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A Theoretical Analysis of a Classic Example of Supramolecular Catalysis

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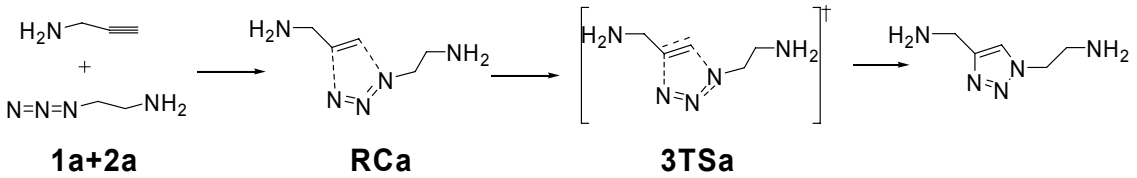
Table S1. Absolute energies for the uncatalyzed reaction (values in a.u.), see text for the structures.

	ΔE	ΔZPE
1	-172.3487806143	0.08903458
2	-299.1038262243	0.11189162
3TS	-471.3670863975	0.20260905
4TS	-471.3537330490	0.20242897
5	-471.5029680651	0.20951572
6	-471.4674052724	0.20890696



Scheme S1. The model reaction.

Table S2. Absolute energies and thermal corrections for the model reaction as depicted in Scheme S1 (values in a.u.)[a].

	ΔE	ΔZPE	$\Delta\Delta H_g$	$\Delta\Delta G_g$
1a	-171.99217789	0.07412	0.08041	0.04576
2a	-298.75031925	0.09717	0.10546	0.06403
RCa	-470.74646595	0.17243	0.18706	0.12828
3TSa	-470.71531384	0.17265	0.18668	0.12963

[a] $\Delta\Delta H_g$ and $\Delta\Delta G_g$ are calculated at 298.15 K and 1 atm.

Table S3. Absolute energies for the CB6-catalyzed reaction (values in a.u.) see text for the structures.

	ΔE
CB6	-3610.49754819216
7	-4082.12788486174
8TS	-4082.09351690946
9	-4082.23975826210

Table S4. Cartesian coordinates for the uncatalyzed reaction.

1 $[NH_3CH_2CCH]^+$

N	-1.496248	-0.469045	-0.000157
H	-1.357184	-1.063924	0.827016
H	-2.470440	-0.138593	-0.000116
C	-0.489753	0.698426	0.000225
H	-0.715240	1.292753	0.890880
H	-0.715652	1.293382	-0.889881
C	0.859269	0.172167	-0.000242
C	1.981759	-0.268540	0.000083
H	2.981524	-0.649786	0.000288
H	-1.357113	-1.063429	-0.827688

2 $[NH_3CH_2CH_2N_3]^+$

H	3.578048	0.313399	-0.000198
N	2.745388	-0.289702	-0.000027
C	1.465627	0.535880	-0.000132
H	2.806298	-0.895820	0.828556
H	1.493797	1.167264	0.889815
H	1.493712	1.166908	-0.890335
H	2.806213	-0.896169	-0.828361
C	0.234013	-0.370055	0.000124
H	0.233090	-1.017278	-0.891066
H	0.233330	-1.017092	0.891454
N	-0.887608	0.567870	0.000197
N	-2.018586	0.043175	0.000013
N	-3.102384	-0.295080	-0.000157

3TS

N	0.003306	-0.008586	-0.000299
N	0.005078	-0.008204	1.167277
C	2.142122	0.000698	1.512941
C	2.642357	0.021803	0.383270
N	0.843912	0.089826	-0.938239
H	3.338809	0.065582	-0.427839
C	2.193780	-0.169965	2.970294
H	1.966786	-1.201684	3.254800
H	3.167591	0.106268	3.383822
C	0.489396	-0.369335	-2.281549
H	1.441297	-0.607649	-2.768349
H	-0.110741	-1.286860	-2.247974
C	-0.237439	0.749007	-3.050185
H	-1.204331	0.985286	-2.600307
H	0.367938	1.656402	-3.098504
N	-0.525411	0.338561	-4.492291
H	-1.014500	1.089445	-4.999663
H	0.335759	0.133735	-5.017627
H	-1.122465	-0.498250	-4.546308
N	1.153207	0.700048	3.675156
H	0.225679	0.534262	3.256745

H	1.108753	0.493844	4.681821
H	1.366138	1.700066	3.568612

4TS

N	-0.027351	0.041578	-0.004486
N	0.134874	0.024278	1.157875
C	2.045443	-0.039623	1.383206
C	2.600496	-0.005669	0.272141
N	0.704787	0.148532	-1.039892
H	2.041766	-0.084990	2.456819
C	0.120766	-0.322504	-2.302076
H	0.937671	-0.332322	-3.030238
H	-0.268918	-1.346036	-2.212653
C	-0.986195	0.650201	-2.750549
H	-1.777106	0.717841	-2.000332
H	-0.590955	1.649192	-2.944684
N	-1.664842	0.187685	-4.038277
H	-2.411855	0.840583	-4.314780
H	-1.009492	0.129997	-4.829264
H	-2.100930	-0.738762	-3.933069
C	3.691390	0.067833	-0.689932
H	3.637105	0.952938	-1.329098
H	3.775598	-0.823951	-1.317758
N	5.036051	0.175848	0.061252
H	5.835874	0.234295	-0.585043
H	5.052078	1.010925	0.662373
H	5.181727	-0.639964	0.671205

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N	-0.450355	0.192144	-0.140027
N	-0.160549	0.255551	1.124661
C	1.158758	-0.028850	1.309073
C	1.728793	-0.280255	0.079945
N	0.690712	-0.131924	-0.788559
H	2.728093	-0.548256	-0.231043
C	1.689600	-0.082682	2.713367
H	1.672177	-1.099094	3.118169
H	2.699642	0.317989	2.819654
C	0.641631	-0.386120	-2.227669
H	1.670680	-0.422061	-2.596195
H	0.179130	-1.366733	-2.393685
C	-0.167776	0.728027	-2.913155
H	-1.151861	0.831983	-2.453752
H	0.349434	1.689247	-2.880427
N	-0.398150	0.403460	-4.382236
H	-0.947724	1.148369	-4.834380
H	0.479142	0.316105	-4.914126
H	-0.924188	-0.472712	-4.509854
N	0.754387	0.742285	3.584963
H	-0.212189	0.619868	3.230554
H	0.797807	0.466254	4.573729
H	0.963412	1.746945	3.528469

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N	-0.209304	0.490071	-0.032089
N	0.153823	0.645458	1.194242
C	1.500356	0.466130	1.286502
C	2.003347	0.180615	0.032215
N	0.896474	0.203620	-0.776489
H	1.993881	0.557259	2.245248
C	0.723682	-0.015002	-2.212689
H	1.324248	0.715689	-2.769847
H	1.071405	-1.022689	-2.474758
C	-0.771679	0.144641	-2.554134
H	-1.389918	-0.582121	-2.026866
H	-1.138329	1.144478	-2.321090
N	-1.008416	-0.074776	-4.044300
H	-2.010570	0.035498	-4.258012
H	-0.505385	0.602585	-4.634005
H	-0.742702	-1.018630	-4.357591
C	3.397799	-0.100842	-0.438252
H	3.764342	0.633272	-1.163810
H	3.513562	-1.100894	-0.869767
N	4.358041	-0.040151	0.737715
H	5.325487	-0.230218	0.439659
H	4.350843	0.887521	1.185634
H	4.116824	-0.733639	1.460300

Table S5. Cartesian coordinates for the model reaction.

1a [NH_2H_2CCH]

N	-1.533480	-0.431240	-0.002050
H	-1.391620	-1.027230	0.813080
C	-0.514170	0.629280	0.001080
H	-0.690840	1.263840	0.878560
H	-0.688740	1.267660	-0.874140
C	0.885290	0.169430	0.001130
C	2.020640	-0.244940	-0.000390
H	3.022160	-0.611030	-0.002120
H	-1.379310	-1.034660	-0.809440

2a [$NH_2H_2CH_2N_3$]

N	2.758140	-0.274930	-0.000420
C	1.522120	0.501590	0.000030
H	2.801560	-0.880250	0.818030
H	1.520280	1.156330	0.878870
H	1.519910	1.157280	-0.878130
H	2.798810	-0.884100	-0.816170
C	0.237510	-0.335790	-0.000090
H	0.209000	-0.984400	-0.888420
H	0.209160	-0.984910	0.887850
N	-0.924770	0.585400	0.000130
N	-2.035010	0.046440	0.000110
N	-3.112410	-0.335810	0.000110

RCa

N	0.370180	0.364340	-0.303130
N	-0.163900	0.508030	0.694110
C	2.986140	-0.155680	2.329240
C	3.485080	0.015850	1.244600
N	1.070110	0.251040	-1.310950
H	3.898590	0.171780	0.278810
C	2.340810	-0.331250	3.645050
H	2.016740	-1.374230	3.762580
H	3.085030	-0.153740	4.441570
C	0.419490	-0.366560	-2.499720
H	1.237800	-0.691220	-3.140670
H	-0.148690	-1.262110	-2.208080
C	-0.481380	0.622040	-3.270090
H	-1.281640	0.964160	-2.608110
H	0.109480	1.511810	-3.537920
N	-1.089180	0.086380	-4.484190
H	-0.372910	-0.220350	-5.137620
H	-1.667960	-0.730720	-4.267460
N	1.171570	0.529340	3.894100
H	0.478310	0.385730	3.147630
H	1.460920	1.512210	3.817140

3TSa

N	0.026890	-0.054370	-0.027550
N	-0.036120	-0.145800	1.132820
C	2.216090	-0.025750	1.565810
C	2.684010	0.011930	0.428400
N	0.839010	0.131550	-0.965870
H	3.347600	0.091040	-0.403020
C	2.157940	-0.101630	3.051270
H	1.930420	-1.134410	3.340460
H	3.154910	0.124360	3.448450
C	0.502160	-0.308820	-2.324110
H	1.460120	-0.545950	-2.801980
H	-0.089940	-1.234180	-2.305830
C	-0.229430	0.776410	-3.140210
H	-1.152260	1.056240	-2.618690
H	0.396180	1.674600	-3.186120
N	-0.579600	0.387210	-4.506360
H	0.255250	0.139950	-5.035660
H	-1.179700	-0.436240	-4.502040
N	1.199930	0.773310	3.736630
H	0.270770	0.596790	3.358680
H	1.413030	1.744120	3.510310

Table S5. Cartesian coordinates for the CB6-catalyzed reaction.

CB6

O	0.213642	-0.205071	-0.078192
C	0.168175	-0.069571	1.125764
N	1.254907	-0.055358	1.997793
N	-0.983373	0.039854	1.902572

C	2.601155	-0.285095	1.518136

C	-0.710700	-0.008650	3.323094
O	3.481160	1.167137	-0.804074
C	3.819336	1.499959	0.311690
N	4.691214	2.536435	0.637203
N	3.460151	0.877699	1.505101
C	5.321435	3.337157	-0.389258
C	4.165967	1.404865	2.652179
O	3.630145	4.348923	-2.480924
C	4.020667	5.068382	-1.586617
N	3.803673	6.440138	-1.473851
N	4.823265	4.690004	-0.512539
C	3.099033	7.171797	-2.504720
C	5.266203	5.813903	0.283806
O	0.095601	2.694914	5.448745
C	0.092134	1.775542	4.657825
N	1.205924	1.083015	4.188210
N	-1.030727	1.171454	4.096471
C	2.540461	1.410505	4.637392
C	0.858478	-0.072491	3.389773
O	3.322838	4.174178	4.671493
C	3.713642	3.422161	3.804559
N	4.631908	3.723771	2.801065
N	3.375158	2.077906	3.661142
C	5.262082	5.024152	2.727818
C	5.038333	2.561359	2.041694
O	3.588049	7.346577	2.987202
C	3.996773	6.984222	1.904727
N	3.803791	7.634405	0.688162
N	4.801632	5.875618	1.653210
C	-2.298339	-0.057068	1.306600
C	4.558227	7.042804	-0.395268
H	2.514452	-0.620320	0.481727
H	3.068603	-1.071323	2.129290
H	6.405228	3.371653	-0.204505
H	5.120777	2.839086	-1.340910
H	3.699139	8.046469	-2.796263
H	2.991403	6.493016	-3.354195
H	3.044219	0.490461	4.969366
H	2.427030	2.098124	5.478993
H	6.350203	4.889653	2.639134
H	5.025006	5.542196	3.660255
H	-2.153036	-0.391729	0.276552
H	-2.889731	-0.799678	1.862705
H	-1.198642	-0.890277	3.767206
H	4.767785	0.609635	3.119198
H	6.365070	5.879393	0.258956
H	1.234046	-0.987851	3.873195
H	6.120410	2.396178	2.162274
H	5.267771	7.779775	-0.802455
N	1.766368	7.609272	-2.153371
C	-2.367373	1.600864	4.443951
C	3.062098	8.873187	0.608135
N	-3.038801	1.183258	1.238308
C	1.456944	8.800544	-1.392813
C	0.637407	7.006952	-2.704890
N	-3.067570	2.342695	3.417460
H	-2.966966	0.721016	4.720185
H	-2.267555	2.269204	5.302653

N	1.741385	8.768725	0.025743

H	2.926826	9.223813	1.634201
H	3.648805	9.606217	0.035026
C	-3.251831	1.831458	0.023828
C	-3.808538	1.751998	2.324000
C	-0.112342	8.868892	-1.448387
H	1.944755	9.674928	-1.851388
O	0.624613	6.083431	-3.490733
N	-0.470712	7.706596	-2.232123
C	-3.275456	3.715320	3.534630
C	0.596208	8.887831	0.810495
O	-2.844326	1.478786	-1.062245
N	-4.073827	2.925593	0.282738
C	-4.519991	2.985348	1.657392
H	-4.515693	1.003308	2.713744
N	-0.496843	8.867371	-0.053183
H	-0.488684	9.780516	-1.938270
C	-1.806444	7.398013	-2.693066
O	-2.889401	4.426677	4.437333
N	-4.061618	4.105387	2.452101
O	0.560560	9.035425	2.013358
C	-4.534760	3.787799	-0.782733
H	-5.618724	2.924400	1.697182
C	-1.841727	9.078540	0.436258
N	-2.656441	6.734365	-1.728581
H	-2.295728	8.326687	-3.022356
H	-1.696803	6.714195	-3.538249
C	-4.563182	5.458323	2.341736
N	-3.895377	5.084369	-0.851740
H	-5.621143	3.928999	-0.684982
H	-4.308061	3.274805	-1.720459
N	-2.688209	7.905946	0.444599
H	-1.750161	9.406457	1.474627
H	-2.322626	9.864756	-0.164669
C	-3.420781	7.402018	-0.697027
C	-2.993133	5.389706	-1.868833
N	-3.942442	6.266267	1.315756
H	-5.648235	5.424675	2.164279
H	-4.356093	5.949923	3.295370
C	-4.294907	6.246471	-0.087059
C	-3.048664	7.284411	1.638268
H	-4.022022	8.210360	-1.141760
O	-2.614029	4.640567	-2.743472
H	-5.376849	6.415407	-0.202871
O	-2.694702	7.605129	2.752656

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O	0.313200	-0.445800	-0.152000
C	0.251700	-0.360400	1.057700
N	1.325900	-0.393700	1.942500
N	-0.907600	-0.265100	1.820200
C	2.682300	-0.588400	1.474200
C	-0.646500	-0.226300	3.238400
O	3.354300	1.102200	-0.764800
C	3.771200	1.335300	0.352700
N	4.644500	2.362800	0.698000
N	3.516100	0.601300	1.502600

C	5.191400	3.244300	-0.306400
C	4.302600	1.044200	2.633800

O	3.330100	4.371600	-2.210200
C	3.833400	5.054500	-1.326400
N	3.732400	6.429200	-1.197300
N	4.647400	4.593000	-0.307600
C	3.151100	7.273700	-2.224400
C	5.112200	5.663000	0.560600
O	0.391700	2.598500	5.110500
C	0.299800	1.571900	4.441400
N	1.334600	0.705200	4.144400
N	-0.859800	1.061900	3.897800
C	2.682600	0.892600	4.642400
C	0.907700	-0.418800	3.329100
O	3.461300	3.640300	4.886800
C	3.858800	2.949800	3.956500
N	4.708400	3.364500	2.951300
N	3.571400	1.616000	3.755700
C	5.236100	4.713800	2.927100
C	5.101100	2.275300	2.066900
O	3.106000	6.678900	3.296900
C	3.671500	6.533700	2.219400
N	3.480800	7.303700	1.080800
N	4.655100	5.596100	1.933200
C	-2.221500	-0.294300	1.209000
C	4.379000	6.923300	-0.002900
C	0.037600	5.860800	5.516600
C	-0.331500	6.489700	4.185700
N	-0.039000	5.486200	3.134000
N	-0.382800	5.747500	1.983400
H	2.612900	-0.907100	0.432000
H	3.166300	-1.374700	2.067400
H	6.280800	3.307500	-0.181600
H	4.960100	2.803600	-1.278000
H	3.800400	8.147600	-2.358300
H	3.129200	6.692900	-3.147800
H	3.110400	-0.093200	4.857600
H	2.622100	1.468500	5.566900
H	6.319100	4.674500	2.757000
H	5.041300	5.145400	3.909800
H	-2.087200	-0.673700	0.194100
H	-2.862600	-0.980100	1.777100
H	-1.216600	-1.007300	3.758600
H	4.950500	0.232500	2.989800
H	6.207100	5.734500	0.528700
H	1.206700	-1.360100	3.808600
H	6.190600	2.141100	2.102500
H	5.051800	7.755400	-0.248300
H	0.255900	7.390300	3.989900
H	-1.392200	6.750700	4.180000
N	1.802600	7.723200	-1.976600
C	-2.170900	1.587900	4.247700
C	2.743500	8.560800	1.085400
N	-2.890900	0.985600	1.098900
C	1.420000	8.818700	-1.111300
C	0.716200	7.097900	-2.563400
N	-2.854400	2.290600	3.186300
H	-2.794700	0.751500	4.593900
H	-2.030500	2.297900	5.064300

N	1.513500	8.566100	0.319600
H	2.473500	8.775600	2.121000

H	3.409300	9.351200	0.710600
C	-2.961600	1.678500	-0.101500
C	-3.639600	1.625600	2.157000
C	-0.129400	8.941500	-1.349600
H	1.976600	9.726800	-1.378600
O	0.765200	6.133000	-3.312600
N	-0.417200	7.790700	-2.192400
C	-3.161200	3.645200	3.298800
C	0.288200	8.732200	0.959600
O	-2.452500	1.351200	-1.158200
N	-3.768500	2.789200	0.107500
C	-4.352700	2.819200	1.435500
H	-4.337100	0.910400	2.614700
N	-0.681200	8.920000	-0.011600
H	-0.419800	9.866400	-1.864600
C	-1.716400	7.443000	-2.724500
O	-2.778000	4.396100	4.177700
N	-4.017000	3.966400	2.253300
O	0.113500	8.743200	2.164300
C	-4.218000	3.603200	-0.997500
H	-5.444000	2.705600	1.375300
C	-2.085200	9.104500	0.331100
N	-2.574300	6.708800	-1.820100
H	-2.238400	8.357200	-3.032200
H	-1.540100	6.815300	-3.599700
C	-4.623400	5.278800	2.114900
N	-3.699800	4.957300	-1.017100
H	-5.315000	3.657000	-0.992400
H	-3.881400	3.108000	-1.910200
N	-2.912000	7.912700	0.303300
H	-2.115700	9.480100	1.355500
H	-2.510300	9.853300	-0.347300
C	-3.500100	7.317300	-0.880600
C	-2.668300	5.332200	-1.850700
N	-4.034100	6.145600	1.111100
H	-5.690000	5.147000	1.892700
H	-4.510000	5.789900	3.072900
C	-4.292300	6.083300	-0.314000
C	-3.242400	7.228700	1.466900
H	-4.135400	8.045800	-1.400500
O	-1.995400	4.575300	-2.544500
H	-5.371100	6.124900	-0.512800
O	-2.924500	7.543400	2.598700
N	-0.625900	5.816400	0.868600
C	0.755600	3.133300	0.821000
C	0.674000	2.757700	-0.321600
H	0.808600	3.467300	1.834200
C	0.585700	2.253000	-1.687000
N	0.613100	3.394200	-2.678100
H	-0.348400	1.704100	-1.828700
H	1.437100	1.601700	-1.894100
H	1.470000	3.969900	-2.576400
H	-0.221500	4.008400	-2.588500
H	0.605800	3.033100	-3.637000
N	1.410600	5.239100	5.432600
H	2.034000	5.707100	4.751100
H	0.044800	6.618800	6.302300

H	-0.651000	5.057700	5.781100

H	1.896500	5.224800	6.332700
H	1.333800	4.247200	5.142700

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O	0.246000	-0.406200	-0.166300
C	0.149200	-0.330300	1.041700
N	1.202000	-0.329000	1.952300
N	-1.034100	-0.268900	1.773700
C	2.574500	-0.484600	1.520400
C	-0.809300	-0.325300	3.205400
O	3.285800	1.174300	-0.742900
C	3.676000	1.429400	0.381700
N	4.544900	2.459400	0.726700
N	3.382000	0.724100	1.539200
C	5.173700	3.282500	-0.281900
C	4.044400	1.265500	2.703800
O	3.329500	4.479300	-2.143800
C	3.908200	5.154600	-1.303600
N	3.894600	6.536600	-1.216700
N	4.741000	4.671500	-0.310300
C	3.221000	7.371900	-2.192200
C	5.326900	5.732500	0.489000
O	-0.200900	2.518700	5.219600
C	-0.135600	1.541800	4.493600
N	1.024700	0.908600	4.074800
N	-1.212000	0.847500	3.961400
C	2.315300	1.300100	4.596800
C	0.758400	-0.313600	3.327800
O	3.054300	4.111700	4.569900
C	3.545500	3.304700	3.787300
N	4.592200	3.561000	2.916100
N	3.193300	1.975500	3.653000
C	5.325300	4.811300	2.906600
C	4.947000	2.404500	2.118100
O	3.668000	7.119400	3.286500
C	4.111700	6.836500	2.180400
N	3.911500	7.560800	1.022500
N	4.932200	5.767400	1.887100
C	-2.327900	-0.393400	1.125600
C	4.671700	7.032600	-0.103700
C	0.184000	5.557400	4.598400
C	-0.401700	5.328300	3.211000
N	0.458700	4.584100	2.271400
N	0.994000	5.187600	1.307200
H	2.543400	-0.829000	0.484800
H	3.065200	-1.240800	2.146300
H	6.263300	3.264000	-0.144600
H	4.920400	2.842800	-1.248600
H	3.835800	8.263500	-2.364800
H	3.144900	6.800200	-3.118700
H	2.835200	0.409900	4.976600
H	2.131600	1.991500	5.421000
H	6.391300	4.585200	2.786400
H	5.166500	5.297900	3.869900
H	-2.137900	-0.739700	0.107700

H	-2.930600	-1.136900	1.661600
H	-1.272500	-1.224900	3.632100
H	4.609300	0.480100	3.223200

H	6.421000	5.715800	0.405900
H	1.159200	-1.180400	3.870700
H	6.023100	2.202500	2.204600
H	5.402200	7.775900	-0.447600
H	-0.726000	6.274000	2.780000
H	-1.289000	4.715500	3.375600
N	1.873600	7.779900	-1.848200
C	-2.582300	1.226100	4.247500
C	3.128500	8.780000	1.023100
N	-3.093500	0.836200	1.018600
C	1.513900	8.874300	-0.966700
C	0.772000	7.181100	-2.433600
N	-3.233400	1.985400	3.193400
H	-3.165200	0.320300	4.456600
H	-2.563500	1.863800	5.133600
N	1.800200	8.673600	0.442900
H	3.014300	9.078500	2.066300
H	3.673700	9.562600	0.481700
C	-3.098000	1.596800	-0.143000
C	-3.930600	1.397700	2.058200
C	-0.055000	8.877700	-1.017900
H	1.968000	9.811900	-1.312000
O	0.793300	6.270600	-3.245900
N	-0.358700	7.832100	-1.970700
C	-3.533600	3.332700	3.362600
C	0.655700	8.507100	1.200700
O	-2.521700	1.337400	-1.182500
N	-3.923300	2.694000	0.080500
C	-4.593200	2.644600	1.366900
H	-4.659700	0.653400	2.404700
N	-0.440000	8.605200	0.362000
H	-0.482400	9.834300	-1.345200
C	-1.676600	7.510100	-2.478900
O	-3.186600	4.032600	4.296800
N	-4.303400	3.734800	2.279900
O	0.613900	8.332500	2.415800
C	-4.252300	3.606800	-0.986800
H	-5.678300	2.542400	1.231500
C	-1.804500	8.749500	0.860500
N	-2.512400	6.715800	-1.601800
H	-2.209000	8.441000	-2.709300
H	-1.526900	6.940800	-3.397700
C	-4.827000	5.085600	2.183400
N	-3.648400	4.928500	-0.876700
H	-5.342300	3.730400	-1.043100
H	-3.886900	3.159100	-1.913000
N	-2.655100	7.590500	0.683700
H	-1.746800	8.934400	1.935100
H	-2.255100	9.620400	0.364800
C	-3.346700	7.254700	-0.551400
C	-2.654200	5.346100	-1.737600
N	-4.099400	5.986300	1.302300
H	-5.871000	5.038200	1.851900
H	-4.779100	5.518700	3.184400
C	-4.241400	6.035900	-0.136300
C	-3.190800	6.918700	1.783400

H	-3.919500	8.115000	-0.923000
O	-2.031900	4.635800	-2.520400
H	-5.297400	6.152100	-0.413300

O	-2.915900	7.131300	2.948800
N	1.310900	5.050400	0.192700
C	-0.278900	2.927100	1.082000
C	0.191800	3.028900	-0.055500
H	-0.836300	2.548800	1.909800
C	0.463700	2.502000	-1.403100
N	0.602100	3.569900	-2.456300
H	-0.364100	1.853300	-1.700500
H	1.390600	1.922500	-1.399600
H	1.449000	4.153400	-2.330600
H	-0.238100	4.177000	-2.496200
H	0.691000	3.130800	-3.378000
N	1.392200	6.454300	4.555000
H	1.294900	7.215400	3.859400
H	-0.582200	6.047700	5.203300
H	0.483200	4.623200	5.071200
H	1.577900	6.880600	5.467200
H	2.241600	5.915200	4.311400

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O	0.234400	-0.339900	-0.215800
C	0.148100	-0.282900	0.994400
N	1.207300	-0.282700	1.896000
N	-1.029900	-0.233800	1.735600
C	2.578100	-0.446000	1.454000
C	-0.796400	-0.290800	3.164500
O	3.307300	1.239200	-0.782500
C	3.720600	1.461400	0.341600
N	4.629100	2.449000	0.696800
N	3.399600	0.751200	1.491000
C	5.266100	3.280700	-0.302100
C	4.073500	1.260100	2.663600
O	3.392800	4.437000	-2.159400
C	3.950300	5.121600	-1.309700
N	3.876600	6.499300	-1.205200
N	4.824500	4.664400	-0.345900
C	3.198700	7.317900	-2.187500
C	5.365700	5.736900	0.468400
O	-0.192200	2.563700	5.159700
C	-0.126700	1.583900	4.436200
N	1.036500	0.957600	4.011200
N	-1.203500	0.879700	3.920500
C	2.331500	1.326200	4.547000
C	0.771100	-0.269300	3.274600
O	3.125900	4.115400	4.533200
C	3.612400	3.303700	3.753600
N	4.673000	3.540300	2.897800
N	3.231400	1.981200	3.611200
C	5.396600	4.797700	2.874200
C	5.010600	2.382000	2.094300
O	3.763900	7.114800	3.300700
C	4.159400	6.819200	2.180200
N	3.920000	7.537800	1.026200
N	4.972100	5.749700	1.866000

C	-2.326400	-0.384100	1.105400
C	4.665600	7.019100	-0.112500
C	0.306400	5.496300	4.578500
C	-0.510400	5.366500	3.303600

N	0.145800	4.722000	2.155300
N	1.336800	5.154000	1.687900
H	2.536600	-0.772000	0.412700
H	3.060900	-1.220200	2.064000
H	6.352200	3.270200	-0.143800
H	5.035000	2.837200	-1.272400
H	3.805000	8.213000	-2.372900
H	3.119700	6.736400	-3.107700
H	2.826900	0.424800	4.933500
H	2.154700	2.021800	5.369100
H	6.461300	4.578000	2.733000
H	5.253100	5.280500	3.842000
H	-2.146000	-0.729900	0.085700
H	-2.912400	-1.133700	1.650900
H	-1.251700	-1.193700	3.592900
H	4.614500	0.454400	3.177200
H	6.460000	5.760500	0.386200
H	1.181900	-1.131800	3.816800
H	6.080100	2.154200	2.192900
H	5.371200	7.776400	-0.478100
H	-0.860200	6.349200	2.987100
H	-1.385900	4.771700	3.560300
N	1.851700	7.720300	-1.836100
C	-2.575100	1.242500	4.222600
C	3.104700	8.735000	1.039000
N	-3.110600	0.835200	1.007800
C	1.495400	8.813600	-0.952100
C	0.751200	7.127600	-2.425500
N	-3.260000	1.989800	3.177600
H	-3.141600	0.329100	4.443400
H	-2.554400	1.883200	5.106400
N	1.774900	8.606600	0.458200
H	2.985300	9.020400	2.085200
H	3.628100	9.537600	0.504600
C	-3.104800	1.606100	-0.143000
C	-3.954500	1.388300	2.047200
C	-0.072000	8.829500	-1.013800
H	1.958400	9.748800	-1.292400
O	0.769700	6.209100	-3.229600
N	-0.376800	7.790100	-1.971800
C	-3.594600	3.328200	3.352600
C	0.623300	8.473400	1.212200
O	-2.480600	1.380000	-1.164200
N	-3.953000	2.685400	0.069800
C	-4.632600	2.626200	1.351600
H	-4.673800	0.636400	2.396500
N	-0.468900	8.555900	0.362400
H	-0.489800	9.790400	-1.341300
C	-1.692500	7.481100	-2.487700
O	-3.270900	4.031900	4.292400
N	-4.358100	3.723700	2.261000
O	0.564400	8.348300	2.432500
C	-4.278500	3.594300	-1.004500
H	-5.715000	2.508600	1.210200
C	-1.835800	8.723500	0.848400

N	-2.540500	6.696300	-1.613800
H	-2.216500	8.415600	-2.721800
H	-1.542500	6.909600	-3.405100
C	-4.893900	5.072700	2.152600

N	-3.678800	4.913200	-0.888600
H	-5.368400	3.711200	-1.068500
H	-3.904100	3.143700	-1.925700
N	-2.706600	7.576600	0.668200
H	-1.785300	8.912600	1.922600
H	-2.270500	9.598500	0.345700
C	-3.385800	7.239900	-0.575500
C	-2.654900	5.322100	-1.723400
N	-4.165400	5.977000	1.274700
H	-5.934100	5.012900	1.812100
H	-4.859900	5.509700	3.152400
C	-4.287200	6.022600	-0.167300
C	-3.262300	6.914100	1.762200
H	-3.952800	8.100200	-0.954600
O	-1.989700	4.599300	-2.454900
H	-5.338700	6.136700	-0.460900
O	-3.007400	7.130900	2.931500
N	1.576200	4.528400	0.564100
C	-0.395900	3.826500	1.294900
C	0.527100	3.703400	0.274200
H	-1.351600	3.360800	1.470900
C	0.500600	2.793300	-0.918500
N	0.699900	3.538600	-2.215100
H	-0.453100	2.270800	-0.997800
H	1.300800	2.052200	-0.874600
H	1.608100	4.046400	-2.236300
H	-0.073200	4.198700	-2.410800
H	0.719900	2.865900	-2.988300
N	1.454900	6.454800	4.440300
H	1.266600	7.216200	3.761800
H	-0.371200	5.891400	5.338800
H	0.705400	4.544400	4.921000
H	1.699800	6.880000	5.338600
H	2.308900	5.971100	4.117200