Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Electrostatic effects in N-heterocyclic carbene catalysis: revealing the nature of catalysed decarboxylation

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Additional computational details

The keyword **int=ultrafine** was used for all DFT calculations, and **opt=(maxstep=x, notrust)** were recommended for geometry optimisations when oscillations occurred. The conversion from 1 atm to 1 M for final free energies was adopted via the addition of 1.89 kcal mol^{-1}.

Colour bar for IRI analysis

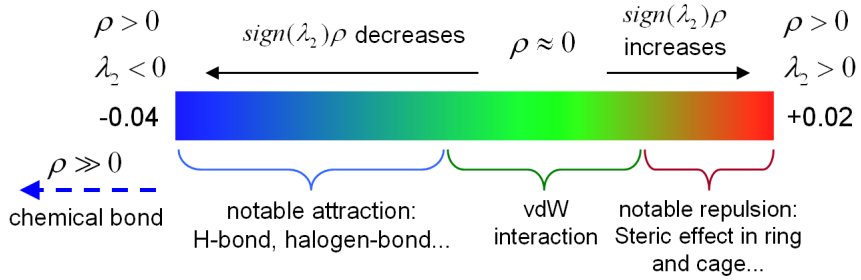

Fig. S1. The colour bar used for IRI analysis is provided in the **/examples** directory of Multiwfn packages.

Energetic data

Sym= symbol, **SP** =single-point energy, **TC**= thermal correction of Gibbs free energy, **GFE**= Gibbs free energy. Unless noted elsewhere, the final GFE(298K,1M)= SP[M06-2X/6-31+G(d,p)/SMD(DCM)]+TC[M06-2X/6-31G(d,p)/IEFPCM(DCM)]+1.89/627.51 in E_h. The calculated free energy barriers are in red, and overall reaction free energies are in green colour.

Table S1. Energetic data used for Fig. 5, where the pre-complex stands for the pre-reaction complex tracked by IRC pathway.

Sym	SP	TC	GFE	kcal mol^{-1}
NHC•H^+ (***3***)	-1052.448937	0.347035	-1052.098890	
truncated NHC•H^+ (***7***)	-360.519971	0.126217	-360.390742	
DABCO•H^+ (***4***)	-345.669876	0.171636	-345.495228	
NMe_3•H^+ (***8***)	-174.857736	0.109976	-174.744748	
MeOH (***9***)	-115.677637	0.029306	-115.645319	
CO_2	-188.515618	-0.005883	-188.518489	
Reactant (***5***)	-579.040893	0.214653	-578.823228	
Product (***6***)	-390.525003	0.200583	-390.321408	-10.5
TS-no HB donor	-578.988828	0.208952	-578.776864	29.1
TS-NHC•H^+	-1631.457397	0.577924	-1630.876461	28.7
TS-truncated NHC•H^+	-939.520794	0.352620	-939.165162	30.6
TS-DABCO•H^+	-924.680081	0.398001	-924.279068	24.7
TS-NMe_3•H^+	-753.867936	0.336829	-753.528095	25.0
TS-MeOH	-694.676729	0.254294	-694.419423	30.8
NHC•H^+ pre-complex	-1631.504086	0.581621	-1630.919453	1.7
truncated NHC•H^+ pre-complex	-939.567233	0.358110	-939.206111	4.9
DABCO•H^+ pre-complex	-924.721610	0.403942	-924.314656	2.4
NMe_3•H^+ pre-complex	-753.909550	0.342862	-753.563676	2.7
MeOH pre-complex	-694.725299	0.259738	-694.462549	3.8

Table S2. Energetic data used for Fig. 7 and 8, where *ri-2* stands for when CFGs are installed on the ring and *up* stands for when CFGs are installed next to the oxygen.

Sym	SP(DCM)	SP(Gas)	TC	GFE(DCM)	GFE(Gas)	kcal mol^{-1} (DCM)	kcal mol^{-1} (Gas)
NHC•H$^+$ *ri*-2-NH_2 (***10***)	-1147.081686	-1146.985595	0.389756	-1146.688918	-1146.592827		
NHC•H$^+$ *ri*-2-NH_3^+ (***11***)	-1147.528369	-1147.267365	0.406592	-1147.118765	-1146.857761		
NHC•H$^+$ *ri*-2-SO_3H (***12***)	-1715.456855	-1715.347608	0.382247	-1715.071596	-1714.962349		
NHC•H$^+$ *ri*-2-SO_3^- (***13***)	-1715.016827	-1714.913580	0.372763	-1714.641052	-1714.537805		
NHC•H$^+$ *up*-2-NH_2 (***14***)	-1147.084372	-1146.987645	0.389190	-1146.692170	-1146.595443		
NHC•H$^+$ *up*-2-NH_3^+ (***15***)	-1147.523090	-1147.252851	0.406300	-1147.113778	-1146.843539		
NHC•H$^+$ *up*-2-SO_3H (***16***)	-1715.448833	-1715.342611	0.383161	-1715.062660	-1714.956438		
NHC•H$^+$ *up*-2-SO_3^- (***17***)	-1715.011840	-1714.923192	0.372684	-1714.636144	-1714.547496		
TS-NHC•H$^+$ *ri*-2-NH_2	-1726.089909	-1725.994663	0.621120	-1725.465777	-1725.370531	29.1	28.6
TS-NHC•H$^+$ *ri*-2-NH_3^+	-1726.536722	-1726.282720	0.639027	-1725.894683	-1725.640681	29.7	25.3
TS-NHC•H$^+$ *ri*-2-SO_3H	-2294.465432	-2294.356943	0.613909	-2293.848511	-2293.740022	29.1	28.6
TS-NHC•H$^+$ *ri*-2-SO_3^-	-2294.025557	-2293.921339	0.603648	-2293.418897	-2293.314679	28.5	29.1
TS-NHC•H$^+$ *up*-2-NH_2	-1726.090519	-1725.994093	0.620315	-1725.467192	-1725.370766	30.2	30.1
TS-NHC•H$^+$ *up*-2-NH_3^+	-1726.533176	-1726.280447	0.636608	-1725.893556	-1725.640827	27.3	16.3
TS-NHC•H$^+$ *up*-2-SO_3H	-2294.457735	-2294.353181	0.613354	-2293.841369	-2293.736815	27.9	26.9
TS-NHC•H$^+$ *up*-2-SO_3^-	-2294.019345	-2293.920999	0.603065	-2293.413268	-2293.314922	28.9	35.0

Final geometries in xyz format with the charge and the multiplicity

The format is as follow:

name

charge multiplicity

[xyz coordinates]

NHC•H$^+$ (***3***)
1 1
C -0.256296 -0.119429 -0.764495
C 0.485004 -1.481128 0.750293
C 2.215833 -0.681282 -0.890834
H 2.136529 -0.862250 -1.966951
N -0.785381 -1.337406 1.009232
N -1.231216 -0.482738 0.050871
N 0.850382 -0.738356 -0.341844
C 1.502406 -2.338025 1.439602
H 1.398550 -3.373756 1.088628
H 1.343172 -2.310798 2.517557
C 3.088224 -1.772624 -0.215572
O 2.785758 -1.827467 1.170821
C 4.292669 0.279080 -0.283366
C 2.967027 0.596402 -0.583282
C 2.523767 1.911237 -0.607799
C 3.437372 2.923792 -0.314599
C 4.764390 2.613812 -0.015852
C 5.202809 1.289366 0.000001
C 4.509123 -1.215815 -0.331882
H 1.493030 2.163025 -0.840265
H 5.462094 3.412574 0.212588
H 6.234327 1.052548 0.240882
H 5.133625 -1.599234 0.477597
H 4.957591 -1.519365 -1.283586
C -2.609019 -0.059835 0.007171
C -2.938000 1.168398 0.579860
C -3.538074 -0.919185 -0.587353
C -4.280283 1.546243 0.529326
C -4.862145 -0.493225 -0.608787
C -5.249059 0.733088 -0.058305
H -4.572589 2.496666 0.966866
H -5.612230 -1.134369 -1.064216
C -3.115421 -2.238691 -1.176001
H -2.626832 -2.866018 -0.425039
H -2.408197 -2.096508 -1.999425
H -3.980905 -2.776726 -1.563469
C -6.695666 1.150219 -0.089543
H -6.819114 2.180918 0.246649

H	-7.294464	0.505479	0.560495
H	-7.103223	1.063621	-1.100056
C	-1.894301	2.045374	1.220086
H	-1.267762	2.533462	0.466494
H	-1.236802	1.468959	1.876774
H	-2.369550	2.827754	1.812484
H	2.949063	-2.758290	-0.674857
H	3.112135	3.958371	-0.318001
H	-0.353170	0.536547	-1.617542

truncated NHC•H^+ (***7***)

1 1

C	0.574048	1.092712	0.004772
C	-0.643106	-0.708118	-0.001214
N	0.601519	-1.112349	-0.003862
N	1.339502	0.019986	0.000176
N	-0.692802	0.665853	0.004234
H	0.906044	2.119718	0.009302
C	-1.900866	1.493482	-0.004607
H	-2.447222	1.321100	-0.931494
H	-2.518440	1.234689	0.854703
H	-1.603235	2.537700	0.058679
C	2.796955	-0.056810	-0.001284
H	3.196361	0.955240	0.003214
H	3.115004	-0.595293	0.889864
H	3.113446	-0.586558	-0.898242
C	-1.840974	-1.583831	0.002096
H	-2.421330	-1.437351	0.916146
H	-2.481232	-1.367433	-0.856046
H	-1.513273	-2.620848	-0.048534

DABCO•H^+ (***4***)

1 1

N	-1.296244	-0.006344	-0.005544
C	-0.799735	-0.591422	-1.251656
C	0.740682	-0.759476	-1.199383
H	-1.085684	0.063168	-2.077482
H	-1.272967	-1.562651	-1.407602
N	1.220392	0.006758	0.005093
H	1.247325	-0.349785	-2.073150
H	1.052009	-1.794959	-1.056227
C	0.729121	-0.657861	1.264278
C	-0.809464	-0.791315	1.129368
H	1.030594	-0.018875	2.095048
H	1.237655	-1.618419	1.346859
H	-1.292799	-0.442327	2.043673
H	-1.091100	-1.834576	0.972249
C	-0.816182	1.371099	0.112240
C	0.724012	1.427420	-0.055847
H	-1.108756	1.755802	1.091549
H	-1.294714	1.986139	-0.651953
H	1.222985	1.983051	0.738216
H	1.033310	1.827386	-1.022352
H	2.242506	0.012475	0.010318

NMe_3•H^+ (***8***)

1 1

H	0.000034	0.000655	-1.369590
C	-1.399034	0.272495	0.104527
H	-2.049212	-0.509922	-0.282507
H	-1.409059	0.270346	1.194077
H	-1.705535	1.245104	-0.276104
C	0.935764	1.074446	0.104612
H	1.930223	0.854947	-0.279621
H	0.582393	2.029657	-0.279022
H	0.941682	1.080811	1.194145
C	0.463314	-1.347055	0.104529
H	-0.226756	-2.098556	-0.273862
H	1.464575	-1.520291	-0.285224
H	0.473172	-1.353266	1.194032
N	-0.000255	0.000172	-0.345477

MeOH (***9***)

0 1

H	-1.130840	-0.760573	-0.000053
O	-0.746620	0.122796	0.000007
C	0.660766	-0.019440	0.000006
H	1.085887	0.986016	-0.000383
H	1.026677	-0.545296	0.890372
H	1.026645	-0.545874	-0.890035

CO_2

0 1

C	0.000002	0.000174	-0.000061
O	0.612371	0.344623	0.924231
O	-0.612373	-0.344754	-0.924185

Reactant (***5***)

0 1

C	0.829283	1.468384	0.324434
C	1.133157	0.022147	0.584269
C	1.851569	-0.803237	-0.474366
C	-1.615675	0.894568	0.213653
C	-0.443809	1.853990	0.213992
H	-0.665004	2.912712	0.082752
O	2.868472	-0.743438	-1.102697
H	-1.935753	0.709998	1.251814
H	1.643617	-0.099815	1.548351
C	0.010428	-1.013427	0.379178
C	-1.173987	-0.446257	-0.409028
H	-0.779417	-0.201687	-1.404736
O	0.898692	-1.766308	-0.541081
C	-0.338511	-1.865226	1.577658
H	-0.953253	-1.291887	2.277812
H	-0.894152	-2.755641	1.276781
H	0.571772	-2.180454	2.093116

C	2.011299	2.391127	0.260699
H	2.704109	2.066645	-0.523123
H	1.702056	3.417642	0.054615
H	2.568929	2.376014	1.203807
C	-2.302759	-1.461380	-0.576170
H	-1.905412	-2.424896	-0.909142
H	-2.842894	-1.619007	0.363252
H	-3.020768	-1.123030	-1.325740
C	-2.800461	1.506805	-0.536738
H	-3.695362	0.886635	-0.453308
H	-3.038295	2.494456	-0.132321
H	-2.560691	1.625331	-1.599189

Product (***6***)

0 1

C	-1.754891	-0.012833	-0.037351
C	-0.965885	-1.249986	-0.131965
C	0.372819	1.239377	-0.339366
C	-1.118809	1.163411	-0.112717
H	-1.679788	2.095975	-0.068598
H	0.547766	1.154641	-1.427613
H	-1.501378	-2.185524	-0.286948
C	0.367540	-1.259105	0.018106
C	1.090745	0.048800	0.322695
H	1.022295	0.191150	1.416900
C	1.150504	-2.540769	0.008949
H	1.915712	-2.542404	-0.774673
H	1.676364	-2.684181	0.960761
H	0.492357	-3.397538	-0.150359
C	-3.243933	-0.140834	0.126252
H	-3.492140	-0.698370	1.035834
H	-3.724427	0.838488	0.179384
H	-3.679539	-0.694026	-0.713219
C	2.573765	0.012646	-0.054816
H	3.090593	-0.827088	0.415022
H	2.692113	-0.080444	-1.140370
H	3.081027	0.925465	0.263657
C	0.925616	2.588229	0.125339
H	1.964669	2.734460	-0.177005
H	0.339017	3.407758	-0.300166
H	0.870528	2.668018	1.216647

TS-no HB donor

0 1

C	-0.772866	1.416456	-0.370706
C	-1.019045	-0.043430	-0.637786
C	-1.867605	-0.821211	0.594732
C	1.685492	0.943790	-0.208807
C	0.479158	1.854408	-0.212890
H	0.662389	2.919418	-0.083889
O	-2.931848	-0.313485	0.887995
H	2.074978	0.853423	-1.235672
H	-1.636453	-0.211285	-1.525779
C	0.132114	-0.902994	-0.578073
C	1.264966	-0.471351	0.289064
H	0.817320	-0.304914	1.278245
O	-1.245794	-1.823679	1.005294
C	0.227783	-2.088265	-1.445463
H	0.918840	-1.803855	-2.255402
H	0.669517	-2.941786	-0.931429
H	-0.733215	-2.349672	-1.885973
C	-1.973254	2.316889	-0.384138
H	-2.672661	2.031376	0.404536
H	-1.677350	3.359276	-0.251061
H	-2.509881	2.225552	-1.335305
C	2.405161	-1.474617	0.402994
H	2.035570	-2.441509	0.752574
H	2.913044	-1.618801	-0.555901
H	3.141340	-1.126134	1.128124
C	2.801431	1.517994	0.666630
H	3.725995	0.945286	0.575466
H	3.014735	2.546364	0.363593
H	2.496958	1.528554	1.718234

TS-NHC•H^+

1 1

C	-2.614628	-2.611166	1.254441
C	-2.045296	-2.877683	-0.120055
C	-0.635136	-2.024066	-0.402271
C	-4.640737	-1.571311	0.192722
C	-3.825775	-2.060527	1.364166
H	-4.266542	-1.939341	2.351819
O	0.249063	-2.253957	0.420394
H	-5.326858	-2.367874	-0.134694
H	-1.728632	-3.918311	-0.244366
C	-2.837410	-2.403782	-1.223416
C	-3.684811	-1.214167	-0.989894
H	-2.994229	-0.471341	-0.555077
O	-0.659164	-1.266474	-1.387114
C	-2.787757	-3.078644	-2.523897
H	-3.786377	-3.517457	-2.679401
H	-2.644356	-2.359109	-3.333569
H	-2.039155	-3.868001	-2.560224
C	1.467741	0.495100	-0.268659
C	1.634337	2.570351	-0.882356
C	-0.718597	1.683195	-0.765557
H	-1.025603	0.908527	-1.473959
N	2.861976	2.166056	-0.719381
N	2.736267	0.866451	-0.334327
N	0.742726	1.561560	-0.624876
C	1.123659	3.922270	-1.273118
H	1.134666	4.025782	-2.366549
H	1.753800	4.696718	-0.835825
C	-1.077910	3.102987	-1.284934
O	-0.179032	4.065798	-0.755850
C	-2.465646	2.555904	0.586014

C	-1.476549	1.570847	0.538777
C	-1.331717	0.641141	1.561794
C	-2.182919	0.731258	2.664323
C	-3.154348	1.729454	2.730169
C	-3.307342	2.646338	1.687817
C	-2.453882	3.387549	-0.674037
H	-0.581200	-0.145191	1.522264
H	-3.803449	1.790341	3.597543
H	-4.069742	3.417500	1.739401
H	-2.575121	4.459192	-0.501537
H	-3.244885	3.063400	-1.358648
C	3.883406	0.036454	-0.083991
C	4.785426	0.435114	0.909019
C	4.031038	-1.132064	-0.837940
C	5.885499	-0.388822	1.130600
C	5.150685	-1.919565	-0.568283
C	6.086395	-1.563920	0.402269
H	6.600270	-0.109081	1.900121
H	5.293155	-2.833765	-1.137973
C	3.036114	-1.548212	-1.892088
H	2.734936	-0.704300	-2.519728
H	2.129905	-1.970077	-1.443568
H	3.476352	-2.310349	-2.536306
C	7.303006	-2.415821	0.651006
H	7.546946	-2.450294	1.715238
H	8.171486	-2.003802	0.127583
H	7.151192	-3.436482	0.294988
C	4.578205	1.687842	1.718903
H	3.543127	1.774860	2.061767
H	4.801353	2.579792	1.128097
H	5.230781	1.680117	2.592788
H	-1.065287	3.148175	-2.380457
H	-2.086482	0.015035	3.474029
H	1.110917	-0.493126	0.014154
C	-4.371767	-0.636276	-2.219439
H	-4.874143	0.296451	-1.960257
H	-3.646006	-0.407918	-3.003863
H	-5.120899	-1.323053	-2.625504
C	-5.477780	-0.350219	0.580266
H	-6.182879	-0.076033	-0.206288
H	-6.053766	-0.571949	1.482478
H	-4.826625	0.504900	0.791395
C	-1.811174	-3.070414	2.435947
H	-0.898675	-2.478125	2.542040
H	-2.401298	-2.990059	3.351051
H	-1.496385	-4.112041	2.311897

TS-truncated NHC•H^+

1 1

C	-2.808241	-1.352879	0.813166
C	-2.067951	-1.155937	-0.488765
C	-0.434022	-1.060582	-0.302356
C	-3.901762	0.888437	0.512449
C	-3.670699	-0.421423	1.225852
H	-4.259390	-0.600736	2.123259
O	0.085229	-2.047255	0.218240
H	-4.741297	0.775270	-0.190765
H	-2.206365	-2.005361	-1.166218
C	-2.295852	0.111312	-1.149868
C	-2.625852	1.279139	-0.301248
H	-1.816266	1.309856	0.443077
O	0.063016	-0.000679	-0.731734
C	-2.258691	0.201611	-2.612306
H	-3.311291	0.328206	-2.917916
H	-1.731273	1.094015	-2.953074
H	-1.865187	-0.699953	-3.078675
C	2.730680	-0.598087	0.404251
C	4.446198	0.712448	0.118988
N	4.186480	0.199560	-1.055466
N	3.122311	-0.611593	-0.852970
N	3.556466	0.232371	1.051401
H	1.885426	-1.154313	0.795702
C	-2.595386	-2.658861	1.521137
H	-2.800491	-3.497726	0.846883
H	-1.557157	-2.759211	1.843928
H	-3.255952	-2.738188	2.386402
C	-2.719918	2.612734	-1.029968
H	-2.861588	3.421031	-0.312315
H	-1.799321	2.823520	-1.578789
H	-3.559613	2.629953	-1.731527
C	-4.265084	1.995531	1.504885
H	-4.564928	2.914085	0.998230
H	-5.103344	1.668154	2.124949
H	-3.418340	2.215417	2.162987
C	3.526165	0.570567	2.473113
H	4.474509	0.290885	2.931246
H	3.354390	1.640661	2.586025
H	2.715332	0.016943	2.940762
C	2.512891	-1.336067	-1.960420
H	1.794608	-2.036577	-1.538222
H	2.002839	-0.622314	-2.605500
H	3.301438	-1.857052	-2.500631
C	5.535473	1.670425	0.433216
H	5.126540	2.599756	0.836898
H	6.222275	1.245523	1.169228
H	6.084010	1.889053	-0.481490

TS-DABCO•H^+

1 1

C	-2.550426	1.720610	0.126198
C	-1.934201	0.694225	1.053759
C	-0.387471	0.377449	0.685562
C	-4.204738	0.001604	-0.663550
C	-3.610815	1.386431	-0.610960
H	-4.097349	2.148733	-1.215942
O	0.382528	1.333853	0.889760

H	-5.021418	-0.072424	0.070314
H	-1.896300	1.062146	2.084595
C	-2.521816	-0.634841	0.984995
C	-3.115353	-1.061710	-0.293554
H	-2.302925	-0.891903	-1.019241
O	-0.148250	-0.761522	0.255478
C	-2.517926	-1.498901	2.165216
H	-3.576337	-1.606192	2.456937
H	-2.179693	-2.507530	1.914085
H	-1.955494	-1.082707	2.998624
C	-1.972947	3.105004	0.171212
H	-0.944234	3.110614	-0.196106
H	-2.575261	3.788729	-0.429443
H	-1.942120	3.476403	1.201139
C	-3.592120	-2.506168	-0.356445
H	-2.790423	-3.197826	-0.088584
H	-4.442843	-2.678449	0.309794
H	-3.902779	-2.750662	-1.372176
C	-4.786934	-0.291720	-2.048459
H	-5.338459	-1.232670	-2.066936
H	-5.480591	0.505804	-2.325928
H	-3.992286	-0.331958	-2.799941
N	4.877430	-0.733304	-0.645674
C	5.127470	0.683801	-0.371961
C	3.866609	1.355978	0.233503
H	5.408624	1.169240	-1.309297
H	5.968482	0.769940	0.319362
N	2.743190	0.378814	0.113306
H	3.573550	2.264263	-0.295184
H	3.978771	1.586460	1.294299
C	3.004972	-0.814824	0.977154
C	4.389999	-1.381997	0.574716
H	2.177923	-1.503828	0.800339
H	2.967747	-0.478604	2.014882
H	4.321698	-2.458332	0.402356
H	5.122580	-1.212428	1.367620
C	3.859533	-0.851463	-1.693452
C	2.586878	-0.053577	-1.310817
H	3.625883	-1.910724	-1.824732
H	4.271740	-0.477654	-2.633312
H	1.668858	-0.640661	-1.357541
H	2.463487	0.853680	-1.905606
H	1.826330	0.821921	0.431585

TS-$NMe_3 \bullet H^+$

1 1

C	-1.345398	1.710273	0.423522
C	-0.776220	0.485219	1.107215
C	0.674950	0.070913	0.535091
C	-3.264411	0.335139	-0.442488
C	-2.500203	1.618413	-0.237720
H	-2.941018	2.518981	-0.660482
O	1.577073	0.890066	0.792464
H	-4.024316	0.234333	0.347014
H	-0.606671	0.668845	2.174014
C	-1.523244	-0.748497	0.897616
C	-2.295186	-0.891306	-0.348802
H	-1.537947	-0.708783	-1.130105
O	0.730921	-1.005347	-0.082104
C	-1.497232	-1.796174	1.917639
H	-2.521051	-1.832912	2.327256
H	-1.324349	-2.778355	1.470766
H	-0.794903	-1.591340	2.723213
C	-0.600968	2.998729	0.618574
H	0.383357	2.955255	0.146853
H	-1.166016	3.832905	0.199265
H	-0.432157	3.189309	1.683853
C	-2.964510	-2.242583	-0.560192
H	-2.239045	-3.056621	-0.501960
H	-3.750918	-2.419327	0.179986
H	-3.415841	-2.283790	-1.551287
C	-3.986249	0.341540	-1.792585
H	-4.653342	-0.514469	-1.902177
H	-4.591996	1.247209	-1.875286
H	-3.264512	0.335903	-2.615270
H	2.895812	0.313213	0.123010
C	3.321085	-0.232067	-1.816809
H	3.171785	0.775933	-2.202962
H	4.112129	-0.735299	-2.375058
H	2.389131	-0.794291	-1.864273
C	3.900109	-1.491011	0.201481
H	4.172159	-1.379723	1.250830
H	2.951568	-2.019257	0.112750
H	4.692216	-2.012150	-0.338572
C	4.920065	0.710822	-0.203341
H	4.715062	1.701336	-0.607969
H	5.138491	0.782946	0.861511
H	5.762815	0.258909	-0.728630
N	3.720010	-0.140424	-0.389198

TS-MeOH

0 1

C	0.830171	1.708369	-0.368899
C	0.137729	0.531913	-1.010426
C	-1.295998	0.121230	-0.274216
C	2.710431	0.196643	0.329442
C	2.024548	1.535959	0.202561
H	2.554870	2.398716	0.600824
O	-2.106081	1.042139	-0.210389
H	3.372857	0.044692	-0.537207
H	-0.151550	0.737595	-2.046256
C	0.802197	-0.740769	-0.865493
C	1.642936	-0.942352	0.340311
H	0.978731	-0.700394	1.182696
O	-1.337946	-1.065298	0.091624
C	0.697782	-1.758522	-1.917437

H	0.553121	-2.758142	-1.505701
H	-0.066703	-1.516654	-2.653782
H	1.681810	-1.761730	-2.415511
H	-3.539257	0.543463	0.832914
O	-4.319320	0.147801	1.261234
C	-4.693615	-0.941484	0.448046
H	-5.459976	-1.514302	0.978182
H	-5.121901	-0.619142	-0.512684
H	-3.844076	-1.602107	0.237784
C	3.570698	0.140088	1.593958
H	4.176393	-0.766689	1.634038
H	4.250171	0.995998	1.612651
H	2.941431	0.183709	2.488576
C	2.208822	-2.345779	0.510728
H	2.726393	-2.427124	1.466831
H	1.409023	-3.089794	0.509977
H	2.919637	-2.592685	-0.283956
C	0.160309	3.044563	-0.503239
H	-0.801873	3.046581	0.012657
H	0.794359	3.834842	-0.096986
H	-0.042747	3.266867	-1.556811

NHC•H^+ pre-complex

1 1

C	-2.989440	-2.785391	0.680481
C	-2.669834	-2.516835	-0.763793
C	-1.485763	-1.635607	-1.116095
C	-5.104156	-1.463683	0.397621
C	-4.147689	-2.343476	1.175537
H	-4.407596	-2.583927	2.205917
O	-0.300967	-1.609853	-0.905097
H	-5.758542	-2.095719	-0.223884
H	-2.613242	-3.453127	-1.333589
C	-3.477235	-1.422383	-1.493959
C	-4.274316	-0.548464	-0.528479
H	-3.533027	-0.062281	0.118389
O	-2.191349	-0.741662	-1.833999
C	-4.182730	-1.838990	-2.762166
H	-5.098333	-2.384037	-2.515856
H	-4.449635	-0.967705	-3.363676
H	-3.540074	-2.491833	-3.357541
C	1.886506	0.320871	-0.379839
C	2.036347	2.485396	-0.336575
C	-0.288691	1.593235	-0.672426
H	-0.574422	0.953274	-1.512252
N	3.255017	2.054763	-0.163825
N	3.139886	0.699730	-0.193691
N	1.161155	1.440543	-0.473954
C	1.536261	3.894001	-0.437789
H	1.724554	4.272049	-1.451859
H	2.059368	4.527150	0.279058
C	-0.614879	3.079431	-0.969943
O	0.164002	3.916510	-0.126195
C	-2.157436	2.237189	0.632320
C	-1.125734	1.299299	0.553962
C	-1.000960	0.278437	1.487617
C	-1.934494	0.209155	2.522729
C	-2.961979	1.148782	2.611824
C	-3.084641	2.167835	1.664711
C	-2.066728	3.224279	-0.508116
H	-0.198984	-0.451704	1.424968
H	-3.671703	1.089527	3.430824
H	-3.884485	2.898182	1.740834
H	-2.274848	4.256695	-0.219813
H	-2.748841	2.949553	-1.319972
C	4.291737	-0.150189	-0.029940
C	4.774534	-0.351350	1.266345
C	4.873102	-0.702479	-1.171305
C	5.895763	-1.164673	1.400570
C	5.994164	-1.510123	-0.979155
C	6.513710	-1.752874	0.292624
H	6.298923	-1.342232	2.394064
H	6.475032	-1.952851	-1.847067
C	4.316224	-0.437729	-2.545280
H	4.110871	0.626311	-2.692496
H	3.380641	-0.982935	-2.706022
H	5.024253	-0.759435	-3.309633
C	7.712636	-2.644881	0.479113
H	7.405354	-3.622978	0.861937
H	8.411541	-2.215457	1.200765
H	8.239284	-2.802789	-0.463625
C	4.110253	0.292564	2.453859
H	3.049319	0.028004	2.508019
H	4.173657	1.382866	2.394146
H	4.588977	-0.029811	3.378883
H	-0.447517	3.339268	-2.021932
H	-1.856999	-0.579764	3.263560
H	1.510273	-0.690683	-0.458658
C	-5.075412	0.538361	-1.239404
H	-5.418664	1.289080	-0.523454
H	-4.454069	1.047954	-1.983021
H	-5.952460	0.129346	-1.751953
C	-5.997596	-0.663615	1.346255
H	-6.765689	-0.110304	0.801605
H	-6.500599	-1.332098	2.050291
H	-5.399699	0.051094	1.920907
C	-1.976708	-3.579877	1.451112
H	-1.010942	-3.061271	1.456862
H	-2.298216	-3.730709	2.483557
H	-1.808237	-4.559233	0.989843

truncated NHC•H^+ pre-complex

1 1

C	3.239590	-1.046562	-0.663350
C	2.152796	-1.228889	0.357048
C	0.728701	-1.493796	-0.094877

C	3.404751	1.371677	0.008970
C	3.837522	0.142489	-0.762249
H	4.668603	0.256829	-1.457047
O	0.137340	-2.289153	-0.776590
H	3.910468	1.383310	0.987603
H	2.441482	-1.981096	1.102572
C	1.532437	0.029053	1.000350
C	1.880771	1.313093	0.244423
H	1.426291	1.208574	-0.750470
O	0.185289	-0.447164	0.565194
C	1.586051	0.102271	2.507410
H	2.588402	0.399201	2.829155
H	0.868654	0.830879	2.890231
H	1.358674	-0.874793	2.940568
C	-2.552688	-0.775184	-0.628777
C	-4.098783	0.632920	-0.028505
N	-3.836131	-0.087224	1.031574
N	-2.876996	-0.954576	0.635476
N	-3.313395	0.227057	-1.081797
H	-1.798374	-1.332695	-1.169725
C	3.612650	-2.262589	-1.459868
H	3.957617	-3.068412	-0.802696
H	2.743087	-2.646035	-2.004459
H	4.403419	-2.035933	-2.177317
C	1.300178	2.558498	0.910823
H	1.365801	3.419731	0.243424
H	0.244119	2.407683	1.154573
H	1.833215	2.804824	1.834751
C	3.814075	2.640336	-0.742331
H	3.619759	3.538603	-0.152888
H	4.882148	2.616576	-0.974042
H	3.264836	2.721053	-1.686865
C	-3.312495	0.794830	-2.430119
H	-4.315806	0.724000	-2.848712
H	-2.996086	1.836546	-2.381662
H	-2.617655	0.226578	-3.044317
C	-2.310525	-1.913556	1.575949
H	-1.661312	-2.585924	1.017782
H	-1.736987	-1.370156	2.325983
H	-3.128507	-2.463212	2.038045
C	-5.094721	1.729538	-0.115110
H	-4.610725	2.668447	-0.394178
H	-5.857972	1.497118	-0.861661
H	-5.570391	1.847271	0.857023

DABCO•H^+ pre-complex

1 1

C	-3.081890	1.548109	-0.261699
C	-2.116544	1.148064	0.817716
C	-0.625885	1.225183	0.564564
C	-3.758892	-0.864977	-0.491604
C	-3.865339	0.612994	-0.802896
H	-4.611579	0.914629	-1.536746
O	0.182269	2.047048	0.206244
H	-4.382965	-1.097066	0.385810
H	-2.350022	1.661003	1.759654
C	-1.828997	-0.354575	1.022998
C	-2.292115	-1.209387	-0.157778
H	-1.701574	-0.875132	-1.022286
O	-0.366777	-0.059688	0.867071
C	-2.096668	-0.907432	2.400811
H	-3.171126	-1.065171	2.530789
H	-1.586181	-1.861224	2.546288
H	-1.754809	-0.205215	3.164298
C	-3.131559	3.009376	-0.599568
H	-2.148094	3.361385	-0.929275
H	-3.856463	3.204758	-1.391737
H	-3.405298	3.603418	0.279211
C	-2.028477	-2.697700	0.060080
H	-1.004034	-2.861417	0.408895
H	-2.714139	-3.122582	0.800087
H	-2.152228	-3.251349	-0.872305
C	-4.281345	-1.693133	-1.667490
H	-4.323022	-2.756668	-1.424346
H	-5.290333	-1.371932	-1.938916
H	-3.637396	-1.563407	-2.544155
N	4.551483	-0.940459	-0.395380
C	4.958597	0.407785	-0.793966
C	3.841387	1.435453	-0.472887
H	5.174719	0.399027	-1.864475
H	5.875631	0.675016	-0.265219
N	2.628749	0.653213	-0.063062
H	3.561956	2.046073	-1.332031
H	4.093617	2.090455	0.362272
C	2.890362	-0.068721	1.227076
C	4.159085	-0.934684	1.015078
H	1.995940	-0.655163	1.441864
H	3.014560	0.686981	2.003772
H	3.969923	-1.960824	1.336369
H	4.992650	-0.543582	1.602491
C	3.416160	-1.367884	-1.214779
C	2.263889	-0.333400	-1.134588
H	3.081120	-2.343688	-0.856371
H	3.745853	-1.481322	-2.249378
H	1.307353	-0.774246	-0.848954
H	2.137250	0.235396	-2.057210
H	1.822519	1.293256	0.067776

NMe_3•H^+ pre-complex

1 1

C	-1.900794	1.743769	-0.021226
C	-0.952996	1.069391	0.929556
C	0.507922	0.923973	0.561950
C	-2.999766	-0.482070	-0.435977
C	-2.867363	1.018562	-0.587684
H	-3.594980	1.520542	-1.223998

O	1.420952	1.634001	0.215652
H	-3.598949	-0.704628	0.461119
H	-1.030265	1.504364	1.934315
C	-0.919852	-0.473674	0.961053
C	-1.597447	-1.101506	-0.257898
H	-1.012279	-0.776697	-1.129701
O	0.559185	-0.410738	0.717357
C	-1.193303	-1.125432	2.293700
H	-2.269683	-1.126666	2.487710
H	-0.838331	-2.157658	2.304757
H	-0.697355	-0.573918	3.095393
C	-1.716735	3.221603	-0.206555
H	-0.710242	3.439886	-0.579588
H	-2.445731	3.622351	-0.913125
H	-1.826077	3.750940	0.746306
C	-1.585516	-2.627641	-0.210223
H	-0.584877	-2.998443	0.032719
H	-2.284588	-3.010631	0.540000
H	-1.866396	-3.045438	-1.178540
C	-3.730472	-1.073921	-1.643298
H	-3.943712	-2.135659	-1.504737
H	-4.681887	-0.559183	-1.800390
H	-3.128365	-0.957278	-2.550981
H	2.868117	0.642248	-0.175852
C	2.952535	-0.953514	-1.457606
H	2.764885	-0.339409	-2.337321
H	3.648727	-1.756881	-1.699084
H	2.017594	-1.358974	-1.071756
C	3.791994	-0.873647	0.852655
H	4.198016	-0.202197	1.607726
H	2.837082	-1.281072	1.182114
H	4.500180	-1.674655	0.639440
C	4.810346	0.559304	-0.874585
H	4.579209	1.151209	-1.758790
H	5.190080	1.201091	-0.081130
H	5.539817	-0.213812	-1.116853
N	3.562513	-0.099531	-0.399572

MeOH pre-complex

0 1

C	-1.214940	1.746521	0.217337
C	-0.104528	0.909561	0.783447
C	1.181730	0.725436	-0.001934
C	-2.590194	-0.341043	-0.055740
C	-2.367198	1.155969	-0.106509
H	-3.193147	1.772010	-0.460259
O	2.027531	1.425532	-0.493995
H	-2.917938	-0.625779	0.956945
H	0.137878	1.224863	1.806571
C	-0.198377	-0.623954	0.647108
C	-1.261403	-1.063211	-0.362715
H	-0.926601	-0.679455	-1.336029
O	1.137088	-0.621202	-0.013852
C	-0.133083	-1.412397	1.933414
H	0.112149	-2.458233	1.738940
H	0.628613	-0.992200	2.594492
H	-1.099105	-1.370506	2.444945
H	3.417053	0.265758	-1.214136
O	4.122748	-0.397703	-1.218928
C	4.473721	-0.608125	0.131261
H	5.261317	-1.365217	0.157346
H	4.861873	0.301535	0.609370
H	3.626826	-0.974715	0.726208
C	-3.695201	-0.745488	-1.033974
H	-3.955777	-1.801148	-0.934221
H	-4.599205	-0.158468	-0.850741
H	-3.377638	-0.564429	-2.066706
C	-1.380835	-2.582627	-0.460039
H	-1.968293	-2.868753	-1.334448
H	-0.392039	-3.039649	-0.561633
H	-1.865162	-3.004620	0.426751
C	-0.949593	3.220173	0.114557
H	-0.073877	3.407743	-0.515992
H	-1.806574	3.746496	-0.310017
H	-0.729896	3.646855	1.099531

NHC•H^+ *ri*-2-NH_2 (***10***)

1 1

C	-0.850915	-0.159540	-0.835989
C	-0.090447	-1.573940	0.619194
C	1.602919	-0.768351	-1.057946
H	1.488282	-0.928767	-2.134251
N	-1.345213	-1.401261	0.931182
N	-1.803629	-0.513362	0.009642
N	0.253582	-0.815967	-0.469065
C	0.932083	-2.467868	1.251215
H	0.803726	-3.489767	0.868953
H	0.801815	-2.474524	2.333470
C	2.484086	-1.880156	-0.428590
O	2.214201	-1.965381	0.963705
C	3.703363	0.162442	-0.498106
C	2.375343	0.497211	-0.752372
C	1.942418	1.817262	-0.749945
C	2.878071	2.812688	-0.477824
C	4.210949	2.480670	-0.228569
C	4.649502	1.154910	-0.238892
C	3.906444	-1.332848	-0.566806
H	0.907552	2.082252	-0.945701
H	4.550678	-1.706227	0.231263
H	4.336338	-1.629649	-1.530326
C	-3.164271	-0.038945	0.036589
C	-3.407423	1.241034	0.536794
C	-4.164722	-0.898439	-0.427510
C	-4.735395	1.668750	0.549891
C	-5.470898	-0.420569	-0.389960
C	-5.773291	0.855987	0.093965

H	-4.960921	2.660063	0.933129
H	-6.273385	-1.059968	-0.748002
C	-3.836554	-2.272843	-0.946322
H	-3.387698	-2.890851	-0.163776
H	-3.125569	-2.223802	-1.777113
H	-4.739693	-2.769780	-1.301405
C	-7.202411	1.327725	0.144313
H	-7.258524	2.412204	0.252787
H	-7.722593	0.876550	0.994881
H	-7.741856	1.038881	-0.760708
C	-2.295018	2.124692	1.039216
H	-1.737481	2.576120	0.211798
H	-1.585494	1.567268	1.657228
H	-2.704008	2.937375	1.640419
H	2.324347	-2.854315	-0.905518
H	-0.963346	0.515243	-1.671830
H	2.569675	3.852323	-0.458253
H	4.926859	3.270213	-0.017038
C	6.085848	0.794679	0.056559
H	6.473781	0.169533	-0.756283
H	6.687374	1.714979	0.067352
H	7.134432	-0.252990	1.457291
H	5.901401	0.605912	2.076562
N	6.167063	0.013084	1.294243

NHC•H^+ *ri*-2-NH_3^+ (***11***)

2 1

C	-0.902737	-0.157480	-0.837101
C	-0.154719	-1.562095	0.636826
C	1.536009	-0.813289	-1.064459
H	1.412092	-0.959651	-2.141614
N	-1.404793	-1.366565	0.950356
N	-1.855805	-0.485882	0.017880
N	0.195228	-0.823010	-0.463401
C	0.853515	-2.470239	1.271981
H	0.690328	-3.496336	0.916637
H	0.745277	-2.448036	2.356285
C	2.386536	-1.952065	-0.448047
O	2.146759	-2.012013	0.949480
C	3.679095	0.045690	-0.536635
C	2.354846	0.423941	-0.761503
C	1.963988	1.754217	-0.743009
C	2.931519	2.728689	-0.497120
C	4.258985	2.363517	-0.292022
C	4.648957	1.019485	-0.307333
C	3.825377	-1.458415	-0.619930
H	0.932265	2.046716	-0.912850
H	4.455151	-1.900047	0.155384
H	4.221837	-1.760509	-1.594985
C	-3.215238	-0.004633	0.040924
C	-3.450887	1.302375	0.468889
C	-4.224604	-0.890352	-0.353165
C	-4.779841	1.729071	0.482763
C	-5.529598	-0.411078	-0.318514
C	-5.825077	0.891751	0.095860
H	-4.998727	2.741164	0.811505
H	-6.337676	-1.070782	-0.623020
C	-3.910141	-2.293883	-0.797449
H	-3.472344	-2.875399	0.018409
H	-3.196687	-2.298097	-1.627294
H	-4.818454	-2.797339	-1.129259
C	-7.253929	1.364246	0.141594
H	-7.310626	2.447620	0.258989
H	-7.780706	0.904107	0.983040
H	-7.786689	1.083897	-0.770302
C	-2.336927	2.226297	0.888814
H	-1.862651	2.693358	0.019247
H	-1.563032	1.703009	1.456890
H	-2.732193	3.027554	1.514262
H	2.187283	-2.922689	-0.915235
H	-1.005329	0.509159	-1.681396
H	2.652538	3.775799	-0.477904
H	5.006134	3.135206	-0.127206
C	6.088322	0.650505	-0.076909
H	6.349882	-0.310584	-0.519100
H	6.765952	1.413046	-0.459390
H	5.840672	-0.214000	1.840734
H	7.375870	0.333240	1.565882
H	6.159873	1.404586	1.894394
N	6.384680	0.534539	1.401639

NHC•H^+ *ri*-2-SO_3H (***12***)

1 1

C	1.898395	-0.251951	0.926859
C	1.033531	-1.541745	-0.586065
C	-0.497719	-0.985869	1.329496
H	-0.264456	-1.239876	2.367860
N	2.246969	-1.295850	-0.996078
N	2.771229	-0.487453	-0.037382
N	0.779751	-0.908267	0.602695
C	-0.020950	-2.406151	-1.206981
H	0.185658	-3.457663	-0.965780
H	-0.013508	-2.281913	-2.289897
C	-1.392627	-2.076917	0.685364
O	-1.281011	-2.003218	-0.727089
C	-2.687898	-0.124280	1.091722
C	-1.354244	0.258693	1.233632
C	-0.982571	1.593323	1.305286
C	-1.980843	2.563902	1.223438
C	-3.315996	2.191461	1.090887
C	-3.687309	0.844397	1.036853
C	-2.814291	-1.629662	1.033431
H	0.055985	1.892572	1.413884
H	-3.512508	-1.979819	0.270287
H	-3.115657	-2.038959	2.003949
C	4.116540	0.021960	-0.139699

C	4.293926	1.331844	-0.586443
C	5.166253	-0.836406	0.199166
C	5.607275	1.792902	-0.675275
C	6.455940	-0.324714	0.091048
C	6.693606	0.982970	-0.342838
H	5.782477	2.808699	-1.018684
H	7.296473	-0.962522	0.351084
C	4.904457	-2.245956	0.657298
H	4.426508	-2.831237	-0.133478
H	4.240967	-2.263890	1.527582
H	5.838650	-2.736528	0.931464
C	8.103714	1.494177	-0.475721
H	8.130691	2.585295	-0.479277
H	8.548442	1.144367	-1.412518
H	8.731135	1.131506	0.341534
C	3.125483	2.209059	-0.951685
H	2.614778	2.581974	-0.058201
H	2.391544	1.668607	-1.555707
H	3.466463	3.073881	-1.521576
H	-1.139861	-3.083592	1.037845
H	2.074215	0.345579	1.809660
H	-1.717774	3.614746	1.264391
H	-4.084667	2.955788	1.026875
C	-5.130460	0.461187	0.863057
H	-5.367027	-0.519980	1.281026
H	-5.809894	1.206460	1.282004
S	-5.519621	0.362877	-0.885220
O	-5.450744	1.691005	-1.468660
O	-4.782903	-0.737904	-1.472657
O	-7.060069	-0.098834	-0.853956
H	-7.637808	0.679711	-0.933540

NHC•H^+ *ri*-2-SO_3^- (***13***)

0 1

C	1.847772	-0.259255	0.923559
C	1.000071	-1.564045	-0.584535
C	-0.547415	-1.001752	1.318626
H	-0.316042	-1.270217	2.354038
N	2.214601	-1.313854	-0.990237
N	2.728369	-0.495864	-0.034034
N	0.736134	-0.925174	0.598414
C	-0.049529	-2.433136	-1.206879
H	0.150418	-3.482170	-0.948022
H	-0.025899	-2.324321	-2.291257
C	-1.446487	-2.083365	0.661999
O	-1.312252	-2.018154	-0.749847
C	-2.728316	-0.120957	1.081541
C	-1.392914	0.249985	1.233376
C	-1.010513	1.580831	1.326255
C	-2.006462	2.554384	1.253334
C	-3.343246	2.188325	1.110471
C	-3.731425	0.846408	1.037511
C	-2.868231	-1.622727	0.992218
H	0.029182	1.873806	1.441678
H	-3.560632	-1.930610	0.205556
H	-3.194111	-2.051582	1.946675
C	4.070205	0.021243	-0.133466
C	4.242105	1.326465	-0.595735
C	5.123665	-0.825837	0.221682
C	5.553258	1.794060	-0.685020
C	6.410929	-0.308246	0.112588
C	6.642819	0.994794	-0.338028
H	5.723971	2.806326	-1.040980
H	7.254008	-0.937581	0.384853
C	4.867510	-2.230557	0.697688
H	4.392355	-2.827876	-0.085740
H	4.203054	-2.240052	1.567405
H	5.803455	-2.713756	0.979149
C	8.050676	1.511887	-0.473423
H	8.071733	2.603026	-0.491021
H	8.500156	1.152586	-1.404388
H	8.677801	1.163363	0.350252
C	3.069715	2.191689	-0.976571
H	2.550986	2.570181	-0.089966
H	2.342613	1.639605	-1.578240
H	3.407658	3.052786	-1.553907
H	-1.204803	-3.092043	1.018209
H	2.015463	0.344804	1.803334
H	-1.739175	3.604230	1.306641
H	-4.107819	2.956699	1.045961
C	-5.167282	0.470826	0.841234
H	-5.398093	-0.506448	1.272056
H	-5.838917	1.213437	1.277438
S	-5.606934	0.364909	-0.916183
O	-5.359837	1.717883	-1.458107
O	-7.033047	-0.026426	-0.910973
O	-4.707561	-0.671379	-1.473616

NHC•H^+ *up*-2-NH_2 (***14***)

1 1

C	-0.317850	-0.426695	0.956546
C	0.475847	1.372216	0.040144
C	2.163087	-0.022342	1.285372
H	2.086915	-0.219862	2.358999
N	-0.792532	1.353230	-0.270456
N	-1.270572	0.221397	0.309559
N	0.805856	0.279146	0.799729
C	1.525505	2.388662	-0.316353
H	1.469909	3.212913	0.409750
C	3.085410	1.195598	1.014429
O	2.779416	1.743624	-0.258416
C	4.192393	-0.803273	0.346610
C	2.854913	-1.148602	0.546097
C	2.352749	-2.373318	0.127597
C	3.217952	-3.259848	-0.513908
C	4.556012	-2.920723	-0.716087

C	5.054161	-1.690973	-0.284981
C	4.478798	0.572121	0.902615
H	1.313360	-2.650270	0.281144
H	5.117895	1.184358	0.263132
H	4.944638	0.507959	1.891480
C	-2.650880	-0.171915	0.168065
C	-2.982900	-1.013867	-0.894700
C	-3.574278	0.323758	1.090780
C	-4.322710	-1.379596	-1.011178
C	-4.898944	-0.074668	0.928232
C	-5.288633	-0.921587	-0.112619
H	-4.617607	-2.035163	-1.825937
H	-5.645033	0.287379	1.630384
C	-3.149027	1.244304	2.203218
H	-2.634857	2.125435	1.808785
H	-2.464260	0.742985	2.894410
H	-4.016494	1.579528	2.772213
C	-6.734900	-1.306414	-0.279488
H	-6.833310	-2.254866	-0.810900
H	-7.266684	-0.543620	-0.856831
H	-7.232920	-1.394512	0.688304
C	-1.938597	-1.497382	-1.865962
H	-1.228217	-2.177148	-1.384218
H	-1.367128	-0.661186	-2.279300
H	-2.406928	-2.033626	-2.691614
H	2.996215	1.964715	1.790003
H	-0.441907	-1.342609	1.515499
H	2.846016	-4.218590	-0.858388
H	5.215373	-3.620210	-1.219058
H	6.094262	-1.428344	-0.450229
C	1.335150	2.954874	-1.720110
H	2.213568	3.574394	-1.916022
H	1.349517	2.121541	-2.436981
H	0.176743	4.388957	-2.574828
H	-0.685930	3.206426	-1.863649
N	0.140387	3.788005	-1.758078

NHC•H$^+$ *up*-2-NH$_3^+$ (***15***)

2 1

C	-0.331604	-0.477607	0.990368
C	0.485807	1.318838	0.112827
C	2.167525	-0.092218	1.317845
H	2.097799	-0.345450	2.380010
N	-0.776995	1.322123	-0.210385
N	-1.275484	0.189055	0.346060
N	0.802844	0.219440	0.853618
C	1.528959	2.344718	-0.229065
H	1.448904	3.184807	0.477794
C	3.078825	1.145239	1.111354
O	2.791046	1.739246	-0.156811
C	4.206407	-0.806362	0.355072
C	2.867347	-1.166413	0.512751
C	2.368828	-2.356587	0.002998
C	3.245210	-3.200279	-0.679772
C	4.587433	-2.851881	-0.832762
C	5.079011	-1.652198	-0.316895
C	4.477566	0.537621	0.991725
H	1.324058	-2.634014	0.110993
H	5.126812	1.186234	0.400351
H	4.920984	0.424429	1.986317
C	-2.661646	-0.183230	0.188496
C	-3.018306	-0.873279	-0.974103
C	-3.558724	0.180972	1.191754
C	-4.359407	-1.217424	-1.108677
C	-4.890458	-0.188486	1.003178
C	-5.304857	-0.884990	-0.132375
H	-4.676509	-1.757352	-1.996876
H	-5.619190	0.078000	1.763178
C	-3.108976	0.930201	2.417591
H	-2.544911	1.828853	2.150678
H	-2.467936	0.307888	3.049956
H	-3.970256	1.232874	3.013434
C	-6.747002	-1.275072	-0.317831
H	-6.841847	-2.358926	-0.425855
H	-7.155696	-0.820099	-1.224353
H	-7.356226	-0.958945	0.530160
C	-1.996578	-1.209649	-2.027100
H	-1.154220	-1.768530	-1.607466
H	-1.593724	-0.301046	-2.484992
H	-2.445806	-1.815814	-2.813749
H	2.970448	1.890077	1.906831
H	-0.468833	-1.404035	1.530812
H	2.878697	-4.132343	-1.095439
H	5.255355	-3.519144	-1.366957
H	6.121368	-1.380363	-0.448664
C	1.381964	2.838566	-1.666223
H	2.202253	3.516245	-1.898044
H	1.387633	1.999943	-2.362556
H	-0.000354	3.883784	-2.829086
H	-0.716837	2.988306	-1.627777
H	0.043803	4.422175	-1.271998
N	0.095623	3.580180	-1.854887

NHC•H$^+$ *up*-2-SO$_3$H (***16***)

1 1

C	-0.260441	-1.505248	0.682341
C	0.492732	0.522925	0.624437
C	2.218661	-1.224123	1.162161
H	2.134699	-1.887126	2.028448
N	-0.782494	0.622926	0.381825
N	-1.237629	-0.653702	0.415064
N	0.855096	-0.781702	0.825569
C	1.511638	1.623227	0.727004
H	1.403934	2.111935	1.705325
C	3.081162	0.015782	1.507032
O	2.792298	1.056150	0.578133

C	4.309268	-1.429794	0.073991
C	2.984931	-1.868658	0.026825
C	2.557993	-2.786779	-0.922400
C	3.487336	-3.260103	-1.848964
C	4.812394	-2.825618	-1.807613
C	5.234496	-1.908978	-0.844050
C	4.507795	-0.445455	1.203817
H	1.528848	-3.131754	-0.962907
H	5.137388	0.407758	0.943790
H	4.939227	-0.934353	2.083447
C	-2.624314	-0.953383	0.163268
C	-3.125296	-0.661851	-1.111355
C	-3.390141	-1.495138	1.196700
C	-4.465577	-0.956242	-1.338864
C	-4.727612	-1.770920	0.908352
C	-5.278802	-1.510132	-0.345163
H	-4.887285	-0.748891	-2.318837
H	-5.352935	-2.191519	1.690947
C	-2.823346	-1.771602	2.565713
H	-2.154517	-0.972671	2.896703
H	-2.264780	-2.712740	2.588267
H	-3.632280	-1.857211	3.292028
C	-6.729973	-1.794791	-0.628277
H	-6.845715	-2.317343	-1.581053
H	-7.296152	-0.860999	-0.696273
H	-7.176124	-2.404618	0.158993
C	-2.259218	-0.054156	-2.183130
H	-1.316015	-0.599584	-2.292251
H	-2.012625	0.985015	-1.944140
H	-2.778312	-0.078149	-3.141911
H	2.921816	0.366963	2.532495
H	-0.356408	-2.577778	0.767836
H	3.175751	-3.970115	-2.607198
H	5.521769	-3.201601	-2.537256
H	6.264754	-1.568457	-0.819487
C	1.395459	2.664445	-0.383023
H	2.232265	3.357230	-0.277759
H	1.415833	2.208344	-1.374461
S	-0.104588	3.649246	-0.267215
O	-0.462312	3.756559	1.131854
O	-1.072951	3.222178	-1.259903
O	0.450319	5.085456	-0.722450
H	0.111763	5.293885	-1.610387

NHC•H^+ *up*-2-SO_3^- (***17***)

0 1

C	-0.277020	-1.502076	0.619154
C	0.473485	0.536246	0.602939
C	2.187588	-1.238307	1.121906
H	2.077083	-1.926990	1.965277
N	-0.809140	0.634832	0.393722
N	-1.258756	-0.644104	0.396108
N	0.837773	-0.779587	0.763776
C	1.500201	1.631039	0.716579
H	1.373083	2.117973	1.692978
C	3.040440	-0.009930	1.522768
O	2.783651	1.040167	0.606485
C	4.311632	-1.424372	0.096191
C	2.987193	-1.854296	-0.005495
C	2.585946	-2.740177	-0.995146
C	3.541176	-3.191846	-1.906378
C	4.866366	-2.766853	-1.810446
C	5.262436	-1.881766	-0.806831
C	4.476031	-0.471722	1.258642
H	1.555663	-3.074484	-1.077166
H	5.117456	0.384685	1.041258
H	4.876397	-0.986807	2.138285
C	-2.647480	-0.932264	0.150469
C	-3.174198	-0.551127	-1.089704
C	-3.394389	-1.546909	1.157107
C	-4.519500	-0.832117	-1.310381
C	-4.736304	-1.806552	0.876498
C	-5.312525	-1.457300	-0.344073
H	-4.960385	-0.555218	-2.264423
H	-5.345686	-2.283400	1.639291
C	-2.801507	-1.909941	2.494720
H	-2.153273	-1.116143	2.875904
H	-2.211606	-2.830418	2.440817
H	-3.597409	-2.075586	3.221707
C	-6.771001	-1.719113	-0.613193
H	-6.921722	-2.085470	-1.631445
H	-7.350053	-0.796522	-0.507510
H	-7.177857	-2.453076	0.084771
C	-2.328819	0.128114	-2.134432
H	-1.408140	-0.434938	-2.322229
H	-2.035497	1.134457	-1.816212
H	-2.881093	0.197529	-3.072594
H	2.847943	0.316809	2.551358
H	-0.367036	-2.576780	0.673695
H	3.249534	-3.875726	-2.696065
H	5.596350	-3.123888	-2.529359
H	6.292924	-1.547009	-0.741472
C	1.423719	2.680239	-0.382256
H	2.301012	3.318255	-0.263123
H	1.448915	2.217920	-1.370829
S	-0.027462	3.770751	-0.288627
O	-0.404169	3.754151	1.142327
O	-1.040063	3.182534	-1.189307
O	0.480935	5.074523	-0.759751

TS-NHC•H^+ *ri*-2-NH_2

1 1

C	-2.059267	-2.976773	1.420601
C	-1.363827	-3.350228	0.131506
C	-0.051461	-2.361851	-0.198024
C	-4.112977	-2.356976	0.112404

C	-3.333140	-2.578763	1.384738
H	-3.855386	-2.384239	2.319543
O	0.794718	-2.358655	0.692953
H	-4.674784	-3.270129	-0.138662
H	-0.914234	-4.347478	0.175022
C	-2.126802	-3.135582	-1.068028
C	-3.119464	-2.038824	-1.050603
H	-2.555892	-1.165918	-0.680697
O	-0.101731	-1.756932	-1.282609
C	-1.916257	-3.972056	-2.253817
H	-2.847123	-4.545344	-2.393191
H	-1.802847	-3.359170	-3.151217
H	-1.083123	-4.663181	-2.139619
C	1.663145	0.436125	-0.331213
C	1.534747	2.413294	-1.217693
C	-0.659915	1.200814	-1.007181
H	-0.825380	0.301817	-1.608364
N	2.803598	2.226958	-0.988195
N	2.862953	0.985790	-0.431935
N	0.797859	1.322489	-0.836480
C	0.837686	3.607976	-1.791741
H	0.869321	3.568836	-2.889071
H	1.329893	4.520248	-1.454381
C	-1.214627	2.465684	-1.718478
O	-0.487550	3.616691	-1.314406
C	-2.564029	1.953907	0.188574
C	-1.432390	1.145916	0.292152
C	-1.178924	0.389989	1.432084
C	-2.079497	0.481025	2.491813
C	-3.203399	1.302224	2.397994
C	-3.471990	2.045184	1.244795
C	-2.636962	2.610714	-1.168486
H	-0.313515	-0.263766	1.509680
H	-2.933045	3.659952	-1.115003
H	-3.349351	2.084918	-1.815682
C	4.113243	0.383895	-0.055578
C	4.916368	1.052182	0.875519
C	4.455688	-0.844589	-0.630065
C	6.120160	0.444681	1.222709
C	5.671700	-1.406248	-0.240303
C	6.515316	-0.777932	0.675061
H	6.761985	0.936832	1.948717
H	5.965682	-2.360103	-0.669753
C	3.565243	-1.554382	-1.618906
H	3.152915	-0.864317	-2.360922
H	2.723308	-2.046410	-1.119552
H	4.135032	-2.320341	-2.146569
C	7.837429	-1.392003	1.052894
H	8.074454	-1.199904	2.101670
H	8.643905	-0.964225	0.448996
H	7.833883	-2.471169	0.888244
C	4.503204	2.361466	1.494801
H	3.454951	2.343473	1.806530
H	4.617605	3.185436	0.786013
H	5.119202	2.570845	2.370255
H	-1.171426	2.367226	-2.809802
H	1.448427	-0.548061	0.079084
C	-3.772083	-1.715378	-2.386682
H	-4.400296	-0.829309	-2.289082
H	-3.018202	-1.498482	-3.147631
H	-4.399504	-2.539232	-2.740674
C	-5.114694	-1.211558	0.275983
H	-5.785456	-1.134376	-0.581429
H	-5.726808	-1.383258	1.165200
H	-4.584823	-0.261233	0.404074
C	-1.293020	-3.163226	2.697376
H	-0.470040	-2.446981	2.766439
H	-1.952577	-3.037102	3.558329
H	-0.845075	-4.161638	2.741806
H	-1.907016	-0.097752	3.393722
H	-3.894344	1.361705	3.234677
C	-4.695076	2.924507	1.138659
H	-5.264187	2.636860	0.245979
H	-5.344679	2.734568	2.005380
H	-5.136625	4.897309	0.868498
H	-3.857422	4.644281	1.838669
N	-4.302362	4.327718	0.980909

TS-NHC•H^+ *ri*-2-NH_3^+

2 1

C	-2.048517	-2.919220	1.494642
C	-1.323017	-3.348029	0.238658
C	-0.043879	-2.343976	-0.121756
C	-4.097911	-2.428217	0.126459
C	-3.329281	-2.549652	1.418636
H	-3.869747	-2.316345	2.334215
O	0.801824	-2.280773	0.768960
H	-4.635177	-3.369101	-0.068473
H	-0.849493	-4.328719	0.349592
C	-2.079578	-3.233387	-0.981715
C	-3.101111	-2.164751	-1.046963
H	-2.559278	-1.256011	-0.736576
O	-0.106430	-1.778051	-1.227870
C	-1.837522	-4.142976	-2.104331
H	-2.756608	-4.742049	-2.213953
H	-1.728412	-3.590746	-3.041105
H	-0.993225	-4.808396	-1.935098
C	1.712414	0.437208	-0.344896
C	1.581927	2.420967	-1.221133
C	-0.597313	1.177220	-1.079932
H	-0.737957	0.254756	-1.650674
N	2.847246	2.243353	-0.968963
N	2.907785	0.998894	-0.419655
N	0.848551	1.319935	-0.861386
C	0.888809	3.609459	-1.814421
H	0.981786	3.589556	-2.908164

H	1.337992	4.527620	-1.435867
C	-1.133536	2.410812	-1.848926
O	-0.463785	3.583389	-1.413256
C	-2.565046	1.940681	0.006569
C	-1.420145	1.160919	0.188941
C	-1.195550	0.461129	1.366219
C	-2.135720	0.566361	2.393112
C	-3.274778	1.346356	2.225539
C	-3.504956	2.041891	1.030721
C	-2.589685	2.528598	-1.387593
H	-0.319200	-0.169752	1.496656
H	-2.909508	3.571468	-1.444369
H	-3.242922	1.937956	-2.039924
C	4.157108	0.397632	-0.037051
C	4.960744	1.069364	0.891131
C	4.497723	-0.834825	-0.605253
C	6.162831	0.461050	1.242560
C	5.712302	-1.396281	-0.211294
C	6.556349	-0.765064	0.701660
H	6.804966	0.955898	1.966369
H	6.005144	-2.352558	-0.635940
C	3.610443	-1.550909	-1.592949
H	3.193594	-0.865327	-2.336714
H	2.772809	-2.050039	-1.093212
H	4.185151	-2.313518	-2.119950
C	7.876821	-1.379957	1.083136
H	8.116350	-1.178859	2.129577
H	8.683325	-0.960313	0.473648
H	7.869446	-2.460502	0.928174
C	4.552128	2.383120	1.503994
H	3.502244	2.372936	1.810459
H	4.676502	3.204220	0.793594
H	5.164949	2.590712	2.382064
H	-1.026914	2.296959	-2.933689
H	1.493117	-0.548994	0.061407
C	-3.750470	-1.950934	-2.406830
H	-4.387821	-1.066149	-2.379536
H	-2.995519	-1.783928	-3.178982
H	-4.367553	-2.805906	-2.698940
C	-5.129375	-1.300394	0.202316
H	-5.795097	-1.301279	-0.662290
H	-5.743093	-1.422202	1.098511
H	-4.623174	-0.330629	0.261550
C	-1.299892	-3.028160	2.790762
H	-0.479341	-2.307052	2.833058
H	-1.973003	-2.860252	3.633699
H	-0.849336	-4.020737	2.896087
H	-1.985054	0.021607	3.319034
H	-4.009130	1.399385	3.025134
C	-4.755108	2.862740	0.868086
H	-5.007604	3.034017	-0.178069
H	-5.607975	2.402729	1.367994
H	-3.816388	4.749480	1.071818
H	-5.437304	4.791637	1.395055
H	-4.387232	4.151728	2.499253
N	-4.587929	4.227464	1.497619

TS-NHC•H^+ *ri*-2-SO_3H

1 1

C	0.638292	3.618389	1.648370
C	-0.226035	3.919227	0.445063
C	-1.203796	2.620082	0.021691
C	2.680463	3.846118	0.204342
C	1.967117	3.644275	1.518912
H	2.590475	3.506000	2.400288
O	-1.953095	2.262585	0.927038
H	2.898439	4.916843	0.066354
H	-0.952212	4.714433	0.640264
C	0.478369	4.099074	-0.793656
C	1.753813	3.367220	-0.958432
H	1.509812	2.325095	-0.692425
O	-1.041373	2.184674	-1.129999
C	-0.055641	4.968957	-1.845722
H	0.659938	5.800567	-1.946348
H	-0.059260	4.456917	-2.811291
H	-1.039755	5.367500	-1.606371
C	-2.074918	-0.523946	-0.427294
C	-1.451063	-2.286215	-1.532097
C	0.298769	-0.492353	-1.321083
H	0.140685	0.473336	-1.809482
N	-2.694672	-2.507521	-1.214061
N	-3.065934	-1.395532	-0.521833
N	-1.035137	-1.062288	-1.075153
C	-0.490062	-3.162047	-2.275663
H	-0.640516	-3.049097	-3.357802
H	-0.650567	-4.204465	-2.000605
C	1.121408	-1.454403	-2.218789
O	0.819003	-2.802581	-1.898384
C	2.453152	-0.748086	-0.365100
C	1.148390	-0.342148	-0.079323
C	0.799121	0.161833	1.166886
C	1.783731	0.229977	2.153613
C	3.083551	-0.186915	1.883500
C	3.438171	-0.665269	0.616614
C	2.574410	-1.207770	-1.799664
H	-0.210054	0.502831	1.385672
H	3.157711	-2.123663	-1.918747
H	3.020747	-0.423576	-2.422288
C	-4.402665	-1.229229	-0.018312
C	-4.904316	-2.196554	0.860118
C	-5.128192	-0.104180	-0.424156
C	-6.201787	-2.011169	1.329681
C	-6.420945	0.029502	0.082954
C	-6.974494	-0.910935	0.950718
H	-6.616451	-2.742730	2.018286
H	-7.009632	0.892693	-0.215439

C	-4.562389	0.936477	-1.357910
H	-4.025240	0.481715	-2.195354
H	-3.866418	1.605289	-0.839486
H	-5.370389	1.546209	-1.764064
C	-8.384912	-0.758942	1.456046
H	-8.469859	-1.097586	2.491061
H	-9.072836	-1.361743	0.854861
H	-8.715542	0.279947	1.400779
C	-4.083509	-3.380126	1.300255
H	-3.064788	-3.083000	1.565124
H	-4.008349	-4.125258	0.504369
H	-4.542820	-3.849391	2.171122
H	0.934816	-1.273202	-3.283893
H	-2.119353	0.437109	0.080132
C	2.375965	3.420542	-2.346175
H	3.243113	2.760166	-2.389587
H	1.667645	3.078872	-3.104963
H	2.705503	4.431244	-2.605583
C	4.007531	3.085078	0.173046
H	4.599354	3.339848	-0.707779
H	4.597073	3.339097	1.057782
H	3.825673	2.004863	0.180776
C	-0.055616	3.396414	2.960434
H	-0.622617	2.461833	2.950333
H	0.671097	3.368008	3.774745
H	-0.775195	4.197270	3.161061
H	1.534747	0.616679	3.136230
H	3.840469	-0.132940	2.660437
C	4.845472	-1.118140	0.343244
H	5.131704	-1.016612	-0.706157
H	5.576451	-0.602217	0.969699
S	4.996405	-2.863149	0.731499
O	4.189701	-3.623575	-0.201423
O	4.845264	-3.052587	2.163372
O	6.529332	-3.156688	0.342438
H	7.079146	-3.134164	1.144652

TS-NHC•H^+ *ri*-2-SO_3^-

0 1

C	0.718337	3.594516	1.633622
C	-0.134709	3.902731	0.425034
C	-1.162381	2.632818	0.014544
C	2.766812	3.754313	0.189727
C	2.047499	3.588037	1.506174
H	2.666451	3.442227	2.389339
O	-1.905443	2.296958	0.932681
H	3.004239	4.818522	0.032647
H	-0.835418	4.724447	0.604896
C	0.574505	4.038181	-0.815524
C	1.831372	3.272892	-0.965724
H	1.567640	2.240777	-0.678586
O	-1.037648	2.202186	-1.143100
C	0.062154	4.901038	-1.885172
H	0.795367	5.714858	-1.999882
H	0.046439	4.370529	-2.840390
H	-0.913447	5.324623	-1.653710
C	-2.060672	-0.500108	-0.408479
C	-1.456192	-2.251857	-1.538587
C	0.319658	-0.488245	-1.283787
H	0.174524	0.481944	-1.767601
N	-2.705260	-2.461080	-1.231930
N	-3.064480	-1.355336	-0.523204
N	-1.025847	-1.042546	-1.058825
C	-0.500832	-3.127585	-2.289769
H	-0.638599	-2.988056	-3.371010
H	-0.683138	-4.172824	-2.039591
C	1.140503	-1.450571	-2.183509
O	0.808261	-2.799215	-1.890566
C	2.460185	-0.771783	-0.309022
C	1.156175	-0.358998	-0.031402
C	0.797507	0.135645	1.216336
C	1.777906	0.181694	2.208440
C	3.077009	-0.241575	1.940537
C	3.448076	-0.707655	0.672887
C	2.590922	-1.231539	-1.741914
H	-0.209765	0.484848	1.430407
H	3.163092	-2.157689	-1.833370
H	3.062081	-0.459320	-2.361787
C	-4.401141	-1.179282	-0.024336
C	-4.917310	-2.149265	0.842760
C	-5.113153	-0.043375	-0.423270
C	-6.215498	-1.955237	1.306903
C	-6.407437	0.098897	0.077919
C	-6.975127	-0.843961	0.933699
H	-6.641177	-2.688721	1.986714
H	-6.985743	0.970802	-0.215504
C	-4.530090	0.999152	-1.344071
H	-3.998642	0.544987	-2.185501
H	-3.823155	1.650144	-0.817952
H	-5.327686	1.626343	-1.744405
C	-8.386850	-0.683016	1.432970
H	-8.476507	-1.013822	2.470211
H	-9.075282	-1.287639	0.834175
H	-8.713245	0.356748	1.369428
C	-4.109887	-3.344490	1.275998
H	-3.091275	-3.058749	1.553523
H	-4.032800	-4.080248	0.471636
H	-4.580649	-3.820885	2.136861
H	0.968536	-1.251876	-3.248469
H	-2.094570	0.453771	0.112546
C	2.456184	3.289053	-2.353348
H	3.313770	2.615766	-2.382398
H	1.744007	2.943102	-3.106799
H	2.800661	4.289823	-2.631850
C	4.079171	2.967611	0.174062
H	4.676463	3.194013	-0.710856

H	4.672897	3.228446	1.054128
H	3.877233	1.891594	0.204506
C	0.018135	3.401541	2.946802
H	-0.561997	2.475169	2.947197
H	0.742856	3.371755	3.762886
H	-0.689699	4.215824	3.135498
H	1.525594	0.557816	3.194931
H	3.828447	-0.205357	2.723929
C	4.848369	-1.161710	0.399166
H	5.135632	-0.994212	-0.642023
H	5.566360	-0.652703	1.046348
S	5.068369	-2.937263	0.705216
O	6.493825	-3.183343	0.398449
O	4.135165	-3.608881	-0.228364
O	4.720904	-3.127085	2.129169

TS-NHC•H^+ *up*-2-NH_2

1 1

C	-3.179269	-2.586354	1.061512
C	-2.620669	-2.832954	-0.321166
C	-1.085192	-2.170582	-0.520275
C	-5.005064	-1.191390	0.046530
C	-4.303207	-1.877499	1.192905
H	-4.749613	-1.766410	2.179270
O	-0.272635	-2.582073	0.303879
H	-5.779623	-1.859352	-0.361983
H	-2.449942	-3.895805	-0.520109
C	-3.303282	-2.164638	-1.392623
C	-3.963758	-0.879172	-1.075441
H	-3.188633	-0.289754	-0.557386
O	-0.973181	-1.357636	-1.451329
C	-3.330639	-2.734620	-2.743512
H	-4.384463	-2.975839	-2.954730
H	-3.037555	-1.988173	-3.486162
H	-2.729027	-3.637088	-2.833575
C	1.336901	0.037014	-0.196385
C	1.786118	2.110636	-0.679377
C	-0.668186	1.521687	-0.611510
H	-1.067766	0.847177	-1.374301
N	2.945843	1.530119	-0.543424
N	2.643799	0.239751	-0.236113
N	0.764715	1.210510	-0.485702
C	1.457693	3.555291	-0.945000
H	1.459523	3.729642	-2.032314
C	-0.838882	3.008156	-1.020558
O	0.170968	3.796003	-0.412717
C	-2.304089	2.506099	0.801075
C	-1.444390	1.411280	0.682973
C	-1.427366	0.400233	1.636654
C	-2.273771	0.515486	2.740636
C	-3.115144	1.618875	2.877042
C	-3.140340	2.621064	1.904663
C	-2.175515	3.419095	-0.394838
H	-0.780585	-0.468983	1.542934
H	-2.165069	4.482181	-0.144728
H	-2.992618	3.244977	-1.103296
C	3.674855	-0.737699	-0.017764
C	4.629565	-0.477628	0.973163
C	3.668902	-1.898736	-0.797129
C	5.618541	-1.438135	1.165367
C	4.682868	-2.826601	-0.555564
C	5.663928	-2.613308	0.411258
H	6.369386	-1.267127	1.932402
H	4.704934	-3.738107	-1.146672
C	2.623263	-2.167117	-1.850197
H	2.412338	-1.276483	-2.449198
H	1.680075	-2.498648	-1.402117
H	2.969180	-2.954053	-2.521701
C	6.765690	-3.616568	0.629228
H	7.005127	-3.712208	1.690805
H	7.678043	-3.300700	0.113638
H	6.487496	-4.599702	0.245079
C	4.591920	0.771871	1.814242
H	3.581307	0.976125	2.180358
H	4.909901	1.644367	1.237883
H	5.253938	0.662203	2.674132
H	-0.804431	3.136948	-2.108853
H	0.847232	-0.908531	0.022489
C	-4.504945	-0.100639	-2.266073
H	-4.879192	0.869696	-1.937475
H	-3.716995	0.085066	-3.000507
H	-5.324912	-0.630957	-2.760019
C	-5.684802	0.098103	0.511302
H	-6.313433	0.528661	-0.270053
H	-6.322280	-0.113867	1.373628
H	-4.933727	0.835709	0.813734
C	-2.481588	-3.239998	2.218390
H	-1.497167	-2.794293	2.383049
H	-3.078384	-3.139869	3.127201
H	-2.316000	-4.304910	2.023142
H	-2.275958	-0.264339	3.495534
H	-3.761969	1.696840	3.744748
H	-3.801641	3.475599	2.010482
C	2.436901	4.515845	-0.273181
H	1.938004	5.493544	-0.240918
H	2.590853	4.189886	0.759133
H	4.444316	4.844232	-0.380660
H	3.667418	5.119897	-1.782869
N	3.706846	4.495265	-0.982870

TS-NHC•H^+ *up*-2-NH_3^+

2 1

C	-3.122762	-2.570995	1.124057
C	-2.602296	-2.824923	-0.274347
C	-1.120785	-2.117503	-0.523852
C	-5.027965	-1.241966	0.163742

C	-4.257646	-1.887775	1.287081
H	-4.669215	-1.775262	2.288283
O	-0.249145	-2.514679	0.251365
H	-5.820108	-1.927066	-0.175852
H	-2.406147	-3.887005	-0.452859
C	-3.365769	-2.220425	-1.337471
C	-4.068250	-0.955986	-1.035691
H	-3.281273	-0.314243	-0.602420
O	-1.068694	-1.272776	-1.434574
C	-3.412259	-2.831605	-2.668221
H	-4.466936	-3.075034	-2.869781
H	-3.128122	-2.099224	-3.429992
H	-2.806221	-3.731977	-2.744932
C	1.314656	0.034998	-0.233212
C	1.791685	2.091641	-0.703942
C	-0.663282	1.580044	-0.680814
H	-1.073690	0.915331	-1.445430
N	2.943324	1.506151	-0.536973
N	2.626494	0.218646	-0.238532
N	0.759973	1.216855	-0.536965
C	1.523780	3.541713	-0.987116
H	1.579448	3.722079	-2.071478
C	-0.782667	3.070439	-1.102682
O	0.248338	3.846320	-0.489170
C	-2.275836	2.625244	0.710908
C	-1.452418	1.502190	0.606526
C	-1.473087	0.496277	1.565256
C	-2.319969	0.648176	2.664165
C	-3.126306	1.779467	2.787209
C	-3.116111	2.774160	1.807102
C	-2.107831	3.528481	-0.488075
H	-0.852211	-0.392822	1.481086
H	-2.065026	4.592002	-0.243677
H	-2.921772	3.379203	-1.205092
C	3.634456	-0.785683	-0.017027
C	4.548568	-0.588488	1.023800
C	3.631590	-1.913931	-0.844168
C	5.506141	-1.580115	1.217395
C	4.612683	-2.874270	-0.598944
C	5.556396	-2.723958	0.416993
H	6.225288	-1.460290	2.023290
H	4.637869	-3.762831	-1.223528
C	2.621728	-2.112224	-1.946243
H	2.469417	-1.197534	-2.526871
H	1.650513	-2.422868	-1.545438
H	2.966027	-2.891428	-2.627059
C	6.623326	-3.762791	0.638247
H	6.846129	-3.876434	1.701349
H	7.550572	-3.468845	0.136444
H	6.320245	-4.732375	0.239158
C	4.504839	0.626727	1.912720
H	3.480092	0.885180	2.193053
H	4.943070	1.495841	1.413602
H	5.072624	0.441614	2.825168
H	-0.731516	3.195172	-2.189637
H	0.810112	-0.910058	-0.023389
C	-4.725211	-0.259901	-2.219408
H	-5.093404	0.720433	-1.915336
H	-4.012797	-0.103298	-3.032621
H	-5.573453	-0.834041	-2.603884
C	-5.688386	0.058787	0.627212
H	-6.374003	0.454351	-0.123971
H	-6.262967	-0.125836	1.538538
H	-4.926754	0.814028	0.849659
C	-2.368894	-3.195029	2.262137
H	-1.386623	-2.731316	2.383717
H	-2.932706	-3.093817	3.191572
H	-2.191921	-4.259336	2.073968
H	-2.350865	-0.124946	3.425169
H	-3.775043	1.884335	3.650482
H	-3.750950	3.649451	1.902335
C	2.501224	4.447247	-0.242494
H	2.240221	5.489420	-0.419829
H	2.478922	4.234291	0.826469
H	4.561034	4.802497	-0.188563
H	4.179345	3.240143	-0.613734
H	4.013913	4.479116	-1.709715
N	3.902329	4.227541	-0.722426

TS-NHC•H^+ *up*-2-SO_3H

1 1

C	4.404877	1.865379	0.926153
C	3.909499	2.177713	-0.468139
C	2.257119	1.976460	-0.615096
C	5.746241	-0.043436	-0.004040
C	5.285589	0.876931	1.099019
H	5.701694	0.702448	2.089441
O	1.608120	2.662905	0.172410
H	6.669360	0.355887	-0.452720
H	4.053052	3.230067	-0.733957
C	4.355821	1.279986	-1.500686
C	4.642379	-0.116014	-1.107387
H	3.738667	-0.434952	-0.560441
O	1.893228	1.161597	-1.479662
C	4.501153	1.738186	-2.885682
H	5.566049	1.630761	-3.143617
H	3.960555	1.073441	-3.565166
H	4.194161	2.773040	-3.023819
C	-0.727877	0.674098	-0.140365
C	-1.815954	-1.176758	-0.437700
C	0.687410	-1.398995	-0.527677
H	1.239292	-0.917704	-1.339688
N	-2.732555	-0.264257	-0.301458
N	-2.035252	0.885858	-0.110545
N	-0.560704	-0.635892	-0.360085
C	-1.988917	-2.655416	-0.632599

H	-2.150660	-2.864069	-1.699629
C	0.350525	-2.874424	-0.868041
O	-0.817459	-3.285790	-0.164890
C	2.003329	-2.805939	0.857529
C	1.527919	-1.499345	0.725166
C	1.881545	-0.503927	1.628219
C	2.706030	-0.846715	2.701082
C	3.162532	-2.155585	2.854143
C	2.820172	-3.144566	1.929105
C	1.523483	-3.668786	-0.286136
H	1.534719	0.521188	1.518126
H	1.194830	-4.665880	0.014668
H	2.308097	-3.784175	-1.041700
C	-2.703602	2.147388	0.065933
C	-3.647411	2.252157	1.094997
C	-2.374746	3.201021	-0.793197
C	-4.282831	3.481960	1.243436
C	-3.042555	4.409192	-0.591792
C	-3.997783	4.567042	0.411297
H	-5.016148	3.596620	2.037372
H	-2.810084	5.245843	-1.244881
C	-1.348241	3.071561	-1.890494
H	-1.450772	2.127730	-2.433959
H	-0.328484	3.121602	-1.493081
H	-1.468234	3.887567	-2.604267
C	-4.727777	5.872899	0.583194
H	-4.911635	6.084106	1.639007
H	-5.699423	5.835705	0.080672
H	-4.161784	6.702354	0.154942
C	-3.961714	1.102290	2.015731
H	-3.047159	0.618222	2.371917
H	-4.556355	0.337952	1.507657
H	-4.518005	1.462606	2.882155
H	0.203782	-3.023500	-1.943495
H	0.042775	1.431771	-0.010147
C	4.936831	-1.082040	-2.245971
H	5.008560	-2.099151	-1.858850
H	4.135650	-1.071095	-2.988980
H	5.880614	-0.842016	-2.745374
C	6.048129	-1.443205	0.535172
H	6.521809	-2.073720	-0.219227
H	6.731733	-1.368473	1.384893
H	5.126786	-1.926210	0.877327
C	3.940145	2.755166	2.042058
H	2.874748	2.610625	2.238967
H	4.505710	2.548350	2.952787
H	4.070138	3.810618	1.780453
H	2.994256	-0.084875	3.418337
H	3.797421	-2.407064	3.697379
H	3.183875	-4.160441	2.048282
C	-3.136744	-3.240618	0.183884
H	-3.101982	-4.326446	0.081680
H	-3.072636	-2.964786	1.237948
S	-4.751459	-2.715253	-0.414451
O	-5.353467	-1.769970	0.506991
O	-4.633201	-2.414643	-1.826078
O	-5.577109	-4.088816	-0.300579
H	-6.190406	-4.034113	0.452581

TS-NHC•H^+ *up*-2-SO_3

0 1

C	4.420070	1.879474	0.921300
C	3.901273	2.194445	-0.463021
C	2.242097	2.007009	-0.589733
C	5.745914	-0.020131	-0.044770
C	5.306911	0.892923	1.074121
H	5.740868	0.713233	2.055891
O	1.608189	2.682075	0.217740
H	6.645535	0.395876	-0.525436
H	4.049568	3.244703	-0.734853
C	4.314926	1.288552	-1.501130
C	4.601989	-0.107179	-1.106366
H	3.719990	-0.420040	-0.522793
O	1.867959	1.212900	-1.469017
C	4.446957	1.742269	-2.889520
H	5.514300	1.651753	-3.145212
H	3.915733	1.069991	-3.567943
H	4.127303	2.773374	-3.028066
C	-0.762756	0.679269	-0.130088
C	-1.843494	-1.187654	-0.406292
C	0.667242	-1.373450	-0.512097
H	1.206087	-0.882264	-1.327191
N	-2.761929	-0.273178	-0.292473
N	-2.071187	0.882699	-0.111564
N	-0.588711	-0.631666	-0.330925
C	-2.001391	-2.673486	-0.568322
H	-2.173336	-2.898871	-1.629596
C	0.342987	-2.850880	-0.849728
O	-0.795579	-3.270767	-0.117522
C	2.031600	-2.766433	0.839101
C	1.526537	-1.468564	0.728448
C	1.872346	-0.476442	1.637990
C	2.723367	-0.812116	2.692514
C	3.212576	-2.111458	2.822102
C	2.874736	-3.097876	1.892365
C	1.544302	-3.628504	-0.302140
H	1.499602	0.541195	1.545231
H	1.240176	-4.633366	-0.001398
H	2.315566	-3.723189	-1.074522
C	-2.758086	2.133245	0.060417
C	-3.751684	2.203487	1.046823
C	-2.408525	3.209982	-0.760920
C	-4.412279	3.420839	1.188071
C	-3.103980	4.404534	-0.567206
C	-4.107441	4.527174	0.391644
H	-5.184541	3.507901	1.948022

H	-2.855433	5.257393	-1.193083
C	-1.331929	3.123121	-1.813751
H	-1.377543	2.180585	-2.366712
H	-0.332253	3.203432	-1.372560
H	-1.448710	3.940293	-2.526996
C	-4.867627	5.816921	0.556390
H	-5.046421	6.034933	1.612012
H	-5.843509	5.751123	0.065240
H	-4.325986	6.655550	0.114719
C	-4.089796	1.034294	1.934938
H	-3.183291	0.587050	2.355868
H	-4.608670	0.244814	1.382449
H	-4.719960	1.369509	2.760276
H	0.173194	-2.997353	-1.922976
H	0.005368	1.437741	-0.004696
C	4.850635	-1.083150	-2.246961
H	4.939749	-2.096838	-1.854229
H	4.016988	-1.078869	-2.953760
H	5.771039	-0.846688	-2.789925
C	6.092502	-1.414553	0.480095
H	6.545313	-2.036337	-0.294230
H	6.809194	-1.328370	1.301071
H	5.194367	-1.913315	0.858846
C	3.969838	2.761642	2.048883
H	2.909278	2.607532	2.263893
H	4.553255	2.555562	2.948512
H	4.086442	3.819113	1.788997
H	3.005973	-0.052361	3.414331
H	3.867795	-2.358006	3.651282
H	3.261206	-4.107272	1.995012
C	-3.131402	-3.266492	0.256846
H	-3.004531	-4.349852	0.230675
H	-3.093730	-2.923635	1.292580
S	-4.794738	-2.926237	-0.405737
O	-5.519956	-4.196832	-0.201184
O	-5.339612	-1.811809	0.395372
O	-4.565733	-2.591327	-1.829419