021 0.421238
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 C -0.387065 1.137362 -0.674001
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 O 0.507189 -0.167812 1.219915
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1d TS
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 C 2.214263 -0.505140 -0.445061
 C 1.791216 0.262916 0.689603
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 H -2.560696 -0.383420 -1.109333
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  22
1d PS
 C -0.014305 -0.642568 -0.030732
 C 1.184696 -1.315487 -0.671864
 C 2.231205 -0.596930 -0.255660
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 H -2.232777 1.840705 -0.681061
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 H -2.949134 -0.342547 -0.810774
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 C -0.747461 0.650208 -0.755894
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 H 0.370208 1.322761 -2.443988
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H 0.864690 -2.773486 -0.550117
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H -0.367867 -2.906889 1.555906
O 4.030104 0.565036 -2.367103
H 4.494770 0.261344 -3.162360
H 4.551731 1.309942 -2.030370
25
1a+wat TS
C -0.926671 -1.168693 -0.302742
C 0.512007 -0.832984 -0.118692
H -1.383688 -1.477003 0.639647
H -1.089690 -1.940627 -1.056196
C 1.687101 -1.252486 -0.798715
C 2.735648 -0.735817 -0.075473
H 1.719103 -1.751098 -1.758631
H 3.785944 -0.739416 -0.333437
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O 0.852211 -0.461362 1.157306
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N -1.679025 0.089901 -0.747517
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H -1.732553 0.103650 -1.770047
H -1.057456 1.401108 0.791943
H -1.504362 2.188703 -0.745285
C 0.484174 1.268183 -0.704722
C 1.534361 1.715649 0.125561
H 0.658776 1.236549 -1.778609
H 1.279133 2.211579 1.059609
H 2.430789 2.105815 -0.345575
O -4.030329 -0.303300 0.638016
H -4.787556 -0.844701 0.365103
H -4.368389 0.276219 1.338546
148
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C -1.299946 4.371891 -1.824631
N -0.210243 4.914874 -1.153146
O -1.269558 3.769802 -2.882504
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N 2.314510 4.698976 1.106833
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N -2.130358 4.463261 1.318602
O -0.671373 3.965536 3.064610
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H -4.023564 4.924716 2.061276
H -3.049523 3.758023 3.014014
C -4.237279 1.768462 2.124564
N -5.199426 1.035950 1.436957
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C -5.670153 1.693202 0.247360
N -5.230633 1.128412 -1.013134
H -6.766805 1.771603 0.261769
C -5.862516 -0.003471 -1.643532
N -5.353140 -1.294527 -1.248274
H -5.694649 0.091174 -2.718054
H -6.939796 0.015275 -1.432567
C -5.664721 -1.964944 -0.006359
C -4.904997 -3.327382 -0.140101
H -6.752419 -2.074617 0.098263
H -5.562366 -4.184185 -0.341504
N -4.251374 -3.473755 1.132100
C -3.632334 -4.683243 1.626038
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C -1.177698 -4.706336 2.011753
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H9 1.356556 2.304600 -0.801042
H10 -0.521576 1.051771 -1.715752
H11 -2.604190 -0.421317 -1.146689
H12 2.371468 0.802253 1.432721
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noCBpath coordinate 4.20
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C2 1.087528 -1.153265 -0.859364
C3 2.175575 -0.413088 -0.455447
C4 1.748995 0.349554 0.677895
O 0.616543 -0.287216 1.173958
H1 0.986207 -1.762751 -1.749716
H2 3.125382 -0.300277 -0.963726
C5 -1.334797 -1.380627 0.241065
H3 -1.537248 -2.254975 -0.380366
H4 -1.513462 -1.642856 1.286308
N -2.351712 -0.305671 -0.138604
H5 -3.250431 -0.444389 0.380318
C6 -1.788567 1.095638 0.065092
H6 -2.545382 1.783085 -0.326660
H7 -1.697736 1.259635 1.141977
C7 -0.466049 1.173240 -0.642511
C8 0.659492 1.852886 -0.114545
H8 0.546546 2.402068 0.820100
H9 1.359265 2.313065 -0.807273
H10 -0.523328 1.050996 -1.723400
H11 -2.590263 -0.423210 -1.152439
H12 2.371799 0.804039 1.441682
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noCBpath coordinate 4.41
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C2 1.066054 -1.139263 -0.859855
C3 2.176886 -0.408290 -0.444441
C4 1.780988 0.296455 0.704493
O 0.613637 -0.266726 1.166777
H1 0.947253 -1.717028 -1.766276
H2 3.120245 -0.289151 -0.960952
C5 -1.329080 -1.379672 0.252327
H3 -1.529743 -2.262172 -0.357742
H4 -1.516669 -1.626962 1.299708
N -2.337808 -0.307878 -0.148684
H5 -3.242811 -0.449733 0.357653
C6 -1.791499 1.097188 0.063349
H6 -2.564694 1.773464 -0.317245
H7 -1.694962 1.256568 1.139383
C7 -0.478585 1.222631 -0.656068

C8 0.617645 1.901535 -0.144761
H8 0.561495 2.383893 0.828632
H9 1.364493 2.311602 -0.817872
H10 -0.528741 1.054588 -1.730674
H11 -2.562235 -0.427763 -1.165517
H12 2.372945 0.802751 1.458044
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noCBpath coordinate 4.62
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C2 1.060129 -1.142423 -0.858664
C3 2.184424 -0.412374 -0.440645
C4 1.809645 0.251055 0.722762
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H2 3.122554 -0.287397 -0.963315
C5 -1.325909 -1.382574 0.258031
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C8 0.582388 1.949852 -0.162669
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H10 -0.534109 1.068898 -1.735204
H11 -2.550823 -0.427699 -1.169541
H12 2.379180 0.797294 1.462221
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C2 1.053893 -1.148043 -0.858060
C3 2.192665 -0.424471 -0.436631
C4 1.836608 0.210063 0.736054
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H1 0.934162 -1.716149 -1.771595
H2 3.131905 -0.310838 -0.959265
C5 -1.321247 -1.380928 0.269167
H3 -1.540106 -2.270981 -0.323912
H4 -1.527496 -1.605437 1.318782
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H11 -2.522072 -0.426319 -1.178248
H12 2.398235 0.770286 1.472582
22
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C2 1.054605 -1.158926 -0.855492
C3 2.201116 -0.440037 -0.432134
C4 1.864036 0.167578 0.752403
O 0.632912 -0.262514 1.153751

H1 0.930684 -1.720456 -1.772609
H2 3.138009 -0.322381 -0.961452
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H3 -1.545754 -2.273356 -0.312329
H4 -1.533284 -1.597591 1.325150
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H5 -3.216332 -0.448594 0.326186
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H7 -1.698348 1.265727 1.141348
C7 -0.540499 1.376311 -0.690184
C8 0.518426 2.048302 -0.188456
H8 0.537444 2.415514 0.833898
H9 1.339262 2.358901 -0.826647
H10 -0.568452 1.143691 -1.753124
H11 -2.512083 -0.425384 -1.182163
H12 2.410219 0.755850 1.476537
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C2 1.053536 -1.174402 -0.852980
C3 2.213021 -0.468536 -0.428656
C4 1.892371 0.123245 0.764860
O 0.646623 -0.270832 1.154436
H1 0.925126 -1.735642 -1.769238
H2 3.151427 -0.366172 -0.957681
C5 -1.313597 -1.379364 0.287397
H3 -1.552438 -2.274797 -0.290933
H4 -1.535246 -1.580786 1.338262
N -2.290422 -0.294511 -0.165418
H5 -3.208747 -0.450020 0.310888
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H7 -1.697589 1.272070 1.144322
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C8 0.484051 2.100967 -0.196889
H8 0.512520 2.447745 0.833679
H9 1.307644 2.411486 -0.832908
H10 -0.598148 1.203437 -1.764078
H11 -2.486758 -0.421747 -1.187688
H12 2.443751 0.704344 1.490957
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C2 1.053166 -1.192790 -0.848845
C3 2.227100 -0.503593 -0.425318
C4 1.923431 0.077093 0.775495
O 0.664998 -0.282356 1.158310
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H2 3.166047 -0.417992 -0.954942
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H4 -1.535872 -1.555380 1.354163
N -2.279628 -0.287201 -0.168797
H5 -3.203404 -0.450096 0.298450
C6 -1.836112 1.146086 0.074586
H6 -2.687758 1.760180 -0.236192
H7 -1.699586 1.273798 1.151818
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C8 0.449753 2.153650 -0.200292
H8 0.490760 2.474176 0.837825

H9 1.275625 2.464619 -0.835693
H10 -0.628999 1.257408 -1.769351
H11 -2.467251 -0.416600 -1.191992
H12 2.478626 0.659285 1.497828
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noCBpath coordinate 5.61
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C2 1.054456 -1.215328 -0.842850
C3 2.240650 -0.541128 -0.420578
C4 1.952209 0.028710 0.787237
O 0.684955 -0.303216 1.166440
H1 0.909425 -1.768521 -1.761269
H2 3.177145 -0.462979 -0.954941
C5 -1.306606 -1.369814 0.313819
H3 -1.568909 -2.272629 -0.240129
H4 -1.537004 -1.536445 1.369391
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H5 -3.195675 -0.449312 0.289483
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H9 1.245203 2.514415 -0.840484
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H11 -2.447227 -0.412180 -1.193216
H12 2.511652 0.611270 1.506566
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C3 2.256603 -0.589175 -0.412825
C4 1.982350 -0.025033 0.799889
O 0.705904 -0.327175 1.175665
H1 0.901660 -1.789375 -1.755971
H2 3.191740 -0.522352 -0.950326
C5 -1.302727 -1.365387 0.327694
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H4 -1.536148 -1.516182 1.385109
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H5 -3.188248 -0.449299 0.281180
C6 -1.857530 1.170252 0.086995
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H7 -1.697132 1.286003 1.161975
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C8 0.385054 2.255637 -0.212277
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H10 -0.695328 1.364978 -1.782756
H11 -2.427186 -0.408031 -1.193776
H12 2.548795 0.552043 1.517993
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C2 1.060265 -1.276097 -0.824714
C3 2.273035 -0.645505 -0.402096
C4 2.011634 -0.081105 0.812442
O 0.726643 -0.350785 1.183861
H1 0.895667 -1.818569 -1.746723
H2 3.209376 -0.595149 -0.940831

C5 -1.299099 -1.360637 0.342069
H3 -1.587045 -2.270366 -0.188438
H4 -1.533944 -1.494395 1.401226
N -2.247673 -0.269249 -0.166525
H5 -3.181121 -0.449819 0.273416
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H7 -1.693916 1.289667 1.168879
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C8 0.350294 2.306756 -0.218190
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H9 1.161194 2.646697 -0.859388
H10 -0.734850 1.424743 -1.789052
H11 -2.407515 -0.403446 -1.193566
H12 2.586264 0.490182 1.528658
22
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C3 2.289166 -0.701429 -0.390265
C4 2.038330 -0.136533 0.825626
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H12 2.619929 0.432352 1.538427
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C4 2.066159 -0.196242 0.840788
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C2 1.072708 -1.381770 -0.790983
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C4 2.094985 -0.261352 0.856666
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H12 2.695369 0.287644 1.568452
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C3 2.337207 -0.892565 -0.349549
C4 2.123714 -0.330833 0.873397
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C3 2.351613 -0.961195 -0.336200
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C4 2.152826 -0.320517 0.834894
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C19 2.291545 6.644605 1.704136
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N 1.744385 5.040786 -1.484249
C21 2.449035 4.558721 -2.649789
N 1.743425 3.507495 -3.339935
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