Supporting Information

Catalytic Metal-Free Intramolecular Hydroaminations of Non-activated Aminoalkenes: A Computational Exploration

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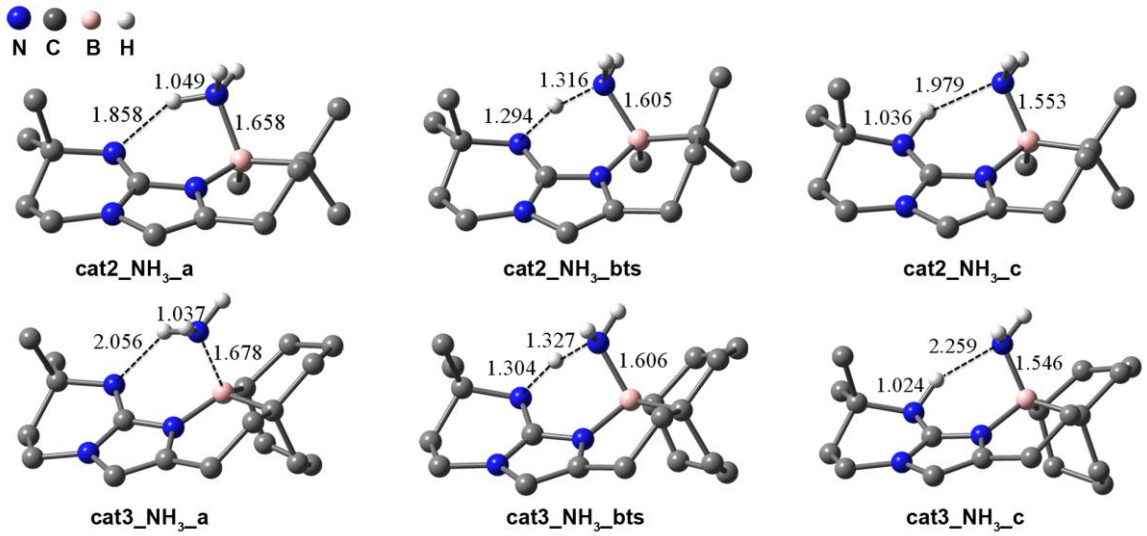
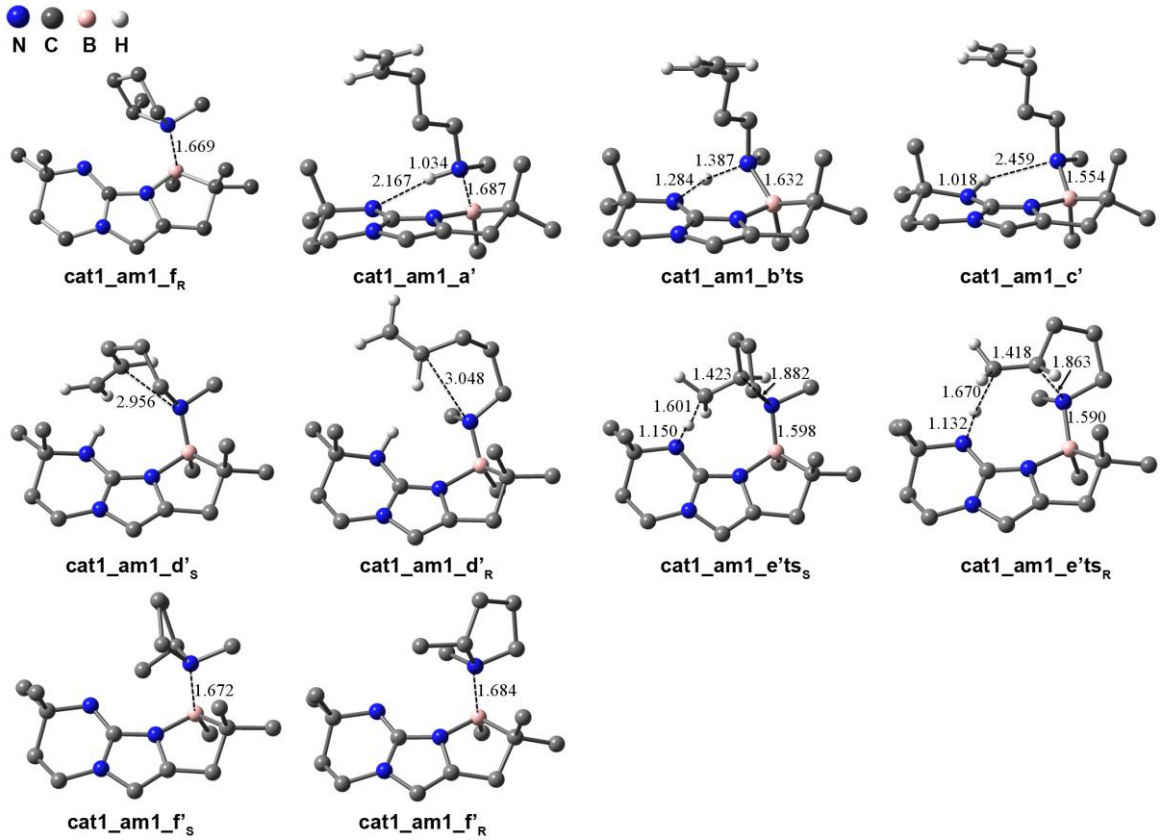
Contents

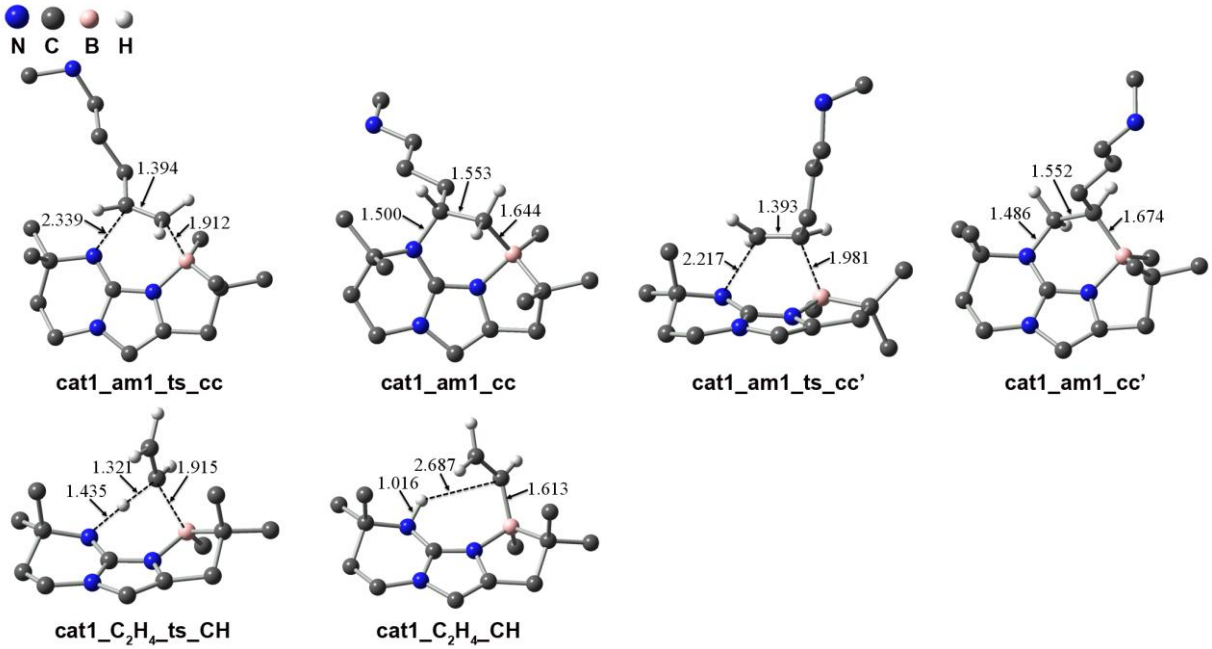
SI1: Optimized geometries mentioned in Fig. 1(A) but not included in Fig. 1B. The key bond lengths are given in Å. Trivial hydrogen atoms are omitted for clarity.



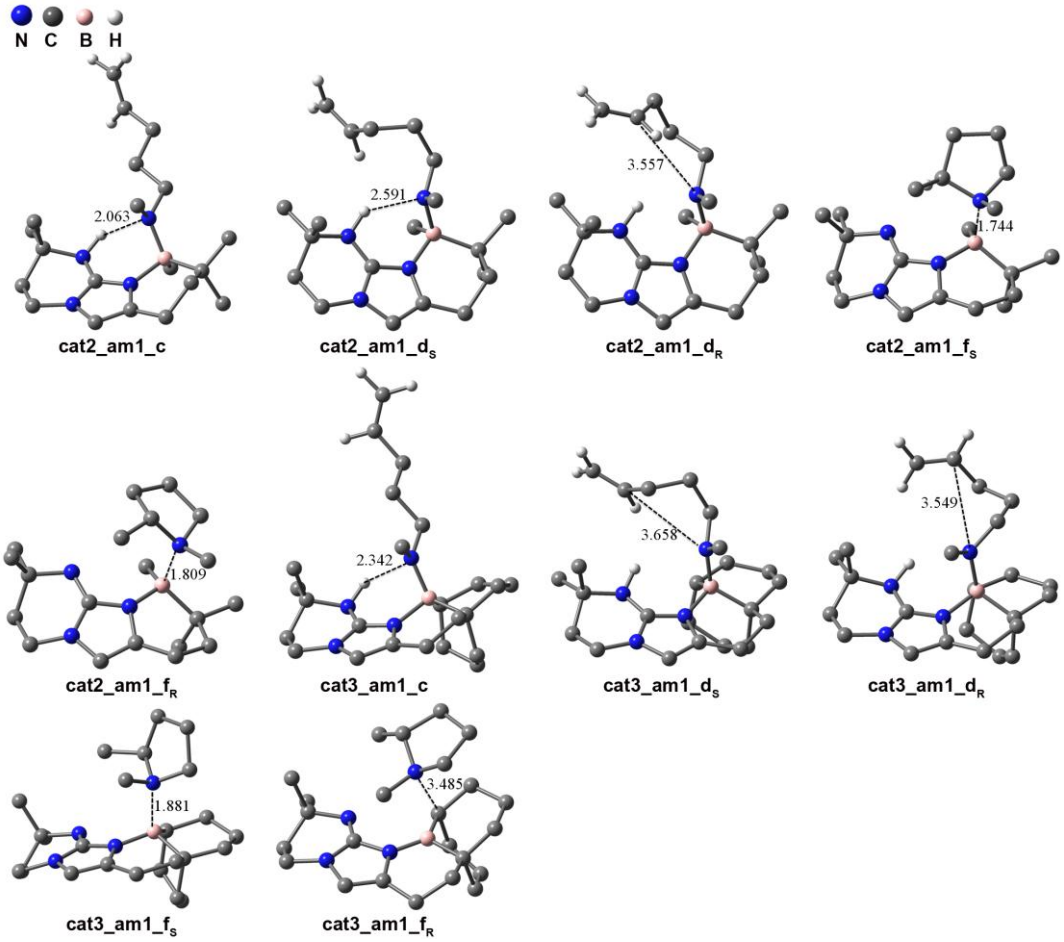
SI2: Optimized geometries mentioned in Fig. 3 but not included in Fig. 4. The key bond lengths are given in Å. Trivial hydrogen atoms are omitted for clarity.



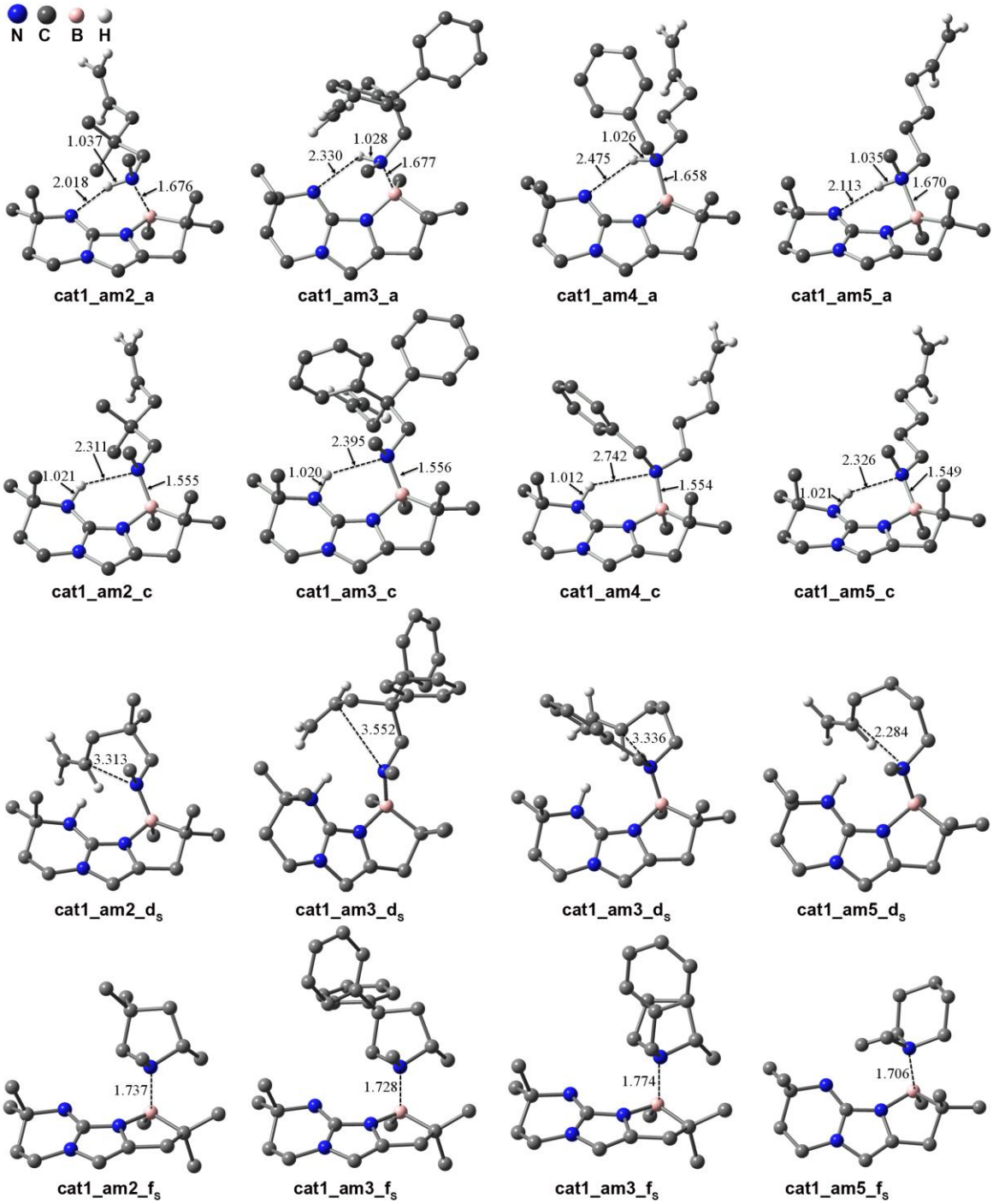
SI3: Optimized geometries of the complexes and transition states mentioned in the undesired side reactions. The key bond lengths are given in Å. Trivial hydrogen atoms are omitted for clarity.



SI4: Optimized geometries mentioned in Fig. 7 but not included in Fig. 8. The key bond lengths are given in Å. Trivial hydrogen atoms are omitted for clarity.



SI5: Optimized geometries mentioned in Fig. 9 but not included in Fig. 10. The key bond lengths are given in Å. Trivial hydrogen atoms are omitted for clarity.



SI6: Cartesian coordinates and absolute energies for the stationary points in the text.

The Cartesian coordinates (Å), SCF energies, enthalpies, and Gibbs free energies (a. u.) at 298.15K and 1.0 atm in toluene at the level of M05-2X/6-311++G(2d,p)//M05-2X/6-31G(d,p) for the optimized structures.

cat1

SCF energy in solution: –697.892831
Enthalpy in solution: –697.528665
Free energy in solution: –697.591417

Cartesian coordinates

Atom	X	Y	Z
C	0.154800	-2.198120	-0.055770
H	0.101780	-3.272201	-0.006343
C	1.202318	-1.369769	-0.162153
C	-2.387944	-1.853987	-0.028330
H	-2.717533	-2.115353	0.981949
H	-2.467958	-2.749301	-0.649071
C	-2.879819	0.638864	0.027771
N	-1.457969	0.951152	-0.138978
B	1.752485	0.933823	-0.149725
C	2.695912	-1.365461	-0.299217
H	2.973262	-1.603313	-1.331147
H	3.183064	-2.097519	0.348769
N	0.711500	-0.044326	-0.192327
C	-0.684648	-0.068282	-0.117296
N	-1.009692	-1.409513	-0.014821
C	3.108253	0.100238	0.032488
C	-3.236234	-0.721803	-0.604135
H	-3.055106	-0.653420	-1.680389
H	-4.294467	-0.944572	-0.451965
C	-3.673919	1.737304	-0.675751
H	-3.390461	2.706958	-0.264459
H	-3.443741	1.741218	-1.742542
H	-4.749231	1.593742	-0.543566
C	-3.215452	0.645481	1.525052
H	-2.986396	1.627694	1.940192
H	-4.274606	0.429381	1.690958
H	-2.616861	-0.090311	2.065826
C	3.461682	0.204501	1.529008
H	2.652245	-0.181640	2.154663
H	4.363583	-0.376218	1.746872
H	3.650860	1.240463	1.820182
C	4.287997	0.582140	-0.809826
H	4.066871	0.524751	-1.878392
H	4.530066	1.621070	-0.573015
H	5.181327	-0.020673	-0.617507
C	1.550284	2.481892	-0.207586
H	0.537260	2.765305	0.074677
H	2.282067	3.015997	0.402207
H	1.705307	2.809647	-1.241921

NH_3

SCF energy in solution: –56.565806
Enthalpy in solution: –56.526912
Free energy in solution: –56.548742

Cartesian coordinates

Atom	X	Y	Z
N	0.000000	0.000000	0.114098
H	0.000000	0.937293	-0.266229
H	-0.811719	-0.468646	-0.266229
H	0.811719	-0.468646	-0.266229

cat1_NH_3_a

SCF energy in solution: –754.487803
Enthalpy in solution: –754.081164
Free energy in solution: –754.14475

Cartesian coordinates

Atom	X	Y	Z
C	-0.008025	2.334150	-0.185441
H	0.066982	3.404712	-0.114968
C	-1.069122	1.502579	-0.283744
C	2.534972	1.888457	-0.119341
H	2.809596	2.189083	0.896856
H	2.708399	2.741847	-0.778819
C	2.899169	-0.626901	0.100704
N	1.486592	-0.888677	-0.172165
B	-1.685371	-0.870481	-0.329434
C	-2.570431	1.469085	-0.289239
H	-2.941510	1.560706	-1.315935
H	-3.019585	2.274293	0.298083
N	-0.593703	0.206762	-0.359666
C	0.756056	0.193574	-0.251600
N	-1.037479	-1.972182	0.715309
N	1.138531	1.512662	-0.179854

C	-1.914395	-1.641809	-1.722518
H	-0.987826	-2.099071	-2.082828
H	-2.678657	-2.424414	-1.656240
H	-2.244161	-0.940784	-2.494075
C	-2.925041	0.049930	0.268048
C	3.358726	0.682667	-0.575571
H	3.240520	0.561638	-1.655878
H	4.415474	0.865882	-0.367683
C	3.126728	-0.548353	1.618084
H	2.848349	-1.500325	2.074291
H	4.173971	-0.340624	1.856737
H	2.504719	0.230071	2.065255
C	3.708702	-1.787850	-0.472650
H	3.357095	-2.724761	-0.036631
H	3.565768	-1.843097	-1.553033
H	4.774328	-1.676141	-0.256850
C	-2.882845	0.125219	1.800003
H	-3.615164	0.845036	2.179471
H	-3.125565	-0.840662	2.257224
H	-1.898097	0.445146	2.157860
C	-4.323858	-0.369673	-0.177021
H	-5.087292	0.326471	0.187583
H	-4.396324	-0.410479	-1.265874
H	-4.575367	-1.362561	0.207931
H	-1.133473	-1.698034	1.688035
H	-1.417631	-2.903789	0.592945
H	-0.019104	-1.964142	0.480073

cat1_NH_3_bts

SCF energy in solution: –754.479544

Enthalpy in solution: –754.077804

Free energy in solution: –754.139299

Cartesian coordinates

Atom	X	Y	Z
C	-0.042604	2.366604	-0.237799
H	0.028160	3.424897	-0.061828
C	-1.101358	1.535429	-0.406537
C	2.499702	1.887072	-0.061655
H	2.627037	2.159343	0.990177
H	2.791987	2.744820	-0.670096
C	2.771018	-0.651372	0.144499
N	1.424644	-0.853977	-0.397780
B	-1.634670	-0.899139	-0.389621
C	-2.589270	1.438452	-0.232997
H	-3.088685	1.479174	-1.206632
H	-2.997765	2.238618	0.389269
N	-0.612351	0.265446	-0.628517
C	0.712602	0.268286	-0.493127
N	-0.756080	-1.932804	0.460160
N	1.111473	1.556201	-0.322814
C	-2.103707	-1.611651	-1.757012
H	-1.255448	-2.050426	-2.292266
H	-2.830664	-2.409922	-1.571501
H	-2.578317	-0.899402	-2.438217
C	-2.785710	0.015459	0.398250
C	3.348153	0.663319	-0.420762
H	3.393149	0.567277	-1.508694
H	4.364820	0.812556	-0.050950
C	2.719803	-0.602490	1.679032
H	2.371312	-1.562962	2.064559
H	3.706789	-0.399715	2.103589
H	2.026098	0.168031	2.023679
C	3.646944	-1.816784	-0.305659
H	3.215756	-2.757518	0.042088
H	3.696367	-1.847972	-1.394848
H	4.657963	-1.726928	0.098347
C	-2.477295	0.119264	1.896760
H	-3.146215	0.829807	2.394551
H	-2.609605	-0.847248	2.393416
H	-1.449822	0.456685	2.073747
C	-4.226143	-0.454635	0.212443
H	-4.938391	0.221275	0.699646
H	-4.488167	-0.516770	-0.845951
H	-4.368041	-1.448991	0.645867
H	-0.830099	-1.803267	1.463609
H	-0.996418	-2.894072	0.251470
H	0.464941	-1.627383	0.085126

cat1_NH_3_c

SCF energy in solution: –754.496937

Enthalpy in solution: –754.090503

Free energy in solution: –754.153808

Cartesian coordinates

Atom	X	Y	Z
C	0.003971	2.326697	-0.214575
H	0.083736	3.394451	-0.116799
C	-1.061589	1.486772	-0.293200
C	2.542890	1.875986	-0.101782
H	2.712269	2.184061	0.933123
H	2.774666	2.721817	-0.750255
C	2.893023	-0.643556	0.145480
N	1.549766	-0.857971	-0.406914

B	-1.718788	-0.950483	-0.329756
C	-2.559933	1.459743	-0.216899
H	-2.979410	1.554246	-1.223984
H	-2.962618	2.275864	0.389888
N	-0.584034	0.200306	-0.407360
C	0.729923	0.229227	-0.370569
N	-1.091674	-2.086650	0.489231
N	1.146274	1.510870	-0.275693
C	-2.067591	-1.448605	-1.830515
H	-1.198629	-1.920052	-2.301054
H	-2.876360	-2.187172	-1.824178
H	-2.386729	-0.631516	-2.485516
C	-2.880147	0.044970	0.356655
C	3.410879	0.669548	-0.466884
H	3.424753	0.549105	-1.552643
H	4.433235	0.850587	-0.130468
C	2.854402	-0.568540	1.677106
H	2.527806	-1.526424	2.086034
H	3.844157	-0.340713	2.080002
H	2.152773	0.195036	2.018593
C	3.776797	-1.801442	-0.305089
H	3.378833	-2.746629	0.069922
H	3.809830	-1.849616	-1.393971
H	4.790427	-1.680230	0.081233
C	-2.715163	0.099973	1.879270
H	-3.395044	0.831070	2.332098
H	-2.936161	-0.872470	2.328179
H	-1.693648	0.375869	2.162905
C	-4.315072	-0.354924	0.024144
H	-5.046013	0.322018	0.482752
H	-4.485595	-0.357089	-1.054761
H	-4.524041	-1.363493	0.393100
H	-1.212536	-1.986263	1.489335
H	-1.475771	-2.985454	0.231404
H	1.017352	-1.675563	-0.089848

cat2

SCF energy in solution: –737.218839

Enthalpy in solution: –736.823875

Free energy in solution: –736.887658

Cartesian coordinates

Atom	X	Y	Z
C	0.187134	2.317144	0.016188
H	0.314726	3.386075	0.047691
C	-0.933563	1.585294	-0.043321
C	2.687197	1.792614	-0.063659
H	3.081533	2.048699	0.924319
H	2.799459	2.668255	-0.707161
C	2.987410	-0.721064	0.028094
N	1.542137	-0.927197	-0.085310
B	-1.509489	-0.873506	-0.079613
C	-3.232572	0.947699	0.618517
H	-4.288383	1.234039	0.556019
H	-2.956937	0.967407	1.678176
N	-0.567360	0.215729	-0.077901
C	0.842064	0.143808	-0.053976
N	1.282198	1.450459	0.024926
C	-3.050772	-0.482252	0.080956
C	3.423798	0.591668	-0.649972
H	3.193798	0.515684	-1.716303
H	4.501273	0.735340	-0.544536
C	3.670562	-1.894865	-0.670198
H	3.323117	-2.829308	-0.227775
H	3.409694	-1.903522	-1.730010
H	4.757326	-1.834653	-0.571166
C	3.371223	-0.718760	1.514016
H	3.084710	-1.671958	1.959986
H	4.448450	-0.578581	1.640898
H	2.846913	0.071127	2.055534
C	-3.757697	-1.445167	1.046771
H	-3.301908	-1.422774	2.040022
H	-4.809372	-1.159301	1.155769
H	-3.728913	-2.474128	0.685990
C	-3.706999	-0.625533	-1.306467
H	-3.261155	0.037744	-2.050963
H	-3.608462	-1.648377	-1.677263
H	-4.775434	-0.393084	-1.242320
C	-1.027254	-2.357651	-0.254374
H	-0.459900	-2.661792	0.630261
H	-1.852225	-3.055371	-0.400862
H	-0.315065	-2.444890	-1.075423
C	-2.371943	1.970226	-0.125973
H	-2.501067	2.970896	0.289597
H	-2.685100	2.018096	-1.174025

cat2_NH_3_a

SCF energy in solution: –793.814147

Enthalpy in solution: –793.376692

Free energy in solution: –793.441303

Cartesian coordinates

Atom	X	Y	Z
C	0.345307	2.447319	-0.029156

H	0.507595	3.507658	0.053100
C	-0.795170	1.723885	-0.049077
C	2.829281	1.808311	-0.170967
H	3.206491	2.096428	0.815250
H	3.007273	2.641601	-0.854327
C	3.007884	-0.713807	0.061708
N	1.563707	-0.864528	-0.104349
B	-1.435038	-0.831968	-0.221281
C	-2.971826	0.997545	0.871508
H	-4.005497	1.311451	1.061022
H	-2.496742	0.864289	1.852231
N	-0.460491	0.376735	-0.166298
C	0.903907	0.265957	-0.150018
N	1.407620	1.539974	-0.110271
C	-2.966376	-0.336133	0.100877
C	3.519198	0.541454	-0.673206
H	3.307365	0.418306	-1.738717
H	4.599969	0.641417	-0.549951
C	3.676243	-1.947659	-0.540376
H	3.279011	-2.844812	-0.062186
H	3.455455	-2.007329	-1.607295
H	4.759698	-1.922408	-0.398645
C	3.348575	-0.629415	1.557714
H	3.036273	-1.551554	2.051815
H	4.422719	-0.496625	1.716781
H	2.819475	0.199486	2.032671
C	-3.724558	-1.377582	0.935269
H	-3.315119	-1.476940	1.946165
H	-4.777532	-1.096964	1.045822
H	-3.698901	-2.362715	0.458052
C	-3.750516	-0.154627	-1.209576
H	-3.223775	0.473737	-1.930362
H	-3.918713	-1.119091	-1.692706
H	-4.729433	0.299258	-1.014719
C	-2.228020	2.112164	0.122643
H	-2.278829	3.052920	0.673713
H	-2.707442	2.284663	-0.844464
N	-0.819741	-1.768333	1.001130
C	-1.251116	-1.739786	-1.544455
H	-1.908468	-2.617844	-1.536926
H	-1.496806	-1.170515	-2.443276
H	-0.220915	-2.086491	-1.650665
H	0.202457	-1.781950	0.765969
H	-0.943447	-1.361867	1.922662
H	-1.201501	-2.706957	0.996581

cat2_NH_3_bts

SCF energy in solution: –793.805449
Enthalpy in solution: –793.372922
Free energy in solution: –793.436682

Cartesian coordinates

Atom	X	Y	Z
C	0.340247	2.486628	-0.062900
H	0.508018	3.544001	0.037896
C	-0.803405	1.759246	-0.102094
C	2.831443	1.806846	-0.119904
H	3.132197	2.086602	0.893573
H	3.081756	2.633757	-0.786840
C	2.951452	-0.733094	0.109101
N	1.528378	-0.832814	-0.213035
B	-1.411233	-0.849325	-0.289582
C	-2.895443	0.980779	0.932041
H	-3.918967	1.276386	1.193057
H	-2.341578	0.887417	1.874407
N	-0.465306	0.423237	-0.246613
C	0.875517	0.327626	-0.238003
N	1.399736	1.575100	-0.165306
C	-2.922911	-0.379740	0.203932
C	3.532028	0.523330	-0.570055
H	3.408195	0.408502	-1.649971
H	4.599993	0.603318	-0.356477
C	3.649594	-1.971167	-0.446240
H	3.212253	-2.869760	-0.006978
H	3.515978	-2.021319	-1.527606
H	4.717202	-1.955213	-0.215237
C	3.149166	-0.663940	1.630701
H	2.783312	-1.584537	2.089688
H	4.205346	-0.546378	1.887919
H	2.589203	0.168901	2.061199
C	-3.531387	-1.413599	1.160731
H	-2.975492	-1.484451	2.100284
H	-4.564838	-1.151388	1.414716
H	-3.547291	-2.408563	0.705084
C	-3.885190	-0.264275	-0.990641
H	-3.511795	0.402387	-1.770510
H	-4.042303	-1.239216	-1.456139
H	-4.862390	0.112470	-0.664779
C	-2.241411	2.101468	0.104794
H	-2.313970	3.061709	0.618145
H	-2.759816	2.207111	-0.851434
N	-0.620526	-1.840780	0.693540
C	-1.341850	-1.552007	-1.748681
H	-1.954363	-2.460835	-1.784996

H	-1.701257	-0.894701	-2.543110
H	-0.316408	-1.837797	-1.999597
H	-0.738363	-1.628594	1.678438
H	-0.900286	-2.803009	0.547322
H	0.608738	-1.581981	0.303052

cat2_NH_3_c

SCF energy in solution: –793.817427

Enthalpy in solution: –793.380159

Free energy in solution: –793.444464

Cartesian coordinates

Atom	X	Y	Z
C	0.353602	2.450950	-0.062338
H	0.524947	3.508698	0.028328
C	-0.790416	1.718437	-0.047407
C	2.835444	1.802039	-0.175736
H	3.124776	2.113862	0.830828
H	3.063747	2.617384	-0.863373
C	3.000944	-0.722116	0.102432
N	1.597297	-0.840195	-0.309485
B	-1.433044	-0.927496	-0.173794
C	-2.925546	0.958155	0.942322
H	-3.947815	1.276583	1.182700
H	-2.413459	0.783622	1.897135
N	-0.454885	0.381327	-0.198868
C	0.871059	0.308535	-0.254444
N	1.404523	1.545160	-0.207123
C	-2.959288	-0.345791	0.124820
C	3.567862	0.526615	-0.590196
H	3.470863	0.385978	-1.669353
H	4.628357	0.628914	-0.353211
C	3.737073	-1.962000	-0.394360
H	3.297047	-2.859994	0.043767
H	3.660118	-2.036234	-1.479564
H	4.790133	-1.921216	-0.108941
C	3.114105	-0.616609	1.629003
H	2.738070	-1.532105	2.089075
H	4.154283	-0.477422	1.933284
H	2.520979	0.214617	2.015056
C	-3.754040	-1.382399	0.927393
H	-3.318938	-1.547446	1.916433
H	-4.793276	-1.061663	1.068400
H	-3.772374	-2.345853	0.408809
C	-3.738332	-0.087339	-1.175302
H	-3.189658	0.542490	-1.879687
H	-3.944213	-1.027752	-1.690064
H	-4.701062	0.397483	-0.967295
C	-2.211564	2.102223	0.208112
H	-2.226741	3.019478	0.800130
H	-2.729898	2.318996	-0.728689
N	-0.775854	-1.807143	0.924581
C	-1.306758	-1.712613	-1.591597
H	-2.002175	-2.559899	-1.618599
H	-1.544740	-1.082468	-2.451767
H	-0.304689	-2.119242	-1.753294
H	-0.952456	-1.461252	1.862076
H	-1.157577	-2.744691	0.890675
H	1.028523	-1.575964	0.146155

cat3

SCF energy in solution: –892.078935

Enthalpy in solution: –891.605841

Free energy in solution: –891.672994

Cartesian coordinates

Atom	X	Y	Z
C	1.323829	2.567835	-0.048253
H	1.710839	3.572649	-0.064727
C	0.057406	2.130468	-0.065315
C	3.619764	1.443717	-0.134529
H	4.076474	1.631671	0.841788
H	3.935586	2.240991	-0.811306
C	3.297319	-1.065006	0.047280
N	1.843868	-0.914623	-0.055879
N	0.083010	0.712325	-0.064547
C	1.430074	0.295892	-0.060297
N	2.175113	1.458379	-0.029237
C	4.034182	0.078466	-0.677293
H	3.783404	0.024053	-1.740219
H	5.114961	-0.042161	-0.576875
C	3.666498	-2.392359	-0.610681
H	3.114677	-3.200118	-0.128193
H	3.390962	-2.376346	-1.666594
H	4.737699	-2.591040	-0.524891
C	3.685510	-1.104653	1.531313
H	3.178796	-1.941651	2.013034
H	4.765491	-1.228800	1.651516
H	3.376464	-0.191252	2.043196
B	-1.109155	-0.076581	-0.011014
C	-2.479617	0.643127	0.308751
C	-1.258367	-1.603224	-0.329280
H	-0.296638	-2.080298	-0.509938
C	-3.062064	-0.101568	1.537332

H	-2.397189	0.100809	2.386523
H	-4.031882	0.341652	1.797711
C	-1.948864	-2.315755	0.852485
H	-1.213920	-2.383691	1.661564
H	-2.195752	-3.346405	0.574741
C	-3.209456	-1.622950	1.400787
H	-3.434560	-2.035691	2.388505
H	-4.074178	-1.858486	0.783030
C	-2.072103	-1.620493	-1.650793
H	-1.453989	-1.160246	-2.430774
H	-2.237559	-2.656683	-1.965042
C	-3.369359	0.505999	-0.952506
H	-2.989572	1.208011	-1.703503
H	-4.386574	0.840233	-0.711262
C	-3.424860	-0.891382	-1.598694
H	-3.802662	-0.783051	-2.619502
H	-4.154260	-1.513892	-1.084661
C	-2.316497	2.128844	0.677300
H	-2.011791	2.207642	1.725452
H	-3.275589	2.650485	0.583850
C	-1.255036	2.831839	-0.178293
H	-1.135367	3.874463	0.120338
H	-1.572181	2.834697	-1.226933

cat3_NH_3_a

SCF energy in solution: –948.672564

Enthalpy in solution: –948.157129

Free energy in solution: –948.225141

Cartesian coordinates

Atom	X	Y	Z
C	-1.355481	2.569893	0.221721
H	-1.741420	3.572946	0.277922
C	-0.094939	2.117512	0.043565
C	-3.623697	1.398145	0.510690
H	-4.143821	1.720867	-0.396993
H	-3.905978	2.078001	1.317879
C	-3.305574	-1.050667	-0.081954
N	-1.849909	-0.904697	-0.057839
N	-0.126994	0.717803	0.075155
C	-1.437658	0.317814	0.138704
N	-2.189995	1.451636	0.320331
C	-3.985374	-0.042689	0.866397
H	-3.645355	-0.254166	1.883874
H	-5.070433	-0.164742	0.838812
C	-3.637203	-2.467982	0.380495
H	-3.115769	-3.186368	-0.254344
H	-3.294757	-2.613944	1.406146
H	-4.711564	-2.663318	0.329419
C	-3.812121	-0.853785	-1.519214
H	-3.370955	-1.616349	-2.164379
H	-4.901220	-0.939242	-1.576934
H	-3.517166	0.124067	-1.906395
B	1.033016	-0.214140	-0.311792
C	2.410969	0.617608	-0.367255
C	1.287917	-1.574348	0.515366
H	0.379799	-2.182304	0.563321
C	3.406652	-0.193861	-1.209249
H	3.045993	-0.208296	-2.247617
H	4.377676	0.316920	-1.249287
C	2.374531	-2.400521	-0.218736
H	1.908185	-2.902899	-1.076563
H	2.712176	-3.221924	0.423851
C	3.629947	-1.639193	-0.718712
H	4.089866	-2.217288	-1.526313
H	4.376256	-1.617580	0.073167
C	1.689074	-1.218135	1.952099
H	0.870609	-0.646356	2.403914
H	1.814321	-2.124404	2.555784
C	2.918396	0.833023	1.083083
H	2.244214	1.539796	1.572628
H	3.902594	1.320998	1.047922
C	2.973078	-0.386900	2.014703
H	3.126230	-0.027039	3.036723
H	3.832326	-1.018942	1.794357
C	2.194012	2.000951	-1.004326
H	1.838172	1.873765	-2.036028
H	3.141307	2.550038	-1.075101
C	1.178076	2.864884	-0.234298
H	0.934634	3.758741	-0.812476
H	1.629092	3.218367	0.695174
N	0.482709	-0.726314	-1.811721
H	1.040235	-1.456423	-2.238406
H	0.364273	0.036246	-2.470771
H	-0.448899	-1.097958	-1.550282

cat3_NH_3_bts

SCF energy in solution: –948.660971

Enthalpy in solution: –948.150869

Free energy in solution: –948.216978

Cartesian coordinates

Atom	X	Y	Z
C	-1.391206	2.578181	0.256640

H	-1.796307	3.574609	0.263775
C	-0.124752	2.130477	0.065527
C	-3.646110	1.359637	0.538970
H	-4.100209	1.708469	-0.392572
H	-3.997934	2.001979	1.348399
C	-3.242678	-1.073660	-0.105020
N	-1.800385	-0.906348	0.098852
N	-0.135837	0.742849	0.198412
C	-1.418379	0.353664	0.311880
N	-2.200758	1.451426	0.445177
C	-4.004626	-0.101124	0.815068
H	-3.748677	-0.344705	1.849465
H	-5.081025	-0.237076	0.691239
C	-3.609748	-2.507934	0.264852
H	-3.029417	-3.204423	-0.342978
H	-3.374186	-2.695238	1.313102
H	-4.672311	-2.696759	0.094598
C	-3.595782	-0.813396	-1.577630
H	-3.096077	-1.550204	-2.209908
H	-4.673306	-0.891646	-1.745122
H	-3.264636	0.177843	-1.895542
B	0.983089	-0.276223	-0.252973
C	2.329956	0.583737	-0.528229
C	1.381147	-1.491458	0.740284
H	0.512102	-2.118734	0.967760
C	3.217182	-0.297267	-1.416809
H	2.702718	-0.442581	-2.375073
H	4.159861	0.214352	-1.654623
C	2.401212	-2.381495	-0.021523
H	1.847558	-3.007445	-0.730969
H	2.858927	-3.094895	0.674554
C	3.546857	-1.669746	-0.793006
H	3.896215	-2.340275	-1.584369
H	4.402568	-1.544057	-0.131392
C	1.945426	-0.971038	2.064948
H	1.192156	-0.332294	2.541605
H	2.143497	-1.798512	2.756562
C	3.031365	0.940273	0.810879
H	2.427820	1.696794	1.317647
H	3.995450	1.420109	0.589328
C	3.226401	-0.163414	1.859359
H	3.521063	0.310040	2.801260
H	4.044538	-0.832912	1.597369
C	2.005851	1.909239	-1.240274
H	1.493874	1.694965	-2.187293
H	2.925567	2.449750	-1.497943
C	1.109879	2.846043	-0.401083
H	0.797882	3.701636	-1.003448
H	1.675217	3.253205	0.438434
N	0.214177	-0.964065	-1.484006
H	-0.905433	-1.187040	-0.807557
H	0.658141	-1.806417	-1.823837
H	0.056563	-0.348770	-2.275653

cat3_NH_3_c

SCF energy in solution: –948.677279

Enthalpy in solution: –948.162114

Free energy in solution: –948.229853

Cartesian coordinates

Atom	X	Y	Z
C	-1.357680	2.559687	0.258491
H	-1.751378	3.557673	0.334826
C	-0.098294	2.103977	0.021904
C	-3.619814	1.378107	0.544930
H	-4.093333	1.754120	-0.364927
H	-3.915589	2.021076	1.374785
C	-3.305631	-1.055800	-0.122735
N	-1.864070	-0.927574	0.139499
N	-0.134051	0.714144	0.048745
C	-1.398690	0.352595	0.212495
N	-2.174364	1.437523	0.391875
C	-4.018422	-0.071699	0.816175
H	-3.757258	-0.335821	1.843738
H	-5.098773	-0.175119	0.701939
C	-3.713240	-2.483890	0.223938
H	-3.154440	-3.193121	-0.390044
H	-3.497991	-2.693670	1.271997
H	-4.778249	-2.633394	0.036849
C	-3.615934	-0.756945	-1.594910
H	-3.120812	-1.492338	-2.231417
H	-4.691504	-0.803269	-1.781316
H	-3.248856	0.228317	-1.888239
B	1.039397	-0.291525	-0.446555
C	2.400649	0.609616	-0.380287
C	1.316520	-1.592235	0.491636
H	0.452290	-2.267520	0.527884
C	3.456574	-0.177353	-1.167622
H	3.114371	-0.234823	-2.207891
H	4.412036	0.365802	-1.188301
C	2.455045	-2.394237	-0.190039
H	2.030118	-2.892478	-1.068017
H	2.785411	-3.207327	0.469049
C	3.709058	-1.602867	-0.639409

H	4.219436	-2.179757	-1.417315
H	4.419890	-1.547918	0.183788
C	1.648247	-1.205487	1.936536
H	0.794274	-0.658977	2.356613
H	1.784665	-2.099019	2.558393
C	2.832022	0.872706	1.084006
H	2.107123	1.557080	1.535084
H	3.795291	1.404163	1.091647
C	2.896210	-0.326517	2.039336
H	2.995548	0.052299	3.061825
H	3.785099	-0.929596	1.861093
C	2.179358	1.970916	-1.058041
H	1.827600	1.803183	-2.083080
H	3.119301	2.532646	-1.138692
C	1.157455	2.855126	-0.319032
H	0.883362	3.712846	-0.937333
H	1.607009	3.262458	0.588509
N	0.467981	-0.758743	-1.805339
H	1.033117	-1.479461	-2.233482
H	0.398392	-0.009176	-2.485634
H	-1.262214	-1.432908	-0.517241

am1

SCF energy in solution: –291.211925

Enthalpy in solution: –291.015727

Free energy in solution: –291.060437

Cartesian coordinates

Atom	X	Y	Z
C	1.291130	-0.433944	0.490422
H	1.512353	-1.428955	0.093321
H	1.138128	-0.545546	1.570405
C	0.000120	0.102365	-0.138650
H	-0.180222	1.117097	0.228842
H	0.110852	0.168559	-1.223226
C	-1.195382	-0.791543	0.178588
H	-1.330342	-0.830439	1.274408
H	-0.965271	-1.807642	-0.153706
N	-2.402773	-0.357498	-0.512669
H	-3.082159	-1.105746	-0.479463
C	-2.993984	0.838348	0.068934
H	-3.967370	1.019210	-0.387387
H	-3.125443	0.778221	1.160968
H	-2.369144	1.706411	-0.144809
C	2.458968	0.475786	0.242171
H	2.369933	1.485306	0.637485
C	3.552005	0.136825	-0.432932
H	3.670594	-0.859597	-0.844508
H	4.360365	0.838575	-0.594839

$py1_S$

SCF energy in solution: –291.241444

Enthalpy in solution: –291.044615

Free energy in solution: –291.084842

Cartesian coordinates

Atom	X	Y	Z
C	-0.412741	-0.625310	0.346522
C	0.940137	-1.288149	0.049244
H	0.865764	-1.854375	-0.881110
H	1.227121	-1.981058	0.840417
C	1.927377	-0.107147	-0.110961
H	2.723700	-0.122292	0.632619
H	2.391157	-0.126243	-1.096499
C	1.038992	1.136082	0.044052
H	1.343888	1.971521	-0.588902
H	1.052066	1.483212	1.093211
N	-0.289793	0.665947	-0.328282
C	-1.323940	1.613812	0.031894
H	-1.130623	2.567685	-0.461468
H	-2.299456	1.257889	-0.299823
H	-1.366805	1.790749	1.121076
C	-1.601477	-1.436621	-0.142858
H	-1.576439	-2.439167	0.288131
H	-2.552282	-0.979209	0.134354
H	-1.557406	-1.519387	-1.230440
H	-0.502227	-0.466949	1.439047

$py1_R$

SCF energy in solution: –291.237245

Enthalpy in solution: –291.040364

Free energy in solution: –291.080716

Cartesian coordinates

Atom	X	Y	Z
C	0.122904	0.801811	-0.501997
H	0.394865	1.166209	-1.497476
C	-1.416403	0.780259	-0.311642
H	-1.940686	1.086292	-1.216487
H	-1.699649	1.476381	0.480325
C	-1.762004	-0.671060	0.083683
H	-2.526606	-0.728486	0.858235
H	-2.109034	-1.227979	-0.786825
C	-0.415555	-1.235327	0.529470

H	-0.356786	-2.323837	0.457024
H	-0.199153	-0.957045	1.576516
N	0.497531	-0.616812	-0.416065
C	1.895315	-0.894650	-0.173704
H	2.070973	-1.967307	-0.278042
H	2.507154	-0.380203	-0.917968
H	2.241028	-0.590952	0.826817
C	0.789867	1.707528	0.540361
H	1.872259	1.752621	0.409815
H	0.398500	2.722659	0.448911
H	0.579676	1.357959	1.554581

cat1_am1_a

SCF energy in solution: –989.135549

Enthalpy in solution: –988.571063

Free energy in solution: –988.653309

Cartesian coordinates

Atom	X	Y	Z
C	-3.412504	1.242015	-0.396348
H	-4.377281	1.619477	-0.684482
C	-2.238471	1.857414	-0.129528
C	-4.127299	-1.235651	-0.290361
H	-4.313550	-1.517364	-1.331655
H	-5.078310	-0.921390	0.145555
C	-2.053635	-2.654195	0.146900
N	-1.247603	-1.462733	0.404608
B	0.070238	1.434433	0.565472
C	-1.597496	3.211376	-0.010925
H	-1.833832	3.636930	0.970505
H	-1.944506	3.920792	-0.766845
N	-1.314216	0.888368	0.207682
C	-1.877799	-0.344109	0.164311
N	1.071349	0.275488	-0.101909
C	0.895484	-0.039000	-1.541010
H	1.172527	-1.075447	-1.726077
H	-0.149164	0.098110	-1.802557
H	1.518647	0.622894	-2.137602
C	2.499763	0.427833	0.256629
H	2.866208	1.326704	-0.247111
H	2.545194	0.607214	1.329183
N	-3.184511	-0.139194	-0.219330
C	0.327509	1.401214	2.163774
H	0.301387	0.379777	2.559081
H	1.253256	1.877517	2.498458
H	-0.491453	1.940198	2.649529
C	-0.054474	2.947580	-0.109066
C	-3.537494	-2.407538	0.496389
H	-3.596481	-2.182061	1.564729
H	-4.127583	-3.306999	0.305353
C	-1.915782	-3.056744	-1.329715
H	-0.870404	-3.288132	-1.543606
H	-2.523581	-3.935046	-1.566978
H	-2.215225	-2.235834	-1.985242
C	-1.518974	-3.779545	1.029573
H	-0.456881	-3.925239	0.823451
H	-1.626197	-3.510104	2.081610
H	-2.046994	-4.718398	0.844254
C	0.330221	3.043096	-1.592482
H	0.144974	4.057397	-1.962850
H	1.392218	2.834335	-1.751489
H	-0.253449	2.358349	-2.211530
C	0.711134	4.034697	0.647983
H	0.513437	5.025688	0.224342
H	0.435603	4.058910	1.703814
H	1.790830	3.864056	0.591353
C	3.361556	-0.780295	-0.095232
H	3.429503	-0.916377	-1.176404
H	2.901067	-1.684993	0.317310
C	4.779665	-0.622630	0.468849
H	5.242602	0.279287	0.058380
H	4.716924	-0.489160	1.554453
C	5.636189	-1.815018	0.154219
H	5.298353	-2.765943	0.559584
C	6.737411	-1.776495	-0.587917
H	7.099575	-0.844465	-1.008040
H	7.312665	-2.669652	-0.795702
H	0.673580	-0.550717	0.376259

cat1_am1_bts

SCF energy in solution: –989.119982

Enthalpy in solution: –988.56166

Free energy in solution: –988.64317

Cartesian coordinates

Atom	X	Y	Z
C	-3.643697	0.197993	0.202947
H	-4.671691	0.326000	0.489461
C	-2.892722	-0.903713	-0.062536
C	-3.004819	2.728386	0.235052
H	-3.044125	2.936655	1.307972
H	-3.958633	3.026960	-0.203075
C	-0.458668	2.910142	-0.090968
N	-0.416701	1.503759	-0.500881

B	-0.519470	-1.542511	-0.527497
C	-2.880272	-2.407883	-0.081590
H	-3.171042	-2.754557	-1.078864
H	-3.570845	-2.853708	0.638313
N	-1.640574	-0.473692	-0.422571
C	-1.566017	0.848524	-0.343765
N	0.709830	-0.733503	0.153325
C	0.636013	-0.509164	1.601445
H	1.226085	0.365291	1.884159
H	-0.397907	-0.317738	1.883799
H	1.001370	-1.369836	2.166213
C	2.057111	-1.165380	-0.238567
H	2.281821	-2.141656	0.214784
H	2.062803	-1.302655	-1.318695
N	-2.790789	1.311012	0.007622
C	-0.181301	-1.823207	-2.087293
H	0.203504	-0.925552	-2.583207
H	0.534994	-2.633685	-2.250200
H	-1.099422	-2.102774	-2.613268
C	-1.381040	-2.804444	0.201762
C	-1.851545	3.484689	-0.435626
H	-1.978502	3.428666	-1.519985
H	-1.896913	4.535967	-0.143271
C	-0.179693	3.051248	1.411634
H	0.836432	2.717280	1.630022
H	-0.275645	4.092180	1.732198
H	-0.866314	2.438497	1.999742
C	0.601834	3.670326	-0.882995
H	1.586095	3.238974	-0.688941
H	0.399736	3.591134	-1.951795
H	0.623546	4.724450	-0.597033
C	-1.247125	-2.956198	1.724374
H	-1.884478	-3.777570	2.072332
H	-0.222935	-3.196315	2.017900
H	-1.557662	-2.058237	2.262482
C	-1.090938	-4.175074	-0.416327
H	-1.743252	-4.947431	0.007674
H	-1.233721	-4.170714	-1.497898
H	-0.057416	-4.475437	-0.219953
C	3.156455	-0.169042	0.128699
H	3.293903	-0.109797	1.210698
H	2.862526	0.829626	-0.215880
C	4.494700	-0.560788	-0.509906
H	4.781422	-1.563491	-0.179653
H	4.368267	-0.603285	-1.597385
C	5.585250	0.411636	-0.166029
H	5.431994	1.436712	-0.496307
C	6.681897	0.106268	0.519298
H	6.863308	-0.905563	0.865167
H	7.432076	0.851144	0.752965
H	0.393067	0.524076	-0.263094

cat1_am1_c

SCF energy in solution: –989.13707

Enthalpy in solution: –988.573324

Free energy in solution: –988.655484

Cartesian coordinates

Atom	X	Y	Z
C	-3.608305	-0.172642	-0.177050
H	-4.679295	-0.185448	-0.084295
C	-2.681262	-1.162336	-0.266281
C	-3.378167	2.398699	-0.081424
H	-3.660173	2.568043	0.960565
H	-4.266217	2.532712	-0.699835
C	-0.895035	2.994189	0.057619
N	-0.587124	1.652736	-0.449871
B	-0.201549	-1.609432	-0.393891
C	-2.544909	-2.655667	-0.304657
H	-2.673046	-2.995425	-1.337856
H	-3.298680	-3.162008	0.304955
N	-1.438845	-0.575504	-0.369397
C	-1.583858	0.732805	-0.351186
N	0.906898	-0.922322	0.430861
C	0.686684	-0.496748	1.799177
H	1.312036	0.371108	2.049228
H	-0.353783	-0.197950	1.942437
H	0.912636	-1.271131	2.546300
C	2.295961	-1.281717	0.211990
H	2.706159	-1.815487	1.085923
H	2.368796	-1.969873	-0.631005
H	0.313809	1.226875	-0.230500
N	-2.894414	1.035781	-0.237708
C	0.242054	-1.783576	-1.949655
H	0.693054	-0.863867	-2.338157
H	0.955913	-2.594969	-2.114668
H	-0.627779	-2.006189	-2.576940
C	-1.084260	-2.933093	0.170440
C	-2.273670	3.364538	-0.518207
H	-2.195311	3.354667	-1.607663
H	-2.539592	4.375267	-0.204101
C	-0.905459	3.020451	1.590964
H	0.092056	2.796268	1.973068
H	-1.203074	4.005366	1.958210

H	-1.591073	2.273732	1.996461
C	0.163330	3.950607	-0.480650
H	1.154229	3.647169	-0.135155
H	0.161042	3.943579	-1.571000
H	-0.025365	4.965467	-0.126582
C	-1.107928	-3.044853	1.699093
H	-1.725313	-3.894548	2.015703
H	-0.101691	-3.201480	2.093024
H	-1.518878	-2.148031	2.170009
C	-0.596797	-4.268911	-0.391794
H	-1.201277	-5.106168	-0.022444
H	-0.632029	-4.283740	-1.482909
H	0.438785	-4.454344	-0.091153
C	3.184043	-0.068327	-0.085058
H	3.079185	0.681220	0.705985
H	2.830166	0.392693	-1.013659
C	4.664342	-0.442793	-0.219974
H	5.024042	-0.874706	0.718433
H	4.759832	-1.219096	-0.988045
C	5.515088	0.736322	-0.589638
H	5.280625	1.213590	-1.538795
C	6.491327	1.234049	0.162729
H	6.749068	0.783970	1.115332
H	7.064199	2.099070	-0.147222

cat1_am1_d$_S$

SCF energy in solution: –989.140742

Enthalpy in solution: –988.577531

Free energy in solution: –988.657001

Cartesian coordinates

Atom	X	Y	Z
C	1.220534	-3.112718	-0.274546
H	1.552900	-4.134281	-0.234881
C	1.886757	-1.932135	-0.377815
C	-1.300049	-3.647173	-0.027125
H	-1.332066	-3.973068	1.015439
H	-1.198263	-4.531934	-0.656547
C	-2.599528	-1.450557	0.194911
N	-1.418724	-0.754077	-0.323265
B	1.559854	0.567034	-0.413356
N	0.955558	-0.917781	-0.387713
C	-0.249087	-1.442585	-0.306607
N	0.622315	1.383570	0.518289
C	0.497713	0.986085	1.911149
H	-0.482596	1.259087	2.321524
H	0.593660	-0.097144	2.001842
H	1.251019	1.443067	2.568546
C	0.682462	2.830918	0.395096
H	1.590485	3.243903	0.871030
H	0.743640	3.080362	-0.664170
C	-0.524287	3.565473	0.999178
H	-0.465087	3.559085	2.091127
H	-0.467746	4.613142	0.690575
C	-1.887043	2.994349	0.581317
H	-1.988491	1.990933	1.011213
H	-2.685887	3.603180	1.013932
C	-2.077461	2.912728	-0.905911
H	-1.357704	2.307011	-1.449317
C	-3.052577	3.526934	-1.569759
H	-3.782539	4.142116	-1.054057
H	-3.150070	3.440656	-2.644874
H	-1.258253	0.223927	-0.078736
N	-0.146112	-2.785698	-0.233485
C	3.263822	-1.353303	-0.517406
H	4.021751	-1.932301	0.017674
H	3.537226	-1.352885	-1.577980
C	1.477308	1.087857	-1.952380
H	1.991373	2.037062	-2.123380
H	1.939135	0.358743	-2.626686
H	0.440255	1.207612	-2.284172
C	3.139653	0.115703	0.002330
C	-2.563503	-2.868726	-0.403760
H	-3.439658	-3.425997	-0.067929
H	-2.615430	-2.773969	-1.490866
C	-2.586663	-1.491095	1.727950
H	-2.662212	-0.477523	2.126579
H	-3.429788	-2.073615	2.106857
H	-1.659929	-1.928086	2.105609
C	-3.834036	-0.709192	-0.307960
H	-3.811835	0.331704	0.022918
H	-3.860784	-0.715459	-1.398140
H	-4.741979	-1.175979	0.078045
C	3.430412	0.089015	1.508779
H	4.457165	-0.251353	1.691688
H	3.331840	1.084221	1.946927
H	2.762321	-0.586321	2.048772
C	4.211891	0.987377	-0.655705
H	5.220712	0.639888	-0.401644
H	4.121697	0.990126	-1.743379
H	4.126699	2.023101	-0.313972

cat1_am1_ets$_S$

SCF energy in solution: –989.099347

Enthalpy in solution: –988.539659
Free energy in solution: –988.613575

Cartesian coordinates

Atom	X	Y	Z
C	-1.446497	-2.832099	0.041154
H	-1.890762	-3.805314	0.148371
C	-0.168722	-2.432676	-0.133113
C	-3.662439	-1.548384	0.161553
H	-3.970691	-1.630602	1.207166
H	-4.115386	-2.373750	-0.389474
C	-3.223500	0.950836	0.094742
N	-1.823565	0.660052	-0.192946
B	1.363486	-0.533155	-0.506397
N	-0.132859	-1.042022	-0.200154
C	-1.395279	-0.595536	-0.114381
N	1.688554	0.848903	0.234928
C	1.009278	1.032830	1.526354
H	0.084638	1.588628	1.345146
H	0.763218	0.079482	1.987039
H	1.633165	1.602565	2.216244
C	3.143130	1.055037	0.338587
H	3.587543	0.422887	1.106814
H	3.573847	0.761291	-0.619375
C	3.405811	2.549589	0.601817
H	3.568895	2.740150	1.663732
H	4.314780	2.857928	0.084089
C	2.168524	3.298376	0.087205
H	1.559936	3.675458	0.912810
H	2.435935	4.159426	-0.527426
C	1.313237	2.365369	-0.752524
H	1.841357	2.014203	-1.635538
C	-0.059830	2.683109	-0.929304
H	-0.407790	3.563163	-0.392821
H	-0.433988	2.615625	-1.946864
H	-1.085410	1.474098	-0.432149
N	-2.218559	-1.664254	0.057600
C	1.187694	-3.027249	-0.317931
H	1.332382	-3.937670	0.270934
H	1.332972	-3.289151	-1.370683
C	1.505066	-0.385789	-2.116857
H	2.477985	-0.012343	-2.451528
H	1.363869	-1.355827	-2.602810
H	0.739005	0.282308	-2.519285
C	2.159050	-1.889791	0.094066
C	-4.085937	-0.207956	-0.433648
H	-5.136894	-0.023618	-0.202263
H	-3.975647	-0.246504	-1.520212
C	-3.418310	1.136061	1.606056
H	-2.840194	1.998316	1.942265
H	-4.470942	1.303249	1.849287
H	-3.063426	0.262772	2.156879
C	-3.596283	2.237815	-0.638028
H	-2.952416	3.054932	-0.310705
H	-3.465918	2.111804	-1.713990
H	-4.635019	2.503250	-0.431431
C	2.270516	-1.983083	1.626282
H	2.771800	-2.917441	1.904589
H	2.841916	-1.166758	2.069856
H	1.283942	-1.994960	2.097955
C	3.535452	-2.163784	-0.516876
H	3.880600	-3.170424	-0.253008
H	3.509582	-2.093539	-1.606269
H	4.288917	-1.462669	-0.152271

cat1_am1_f_S

SCF energy in solution: –989.151206
Enthalpy in solution: –988.584733
Free energy in solution: –988.659045

Cartesian coordinates

Atom	X	Y	Z
C	-1.615428	2.436149	-0.968673
H	-2.060246	3.301266	-1.427947
C	-0.335415	2.127553	-0.688560
C	-3.831712	1.254520	-0.491213
H	-4.245810	1.005612	-1.473735
H	-4.233099	2.227339	-0.196954
C	-3.341403	-1.082817	0.349247
N	-1.916146	-0.787632	0.467249
B	1.081210	0.522382	0.545448
C	1.029238	2.706039	-0.841124
H	1.045907	3.789445	-0.692404
H	1.404307	2.524075	-1.855387
N	-0.288807	0.873720	-0.085818
C	-1.567688	0.371936	-0.002876
N	-2.387496	1.339625	-0.556048
C	0.854798	0.096459	2.090769
H	0.065468	-0.653985	2.163160
H	1.725880	-0.257718	2.644038
H	0.475099	0.967298	2.627895
C	1.908041	1.964783	0.212301
C	-4.194852	0.187024	0.537033
H	-4.003280	0.575705	1.540961

H	-5.258749	-0.049264	0.460173
C	-3.619947	-1.713855	-1.024000
H	-3.058666	-2.646013	-1.110866
H	-4.683881	-1.932028	-1.157229
H	-3.293663	-1.052456	-1.829311
C	-3.696375	-2.085351	1.445302
H	-3.057560	-2.965111	1.349536
H	-3.516893	-1.642444	2.426438
H	-4.742207	-2.396768	1.378128
C	3.354923	1.984824	-0.301580
H	3.668777	3.023582	-0.455389
H	4.063141	1.544132	0.402111
H	3.469826	1.482785	-1.265419
C	1.880434	2.819797	1.491668
H	2.342467	3.795506	1.305018
H	0.855547	2.994245	1.827100
H	2.422368	2.338278	2.308973
C	3.121225	-1.220181	-0.266190
C	3.171304	-2.683302	-0.777548
H	3.879564	-3.253721	-0.176611
H	3.515058	-2.736305	-1.810630
C	1.729616	-3.225484	-0.632677
H	1.288497	-3.435859	-1.607219
H	1.690068	-4.147734	-0.054792
C	0.980142	-2.103801	0.087265
H	1.121122	-2.184446	1.161756
H	-0.091414	-2.022751	-0.094812
N	1.659572	-0.839410	-0.348385
C	1.344759	-0.609029	-1.785120
H	0.267144	-0.636395	-1.918120
H	1.715036	0.372062	-2.070279
H	1.814914	-1.366577	-2.410666
H	3.666220	-0.548398	-0.924416
C	3.705398	-1.123878	1.136667
H	3.593910	-0.131616	1.564232
H	3.247216	-1.847584	1.811919
H	4.769667	-1.358500	1.070380

cat1_am1_d_R

SCF energy in solution: –989.137797

Enthalpy in solution: –988.574879

Free energy in solution: –988.655372

Cartesian coordinates

Atom	X	Y	Z
C	3.341922	0.685928	0.274883
H	4.368512	0.841146	0.553183
C	2.304771	1.541151	0.071533
C	3.482565	-1.894928	0.204437
H	3.607410	-2.097475	1.270951
H	4.472054	-1.862261	-0.252994
C	1.124601	-2.835104	-0.142368
N	0.719171	-1.512715	-0.628872
B	-0.153614	1.635070	-0.469611
N	1.199672	0.794874	-0.274671
C	1.536071	-0.477006	-0.301185
N	-1.276107	0.759618	0.135852
C	-1.179621	0.269979	1.502254
H	-0.141939	0.031320	1.748134
H	-1.535731	0.979476	2.260816
H	-1.773075	-0.643910	1.628394
C	-2.647773	1.137107	-0.202323
H	-3.270749	1.102743	0.700026
H	-2.688548	2.170971	-0.561530
C	-3.280728	0.229667	-1.262964
H	-4.259259	0.633325	-1.549618
H	-2.651025	0.245909	-2.154048
C	-3.457436	-1.220276	-0.796007
H	-3.758940	-1.832441	-1.653160
H	-2.498439	-1.611450	-0.441785
C	-4.488700	-1.367089	0.286450
C	-4.311747	-2.014810	1.433699
H	-5.100277	-2.095310	2.171317
H	-3.365000	-2.490736	1.668397
H	-0.258311	-1.227405	-0.560510
N	2.837944	-0.602678	0.028453
C	1.954308	2.999975	0.067607
H	2.506458	3.567981	0.821777
H	2.207623	3.418978	-0.912127
C	-0.358330	1.831175	-2.072215
H	-1.253321	2.405598	-2.328873
H	0.491167	2.359310	-2.518440
H	-0.432861	0.862947	-2.578444
C	0.408297	3.041281	0.281892
C	2.623364	-2.970760	-0.466432
H	2.974556	-3.954267	-0.149394
H	2.739069	-2.900388	-1.550424
C	0.861619	-2.979301	1.361525
H	-0.209054	-2.896333	1.559805
H	1.205970	-3.950965	1.722910
H	1.364326	-2.195191	1.931372
C	0.333117	-3.882029	-0.918744
H	-0.737484	-3.749537	-0.745548
H	0.524176	-3.785435	-1.987837

H	0.609004	-4.886280	-0.592633
C	0.152470	3.071567	1.792510
H	0.578768	3.978061	2.239958
H	-0.918929	3.069875	2.004402
H	0.597526	2.212455	2.301155
C	-0.163212	4.328083	-0.316485
H	0.275697	5.217871	0.151553
H	0.017070	4.389180	-1.391350
H	-1.244453	4.376772	-0.157993
H	-5.452041	-0.901231	0.086867

cat1_am1_ets$_R$

SCF energy in solution: –989.093433

Enthalpy in solution: –988.532947

Free energy in solution: –988.606172

Cartesian coordinates

Atom	X	Y	Z
C	-1.338561	-2.819131	-0.218168
H	-1.739778	-3.814363	-0.284089
C	-0.073268	-2.347447	-0.237202
C	-3.619663	-1.650498	-0.148517
H	-4.026302	-1.846392	0.846892
H	-3.973006	-2.435926	-0.817870
C	-3.309468	0.859892	0.071361
N	-1.871343	0.658162	-0.074142
B	1.371599	-0.339935	-0.317106
N	-0.103267	-0.961598	-0.111975
C	-1.389920	-0.581993	-0.091876
N	1.611271	0.918518	0.663603
C	0.855351	0.816722	1.918827
H	-0.191989	1.035829	1.709310
H	0.930793	-0.169242	2.370922
H	1.224479	1.558084	2.631905
C	3.039547	1.199724	0.891602
H	3.114176	1.837986	1.777226
H	3.614834	0.298738	1.088557
C	3.565852	1.965961	-0.327058
H	4.422769	2.574370	-0.034420
H	3.911988	1.270005	-1.090306
C	2.391049	2.815920	-0.842467
H	2.630914	3.881505	-0.823122
H	2.133888	2.565626	-1.869946
C	1.172266	2.616922	0.046032
C	-0.144372	2.818760	-0.441064
H	-0.752380	3.502793	0.143895
H	-0.245157	2.948892	-1.515694
H	-1.150765	1.512177	-0.212406
N	-2.168571	-1.696426	-0.114515
C	1.311578	-2.853010	-0.470117
H	1.496992	-3.819728	0.006784
H	1.467142	-2.982688	-1.546014
C	1.459460	0.026577	-1.895051
H	2.435814	0.365387	-2.243274
H	1.211077	-0.862749	-2.483698
H	0.723517	0.791838	-2.152653
C	2.237453	-1.733174	0.074392
C	-4.046765	-0.276675	-0.658290
H	-5.124723	-0.160050	-0.529751
H	-3.818501	-0.202746	-1.724483
C	-3.682034	0.886957	1.560111
H	-3.186053	1.731240	2.041427
H	-4.762092	0.992004	1.693289
H	-3.351131	-0.023562	2.063229
C	-3.670145	2.193988	-0.578208
H	-3.133558	3.008170	-0.090595
H	-3.394519	2.188436	-1.633879
H	-4.742556	2.378420	-0.488674
C	2.405154	-2.045185	1.573575
H	2.968147	-2.978010	1.693454
H	2.939922	-1.273264	2.128724
H	1.434619	-2.192533	2.055378
C	3.601038	-1.856336	-0.614757
H	4.017656	-2.859554	-0.466676
H	3.517722	-1.684878	-1.689813
H	4.332677	-1.146404	-0.221636
H	1.341454	3.051829	1.033989

cat1_am1_f$_R$

SCF energy in solution: –989.157169

Enthalpy in solution: –988.591295

Free energy in solution: –988.665628

Cartesian coordinates

Atom	X	Y	Z
C	-0.970471	-2.971012	0.081727
H	-1.281003	-3.994284	0.197355
C	0.246678	-2.408977	-0.041144
C	-3.339311	-2.014595	0.015050
H	-3.725808	-2.132308	1.032570
H	-3.632165	-2.898585	-0.556125
C	-3.206106	0.513494	-0.067409
N	-1.758458	0.468823	-0.251413
B	1.487912	-0.377161	-0.495149

C	1.679314	-2.818951	-0.151970
H	1.900557	-3.126656	-1.179332
H	1.932883	-3.659166	0.500508
N	0.103233	-1.028248	-0.163076
C	-1.233245	-0.720889	-0.152028
N	-1.895740	-1.919554	0.025744
C	1.698542	-0.292367	-2.101556
H	0.894045	0.250764	-2.602864
H	2.653429	0.135756	-2.422315
H	1.672014	-1.309187	-2.502777
C	2.483186	-1.534698	0.203940
C	-3.888795	-0.747575	-0.632763
H	-3.694055	-0.782860	-1.708249
H	-4.970035	-0.699114	-0.483710
C	-3.521759	0.669604	1.428251
H	-3.068607	1.593884	1.793373
H	-4.599726	0.710436	1.611994
H	-3.098002	-0.156283	2.003515
C	-3.734174	1.732619	-0.821756
H	-3.244275	2.634877	-0.450045
H	-3.508454	1.637748	-1.885359
H	-4.814168	1.843359	-0.693680
C	2.583951	-1.528392	1.739403
H	3.086347	-2.441232	2.077849
H	3.171178	-0.693793	2.130834
H	1.595539	-1.504349	2.204777
C	3.894919	-1.656844	-0.376661
H	4.386366	-2.562373	-0.002964
H	3.875414	-1.715624	-1.466382
H	4.529979	-0.811501	-0.099315
C	0.761553	2.188277	-0.643372
H	-0.067062	1.620543	-1.059222
C	0.176376	3.176944	0.391650
H	-0.909777	3.100922	0.346241
H	0.467333	4.205471	0.173079
C	0.674059	2.712731	1.765212
H	1.574612	3.248134	2.072297
H	-0.071180	2.848075	2.548649
C	0.950976	1.236393	1.530748
H	0.010903	0.692984	1.485849
H	1.614497	0.778580	2.257473
N	1.567704	1.155315	0.161169
C	2.990241	1.563329	0.249499
H	3.494841	0.919326	0.962536
H	3.460415	1.449692	-0.723634
H	3.074479	2.600013	0.573830
C	1.529162	2.907040	-1.745506
H	1.973475	2.229675	-2.470024
H	0.807700	3.531904	-2.275258
H	2.301017	3.569852	-1.350584

cat1_am1_a'

SCF energy in solution: –989.131389

Enthalpy in solution: –988.566819

Free energy in solution: –988.64874

Cartesian coordinates

Atom	X	Y	Z
C	0.361057	-0.810254	-2.567297
H	0.565161	-0.791022	-3.622992
C	-0.794315	-0.787648	-1.864975
C	2.816253	-1.102809	-1.837774
H	3.320132	-0.154252	-2.047070
H	2.950382	-1.751136	-2.706576
C	2.926434	-1.051023	0.708235
N	1.467207	-1.023040	0.803472
B	-1.693384	-0.974023	0.401593
C	-2.285364	-0.838315	-2.042501
H	-2.572996	-1.855293	-2.329716
H	-2.646671	-0.168331	-2.827150
N	-0.481165	-0.853001	-0.522048
C	0.861861	-0.944428	-0.351709
N	-1.260837	-0.030839	1.724350
C	-1.097887	1.451357	1.621245
H	-0.788300	1.799130	2.612498
H	-2.077918	1.879687	1.421309
C	-2.106955	-0.323158	2.902095
H	-3.138009	-0.060995	2.663246
H	-2.052645	-1.379606	3.139252
N	1.400051	-0.892346	-1.617633
C	-1.824593	-2.492632	0.951603
H	-0.948042	-2.784840	1.539829
H	-2.725015	-2.708827	1.532954
H	-1.845423	-3.157434	0.082540
C	-2.905353	-0.494861	-0.641499
C	3.387149	-1.763169	-0.581990
H	3.037505	-2.798400	-0.537422
H	4.478085	-1.774902	-0.640291
C	3.486960	0.379781	0.745130
H	3.199795	0.856557	1.684925
H	4.578760	0.383003	0.673397
H	3.081710	0.979435	-0.073508
C	3.453305	-1.826745	1.913976
H	3.097012	-1.354447	2.831243

H	3.074069	-2.849687	1.890697
H	4.546067	-1.849474	1.929106
C	-3.272699	0.996689	-0.647569
H	-4.000920	1.195195	-1.441740
H	-3.743767	1.299462	0.292098
H	-2.411408	1.642110	-0.831149
C	-4.211248	-1.275506	-0.458589
H	-4.938844	-1.009637	-1.233703
H	-4.048185	-2.353092	-0.506031
H	-4.669523	-1.052724	0.509935
C	-0.066005	1.938966	0.613800
H	0.894035	1.473965	0.844466
H	-0.324918	1.644390	-0.402335
C	0.051133	3.466938	0.688033
H	0.251455	3.763766	1.724637
H	-0.895877	3.931822	0.396597
C	1.154001	3.973452	-0.195859
H	2.153168	3.613302	0.038880
C	0.978789	4.791150	-1.227954
H	1.808820	5.115652	-1.842557
H	-0.006361	5.161744	-1.489269
H	-1.775642	0.262015	3.760668
H	-0.310722	-0.409145	1.879865

cat1_am1_b'ts

SCF energy in solution: –989.11173

Enthalpy in solution: –988.55294

Free energy in solution: –988.632477

Cartesian coordinates

Atom	X	Y	Z
C	0.290612	-0.480917	-2.714499
H	0.416357	-0.274853	-3.761740
C	-0.803232	-0.761945	-1.953762
C	2.821276	-0.316149	-2.048086
H	3.048441	0.751750	-2.104691
H	3.114460	-0.775069	-2.993482
C	3.025081	-0.585901	0.512721
N	1.590080	-0.873136	0.567785
B	-1.411321	-1.275350	0.418130
C	-2.295967	-0.969679	-1.963931
H	-2.505216	-1.995534	-2.284944
H	-2.817453	-0.300438	-2.652440
N	-0.366052	-0.975425	-0.675492
C	0.944612	-0.812569	-0.593667
N	-0.734708	-0.527863	1.701770
C	-0.944257	0.925196	1.869238
H	-0.532231	1.211342	2.844715
H	-2.014718	1.144178	1.913530
C	-1.042154	-1.172865	2.984838
H	-2.104692	-1.073832	3.235526
H	-0.793913	-2.229026	2.946543
H	0.600127	-0.703430	1.367301
N	1.400566	-0.522172	-1.834450
C	-1.415333	-2.879120	0.679948
H	-0.434374	-3.228744	1.018892
H	-2.164436	-3.218926	1.400765
H	-1.621421	-3.397161	-0.261824
C	-2.774507	-0.775877	-0.468480
C	3.561028	-0.987893	-0.882273
H	3.455063	-2.071248	-0.985843
H	4.623968	-0.745175	-0.944999
C	3.318338	0.897089	0.777273
H	2.949867	1.178052	1.766007
H	4.394273	1.087967	0.745286
H	2.830092	1.537063	0.039540
C	3.720341	-1.435928	1.574669
H	3.327406	-1.184473	2.561822
H	3.528264	-2.493539	1.390411
H	4.798432	-1.259573	1.574870
C	-3.246783	0.680880	-0.336265
H	-4.064148	0.868165	-1.042594
H	-3.639772	0.887656	0.661492
H	-2.461063	1.404384	-0.556356
C	-4.007797	-1.652596	-0.222590
H	-4.830512	-1.371578	-0.890492
H	-3.796906	-2.711029	-0.378421
H	-4.365269	-1.533793	0.804418
C	-0.271910	1.814944	0.825502
H	0.809575	1.748663	0.945701
H	-0.495760	1.489418	-0.190122
C	-0.716239	3.272332	0.997646
H	-0.539498	3.578564	2.035702
H	-1.792269	3.354766	0.817533
C	0.022412	4.191055	0.068708
H	1.099987	4.247988	0.209467
C	-0.544985	4.894706	-0.905259
H	0.036451	5.530267	-1.561283
H	-1.615619	4.854620	-1.073921
H	-0.459297	-0.709090	3.785290

cat1_am1_c'

SCF energy in solution: –989.130137

Enthalpy in solution: –988.566764

Free energy in solution: –988.647771

Cartesian coordinates

Atom	X	Y	Z
C	0.372270	-1.113438	-2.504592
H	0.571712	-1.195593	-3.557628
C	-0.780340	-1.014255	-1.791156
C	2.847442	-1.205851	-1.772804
H	3.234890	-0.236260	-2.094154
H	3.041312	-1.929466	-2.565165
C	3.008069	-0.854343	0.750953
N	1.558864	-1.059886	0.826498
B	-1.720405	-0.899981	0.542430
C	-2.268875	-1.055208	-1.967653
H	-2.569676	-2.098667	-2.108957
H	-2.601789	-0.499651	-2.848932
N	-0.453638	-0.943871	-0.454946
C	0.856073	-1.025676	-0.334868
N	-1.333646	0.017000	1.735304
C	-1.211247	1.466076	1.596379
H	-0.929889	1.869252	2.579606
H	-2.167586	1.951117	1.352498
C	-2.101953	-0.243547	2.946061
H	-3.146882	0.104216	2.878549
H	-2.118966	-1.306600	3.172146
H	1.015433	-0.697702	1.607208
N	1.411571	-1.118983	-1.561603
C	-1.903034	-2.444562	1.034940
H	-1.068941	-2.754911	1.674456
H	-2.828699	-2.628938	1.585818
H	-1.911926	-3.120665	0.172858
C	-2.874950	-0.502164	-0.637582
C	3.498105	-1.660096	-0.465402
H	3.260777	-2.712553	-0.293107
H	4.581810	-1.562552	-0.549435
C	3.372234	0.628751	0.602445
H	3.099466	1.173839	1.508139
H	4.448079	0.742402	0.447932
H	2.845256	1.088757	-0.235811
C	3.628236	-1.421887	2.023754
H	3.234464	-0.901235	2.899394
H	3.395251	-2.482750	2.119118
H	4.711617	-1.290736	2.009177
C	-3.155330	0.993509	-0.846312
H	-3.835144	1.133097	-1.696191
H	-3.642042	1.427742	0.028518
H	-2.251618	1.570718	-1.055581
C	-4.230450	-1.173035	-0.387252
H	-4.945353	-0.935073	-1.184575
H	-4.141359	-2.259046	-0.330172
H	-4.662723	-0.826096	0.555740
C	-0.143796	1.951586	0.619162
H	0.834471	1.625816	0.981516
H	-0.274452	1.519250	-0.373000
C	-0.155593	3.479761	0.491787
H	-0.133167	3.923098	1.494235
H	-1.088088	3.801062	0.018713
C	1.015706	3.976447	-0.304556
H	1.996721	3.811083	0.137651
C	0.932611	4.559236	-1.496320
H	1.814711	4.880381	-2.036217
H	-0.028645	4.736582	-1.966179
H	-1.650134	0.272343	3.801019

cat1_am1_d's

SCF energy in solution: –989.135035

Enthalpy in solution: –988.572458

Free energy in solution: –988.650688

Cartesian coordinates

Atom	X	Y	Z
C	-0.021318	-3.182889	-0.109377
H	0.019010	-4.242713	-0.285058
C	-1.054637	-2.325191	0.064257
C	2.515841	-2.861897	-0.153372
H	2.723826	-3.055524	-1.208570
H	2.639377	-3.797135	0.393763
C	3.046120	-0.378793	-0.067999
N	1.687361	-0.147675	0.436929
B	-1.741150	0.033691	0.539698
C	-2.543833	-2.353682	0.182339
H	-2.811751	-2.635775	1.206061
H	-3.001946	-3.083592	-0.492356
N	-0.545517	-1.046379	0.241819
C	0.775604	-1.131070	0.224564
N	-1.417206	1.397795	-0.108795
C	-0.783364	1.516331	-1.407148
H	-1.492452	1.378132	-2.241595
H	-0.031940	0.727022	-1.512070
C	-2.522848	2.330079	0.015568
H	-3.245393	2.250794	-0.815089
H	-3.063379	2.144877	0.942284
H	1.317551	0.790300	0.543921
N	1.141522	-2.414354	-0.004631

C	-1.804207	0.165186	2.162236
H	-0.879762	0.620210	2.533037
H	-2.631376	0.783120	2.521811
H	-1.912289	-0.809872	2.650471
C	-2.981999	-0.896158	-0.102462
C	3.446968	-1.787860	0.400464
H	3.415361	-1.800628	1.492166
H	4.469064	-2.001562	0.083409
C	3.091881	-0.272579	-1.598432
H	2.865618	0.748470	-1.909958
H	4.083945	-0.535939	-1.973140
H	2.355789	-0.930956	-2.063667
C	3.993953	0.637046	0.558169
H	3.766516	1.645239	0.210099
H	3.915762	0.612682	1.645936
H	5.020764	0.407116	0.268629
C	-3.092917	-0.738514	-1.623450
H	-3.841910	-1.426310	-2.035571
H	-3.392398	0.275683	-1.892853
H	-2.140314	-0.947803	-2.119126
C	-4.352588	-0.638120	0.523314
H	-5.107942	-1.327666	0.126309
H	-4.322868	-0.759923	1.608567
H	-4.695208	0.377455	0.310144
C	-0.105900	2.875950	-1.639588
H	0.290127	2.884071	-2.659879
H	-0.859907	3.667220	-1.608733
C	1.032126	3.246336	-0.679882
H	1.403699	4.234105	-0.976058
H	1.876047	2.560608	-0.813508
C	0.657258	3.306363	0.780231
H	-0.363123	3.591566	1.005494
C	1.497491	3.087074	1.790784
H	1.172458	3.182023	2.818739
H	2.534843	2.819066	1.627701
H	-2.194951	3.375811	0.041639

cat1_am1_e'ts$_S$

SCF energy in solution: –989.090971

Enthalpy in solution: –988.531581

Free energy in solution: –988.605296

Cartesian coordinates

Atom	X	Y	Z
C	0.917375	-2.990491	-0.178057
H	1.213153	-4.012110	-0.334704
C	-0.287401	-2.415998	0.021369
C	3.298921	-2.045660	-0.206844
H	3.633184	-2.127595	-1.244328
H	3.602302	-2.952247	0.318416
C	3.229983	0.481895	-0.050941
N	1.786666	0.408219	0.160462
B	-1.529986	-0.350371	0.537955
C	-1.713688	-2.820154	0.177901
H	-1.898029	-3.126411	1.212488
H	-1.985786	-3.660275	-0.467714
N	-0.122493	-1.039169	0.150088
C	1.192048	-0.779094	0.064726
N	-1.685262	1.126832	-0.051844
C	-1.082442	1.423130	-1.358348
H	-1.543123	0.842597	-2.158913
H	-0.026525	1.159726	-1.296447
C	-3.116417	1.471907	-0.047903
H	-3.635869	1.023279	-0.895617
H	-3.568595	1.108039	0.871840
H	1.181297	1.216184	0.711337
N	1.850954	-1.948316	-0.153028
C	-1.648657	-0.315710	2.156596
H	-0.796710	0.200105	2.599551
H	-2.554477	0.178252	2.521439
H	-1.661158	-1.328105	2.571230
C	-2.515067	-1.533309	-0.150386
C	3.889051	-0.809388	0.465146
H	3.722924	-0.872086	1.543645
H	4.965530	-0.776917	0.285694
C	3.516843	0.677141	-1.546183
H	3.086939	1.624241	-1.875348
H	4.592518	0.691951	-1.741429
H	3.061816	-0.117232	-2.140776
C	3.768546	1.674859	0.735068
H	3.301618	2.596747	0.386212
H	3.550375	1.562699	1.798308
H	4.848388	1.759009	0.597510
C	-2.625677	-1.485514	-1.683352
H	-3.138420	-2.382037	-2.051132
H	-3.200058	-0.627421	-2.037008
H	-1.640193	-1.451896	-2.155980
C	-3.921206	-1.678595	0.438855
H	-4.378308	-2.619113	0.109044
H	-3.897998	-1.684217	1.530841
H	-4.585700	-0.873625	0.118920
C	-1.232418	2.926262	-1.576642
H	-0.527485	3.277835	-2.330747
H	-2.232103	3.159372	-1.946422

C	-0.971550	3.585638	-0.204000
H	-1.720981	4.350729	0.006960
H	-0.004546	4.085661	-0.221445
C	-0.935095	2.546559	0.930312
H	-1.790748	2.568208	1.604366
C	0.348142	2.328778	1.505586
H	0.376872	2.028426	2.547693
H	1.082766	3.091245	1.263277
H	-3.259730	2.552351	-0.087697

cat1_am1_f'$_S$

SCF energy in solution: –989.141073

Enthalpy in solution: –988.574965

Free energy in solution: –988.649374

Cartesian coordinates

Atom	X	Y	Z
C	1.128791	-2.895279	0.041284
H	1.474348	-3.909105	-0.058347
C	-0.106665	-2.378491	0.155615
C	3.454948	-1.858350	0.036785
H	3.831099	-2.066019	-0.970179
H	3.781271	-2.672256	0.688632
C	3.231737	0.647938	-0.133839
N	1.797482	0.575237	0.116480
B	-1.492774	-0.441646	0.536356
C	-1.515475	-2.864519	0.177637
H	-1.814831	-3.150234	1.190440
H	-1.665667	-3.736431	-0.465807
N	-0.029872	-0.984039	0.233297
C	1.297413	-0.628165	0.146621
N	-1.743763	1.115675	-0.019172
C	-0.952018	1.436670	-1.250733
H	-1.261639	0.780530	-2.059508
H	0.096201	1.258677	-1.006314
C	-3.199554	1.215920	-0.319679
H	-3.433733	0.628950	-1.199852
H	-3.753170	0.830143	0.533735
N	2.008021	-1.809085	0.037230
C	-1.847015	-0.494523	2.129199
H	-0.946353	-0.418157	2.738760
H	-2.539309	0.282449	2.470984
H	-2.311091	-1.445365	2.398141
C	-2.338021	-1.638556	-0.304565
C	3.975322	-0.517848	0.543150
H	3.804146	-0.447844	1.620864
H	5.050544	-0.448867	0.362311
C	3.490437	0.639260	-1.649116
H	3.011144	1.510832	-2.098873
H	4.560851	0.673366	-1.874040
H	3.061820	-0.250969	-2.113617
C	3.734126	1.966155	0.452465
H	3.171308	2.793214	0.014512
H	3.572997	1.979727	1.532233
H	4.797589	2.114716	0.248125
C	-2.194607	-1.627726	-1.838351
H	-2.571871	-2.569743	-2.251628
H	-2.766757	-0.832451	-2.322839
H	-1.149689	-1.530074	-2.141211
C	-3.811585	-1.886925	0.039570
H	-4.108102	-2.889015	-0.290388
H	-3.999165	-1.827086	1.113766
H	-4.483105	-1.184989	-0.459043
C	-1.200753	2.919306	-1.504120
H	-0.373629	3.358277	-2.060304
H	-2.108993	3.080958	-2.086365
C	-1.325996	3.511874	-0.085322
H	-2.168957	4.199409	-0.008084
H	-0.427952	4.070221	0.175633
C	-1.468446	2.315668	0.898035
H	-2.360756	2.419331	1.515576
C	-0.250601	2.211857	1.799494
H	-0.386944	1.484499	2.592831
H	-0.114627	3.191344	2.264670
H	-3.481760	2.253696	-0.490328
H	0.643356	1.946387	1.234128

cat1_am1_d'$_R$

SCF energy in solution: –989.133533

Enthalpy in solution: –988.570541

Free energy in solution: –988.649905

Cartesian coordinates

Atom	X	Y	Z
C	1.309671	-2.900041	-0.639718
H	1.723282	-3.757318	-1.139664
C	0.041619	-2.565450	-0.296215
C	3.541727	-1.657607	-0.457809
H	3.734769	-1.524947	-1.525020
H	4.055388	-2.561692	-0.128782
C	3.068766	0.749881	0.183666
N	1.772141	0.325832	0.735391
B	-1.489397	-0.863027	0.725782
C	-1.360189	-3.037938	-0.513421

H	-1.682505	-3.688987	0.302959
H	-1.456532	-3.600718	-1.446497
N	0.062357	-1.325691	0.320984
C	1.306024	-0.886472	0.299823
N	-1.544722	0.673326	0.715963
C	-2.854887	1.233162	0.415375
H	-3.555283	1.072250	1.257313
H	-3.276117	0.710150	-0.441213
H	1.043141	1.030167	0.719093
N	2.112919	-1.826871	-0.243671
C	-1.833424	-1.523854	2.177301
H	-1.129440	-1.230558	2.960451
H	-2.824561	-1.185945	2.502661
H	-1.859935	-2.617132	2.176516
C	-2.194975	-1.720793	-0.520880
C	4.017126	-0.446768	0.342024
H	4.065705	-0.703085	1.402853
H	5.018241	-0.166082	0.010812
C	2.942657	1.164867	-1.288037
H	2.328539	2.062066	-1.378611
H	3.926793	1.380223	-1.710865
H	2.470923	0.381203	-1.884050
C	3.563214	1.919965	1.026612
H	2.842379	2.740262	0.993491
H	3.686717	1.612787	2.065602
H	4.516902	2.287306	0.643879
C	-1.988401	-1.077648	-1.902290
H	-2.289654	-1.767943	-2.699437
H	-2.573424	-0.166331	-2.028034
H	-0.939920	-0.812453	-2.065781
C	-3.670050	-2.077471	-0.329604
H	-4.017223	-2.750633	-1.122664
H	-3.832017	-2.576052	0.628569
H	-4.308182	-1.191594	-0.352612
C	-2.856545	2.729516	0.090923
H	-3.896854	3.025955	-0.076336
H	-2.501710	3.315903	0.942496
C	-2.040373	3.110352	-1.157174
H	-2.284865	4.139588	-1.434776
H	-2.350957	2.466972	-1.987149
C	-0.550678	3.005351	-0.975547
H	-0.143676	2.000427	-1.008257
C	0.236787	4.055200	-0.750064
H	1.306832	3.957713	-0.607648
H	-0.169144	5.060344	-0.703915
C	-1.053582	1.278931	1.950240
H	-1.819192	1.302247	2.742893
H	-0.207913	0.715760	2.347220
H	-0.719312	2.310016	1.783693

cat1_am1_e'ts$_R$

SCF energy in solution: –989.094692

Enthalpy in solution: –988.534515

Free energy in solution: –988.607114

Cartesian coordinates

Atom	X	Y	Z
C	1.420990	-2.744255	-0.422610
H	1.856922	-3.696413	-0.666403
C	0.137644	-2.344669	-0.271415
C	3.658172	-1.523059	-0.160465
H	4.041344	-1.493048	-1.183180
H	4.058469	-2.413444	0.326799
C	3.227859	0.952271	0.143697
N	1.803457	0.679655	0.386123
B	-1.356971	-0.621446	0.623212
C	-1.232768	-2.940767	-0.282403
H	-1.387065	-3.529543	0.626271
H	-1.387316	-3.610644	-1.133144
N	0.121974	-0.996733	0.068071
C	1.390910	-0.575621	0.121301
N	-1.680136	0.929068	0.482958
C	-3.126874	1.179734	0.477896
H	-3.575438	0.931501	1.445045
H	-3.571501	0.530500	-0.272547
H	1.106368	1.383837	-0.161954
N	2.207824	-1.617574	-0.175864
C	-1.385362	-1.049052	2.198022
H	-0.576151	-0.590128	2.771411
H	-2.326802	-0.771573	2.684563
H	-1.276859	-2.129779	2.321557
C	-2.203074	-1.724855	-0.309990
C	4.040886	-0.263498	0.611423
H	3.847789	-0.419003	1.676021
H	5.106778	-0.065920	0.481942
C	3.487488	1.237342	-1.343307
H	2.991041	2.162526	-1.636280
H	4.559541	1.340969	-1.531432
H	3.094700	0.438942	-1.975983
C	3.601995	2.176224	0.974922
H	2.962781	3.016052	0.695946
H	3.455532	1.970099	2.036055
H	4.643174	2.457813	0.802713
C	-2.380784	-1.359352	-1.792874

H	-2.785700	-2.216468	-2.343452
H	-3.076734	-0.531687	-1.946047
H	-1.426837	-1.089284	-2.253538
C	-3.553967	-2.181347	0.252068
H	-3.928536	-3.046488	-0.307465
H	-3.471783	-2.472906	1.301011
H	-4.315379	-1.401641	0.182644
C	-3.344952	2.641729	0.080617
H	-4.336652	2.768891	-0.354280
H	-3.296571	3.289241	0.957331
C	-2.216494	2.983189	-0.910608
H	-1.655491	3.858193	-0.577196
H	-2.614464	3.228029	-1.897404
C	-1.244514	1.816461	-1.096710
H	-1.652630	1.034081	-1.726687
C	0.126512	2.112882	-1.301327
H	0.608448	1.576288	-2.112912
H	0.411464	3.159035	-1.226973
C	-1.043695	1.722655	1.548495
H	-1.575075	1.589103	2.493345
H	-0.010392	1.411654	1.672133
H	-1.043788	2.781453	1.286606

cat1_am1_f'$_R$

SCF energy in solution: –989.152035

Enthalpy in solution: –988.586136

Free energy in solution: –988.660268

Cartesian coordinates

Atom	X	Y	Z
C	-1.474363	2.600551	-0.710204
H	-1.904751	3.527877	-1.045168
C	-0.212187	2.260801	-0.391512
C	-3.706713	1.388804	-0.490121
H	-4.079552	1.179192	-1.497654
H	-4.107405	2.357187	-0.181768
C	-3.290363	-0.981993	0.283536
N	-1.868183	-0.712326	0.463432
B	1.198342	0.587774	0.656803
C	1.097233	2.937810	-0.149862
H	1.044493	3.478515	0.801263
H	1.357865	3.667359	-0.921755
N	-0.179967	0.922163	0.002342
C	-1.472700	0.450232	0.036639
N	1.669167	-0.997954	0.340088
C	3.124405	-1.143123	0.654056
H	3.277537	-1.039193	1.725722
H	3.644128	-0.334715	0.148436
N	-2.259678	1.460027	-0.487440
C	1.079318	0.751158	2.267224
H	0.220860	0.202838	2.661776
H	1.966505	0.461666	2.840284
H	0.896880	1.806085	2.491874
C	2.143928	1.793210	-0.046980
C	-4.130553	0.293918	0.483952
H	-3.973261	0.643696	1.507940
H	-5.194039	0.079242	0.355307
C	-3.530773	-1.562133	-1.119330
H	-2.987028	-2.503360	-1.218705
H	-4.593682	-1.751417	-1.297715
H	-3.161172	-0.882729	-1.890452
C	-3.699286	-2.014600	1.331766
H	-3.077362	-2.905455	1.223793
H	-3.541930	-1.610077	2.333196
H	-4.748545	-2.300771	1.221915
C	2.651200	1.583644	-1.485482
H	3.097215	2.514974	-1.851382
H	3.429157	0.819883	-1.569278
H	1.833382	1.326887	-2.164736
C	3.319321	2.290136	0.803645
H	3.728666	3.216142	0.383788
H	3.010636	2.497435	1.829217
H	4.141629	1.571177	0.845500
C	3.547987	-2.495221	0.071284
H	4.594403	-2.470377	-0.229974
H	3.437946	-3.292948	0.805542
C	2.588968	-2.695890	-1.120443
H	2.032275	-3.630585	-1.032717
H	3.112970	-2.724371	-2.075772
C	1.628358	-1.488313	-1.095397
H	2.070103	-0.684599	-1.673073
C	0.259493	-1.803729	-1.668284
H	-0.343743	-0.907725	-1.781887
H	0.415750	-2.251895	-2.652486
C	0.907378	-1.946302	1.209427
H	1.222986	-1.796360	2.238384
H	-0.158573	-1.735815	1.109014
H	1.123807	-2.973544	0.915987
H	-0.293135	-2.510224	-1.050877

cat1_am1_ets_anti_H

SCF energy in solution: –989.034792

Enthalpy in solution: –988.473444

Free energy in solution: –988.545136

Cartesian coordinates

Atom	X	Y	Z
C	-1.027629	-2.943212	-0.178838
H	-1.369085	-3.963143	-0.173777
C	0.205997	-2.402157	-0.216573
C	-3.369620	-1.991292	-0.142404
H	-3.726156	-2.238345	0.860783
H	-3.641771	-2.811300	-0.808932
C	-3.310494	0.507989	0.097090
N	-1.862917	0.506226	-0.134516
B	1.674636	-0.430663	-0.439461
C	1.618186	-2.888730	-0.289527
H	1.883149	-3.121601	-1.324664
H	1.766470	-3.800455	0.294975
N	0.102995	-1.015758	-0.195619
C	-1.233242	-0.691451	-0.153342
N	1.891667	1.124715	0.220904
C	2.645294	1.245248	1.480575
H	2.647986	2.287522	1.797124
H	2.155736	0.654966	2.248249
H	3.668475	0.897979	1.340970
C	2.384193	2.179862	-0.732308
H	3.475256	2.126399	-0.754018
H	2.017291	1.923720	-1.720523
C	1.885125	3.600507	-0.412761
H	2.262689	3.948370	0.552880
H	2.328008	4.250219	-1.175805
C	0.343825	3.682759	-0.412860
H	0.031807	4.716468	-0.246701
H	-0.006456	3.407442	-1.419622
C	-0.235905	2.729694	0.623743
H	-0.192525	3.127088	1.640951
C	0.415928	1.433939	0.444809
H	0.077448	1.104235	-0.534137
H	0.125518	0.732054	1.220588
N	-1.921140	-1.874273	-0.137887
C	1.848300	-0.356490	-2.044636
H	1.098730	0.283740	-2.518846
H	2.835960	-0.008968	-2.360039
H	1.707545	-1.348890	-2.477767
C	2.477262	-1.707237	0.237055
C	-3.958707	-0.675991	-0.626419
H	-3.774683	-0.567109	-1.698213
H	-5.037932	-0.670933	-0.460920
C	-3.584717	0.461844	1.607442
H	-3.147934	1.347469	2.072348
H	-4.658441	0.447590	1.813567
H	-3.126480	-0.416306	2.067154
C	-3.849171	1.817003	-0.479052
H	-3.317757	2.658955	-0.031966
H	-3.688717	1.845888	-1.558077
H	-4.917090	1.915525	-0.272368
C	2.458991	-1.824419	1.772756
H	2.714499	-2.847824	2.066562
H	3.191902	-1.174195	2.248056
H	1.472010	-1.600635	2.187988
C	3.920750	-1.852940	-0.249500
H	4.374766	-2.769895	0.141812
H	3.973667	-1.890304	-1.339101
H	4.539794	-1.015253	0.085491
H	-1.397292	1.586915	0.211631

Ir_IM

SCF energy in solution: –1477.636634

Enthalpy in solution: –1477.091356

Free energy in solution: –1477.169815

Cartesian coordinates

Atom	X	Y	Z
Ir	-1.230487	0.082591	0.142783
C	-1.158835	-1.002240	-1.703801
C	-2.470243	-0.527193	-1.522509
C	-3.636785	-1.434679	-1.153554
C	-3.891075	-1.424111	0.357805
C	-2.616567	-1.186398	1.140257
C	-1.393896	-1.898321	0.940048
C	-1.245265	-2.997348	-0.112671
C	-0.762112	-2.450941	-1.472072
H	-0.538751	-0.462691	-2.416924
H	-2.740068	0.361400	-2.082197
H	-2.777500	-0.793839	2.138428
H	-0.767672	-2.003327	1.820443
H	-4.528142	-1.096750	-1.685013
H	-3.432346	-2.444644	-1.512702
H	-4.574274	-0.606155	0.597103
H	-4.379871	-2.350971	0.680258
H	-0.527198	-3.738585	0.243996
H	-2.189362	-3.534470	-0.227362
H	0.329278	-2.509748	-1.512955
H	-1.126877	-3.069518	-2.300871
Cl	-0.665307	0.880459	2.382378
N	1.097559	0.133622	-0.128595
C	1.752716	1.427285	0.165523

C	1.259828	2.624382	-0.653889
C	-0.176627	3.033524	-0.279738
C	-1.271995	2.103479	-0.738960
C	-2.448402	1.891350	0.007437
H	2.830122	1.321091	-0.005812
C	2.183610	3.794373	-0.288217
C	1.395205	2.346544	-2.154426
H	-0.359449	4.020394	-0.725387
H	-0.236751	3.150641	0.805073
H	1.591597	1.623878	1.226791
H	-1.352573	2.005824	-1.820598
H	-3.393030	1.698560	-0.485293
H	-2.523079	2.307988	1.004908
C	1.734092	-0.947193	0.666404
H	1.254652	-0.075561	-1.109562
H	2.430711	2.099560	-2.405791
H	0.756823	1.522800	-2.481699
H	1.108099	3.229471	-2.731055
H	2.119683	4.016723	0.779817
H	3.224508	3.566501	-0.530230
H	1.894593	4.691976	-0.839251
H	1.553008	-0.709217	1.715371
H	1.205564	-1.872289	0.441322
C	3.210067	-1.123056	0.386079
C	3.625958	-1.651063	-0.838488
C	5.933638	-1.431126	-0.182535
C	4.174919	-0.755405	1.323128
C	5.530084	-0.909788	1.042671
H	6.269110	-0.621502	1.779834
H	3.858539	-0.344289	2.275423
C	4.978044	-1.802281	-1.125395
H	2.883530	-1.956974	-1.570332
H	6.987088	-1.551621	-0.401483
H	5.286668	-2.216062	-2.077402

Ir_TS

SCF energy in solution: –1477.582837

Enthalpy in solution: –1477.042157

Free energy in solution: –1477.119184

Cartesian coordinates

Atom	X	Y	Z
Ir	-1.258549	-0.080330	-0.245939
C	-3.338359	0.246579	-0.732858
C	-2.990820	-1.040906	-1.165081
C	-3.456092	-2.297986	-0.443284
C	-2.409139	-2.804791	0.555429
C	-1.573175	-1.678353	1.132880
C	-2.104342	-0.477121	1.683095
C	-3.602425	-0.199634	1.765590
C	-4.140592	0.531718	0.520598
H	-3.346887	1.042957	-1.469396
H	-2.760982	-1.158824	-2.218458
H	-0.634729	-2.025794	1.549213
H	-1.500466	0.024490	2.432765
H	-3.666182	-3.072941	-1.182371
H	-4.401463	-2.085620	0.057675
H	-1.724963	-3.482024	0.038521
H	-2.884599	-3.381629	1.357528
H	-3.796190	0.417720	2.643148
H	-4.135995	-1.139330	1.930393
H	-4.076455	1.604909	0.690144
H	-5.194196	0.283034	0.345863
Cl	-1.461885	2.451997	0.198184
N	0.969020	0.115447	0.087265
C	1.468404	1.172553	1.025638
C	2.234522	2.222893	0.192355
C	1.571466	2.087199	-1.187143
C	1.218316	0.605734	-1.330496
C	-0.064982	0.329004	-2.117998
H	2.102128	0.721242	1.789560
C	2.034019	3.619887	0.781279
C	3.735670	1.924975	0.099599
H	2.235251	2.410689	-1.992369
H	0.657741	2.679335	-1.215025
H	0.603113	1.636172	1.496330
H	2.072678	0.060143	-1.733815
H	0.098163	-0.306630	-2.989516
H	-0.575796	1.233295	-2.444110
H	-0.642258	-0.901451	-1.486192
C	1.556075	-1.230805	0.362339
H	4.187635	1.884957	1.094016
H	3.948507	0.979859	-0.401542
H	4.226856	2.723543	-0.462170
H	0.971050	3.852598	0.853302
H	2.480791	3.687353	1.777081
H	2.516600	4.368282	0.148177
H	1.069531	-1.929779	-0.319363
H	1.252718	-1.494727	1.374564
C	3.057085	-1.378834	0.257297
C	3.657229	-1.731404	-0.955294
C	5.841909	-1.644829	0.058506
C	3.872287	-1.219034	1.380618
C	5.254247	-1.342811	1.283128

H	5.870666	-1.208390	2.163144
H	3.421785	-1.001436	2.342434
C	5.039114	-1.852010	-1.059597
H	3.035781	-1.924523	-1.822942
H	6.917744	-1.738457	-0.020091
H	5.487058	-2.117810	-2.008790

cat1_am1_ts_cc

SCF energy in solution: –989.079202

Enthalpy in solution: –988.517605

Free energy in solution: –988.59898

Cartesian coordinates

Atom	X	Y	Z
C	-3.216595	1.814732	0.133560
H	-4.014089	2.510089	0.326864
C	-3.211046	0.478133	-0.072086
C	-1.350350	3.589030	0.042019
H	-1.281974	3.960585	1.068813
H	-2.023295	4.247796	-0.510864
C	0.881389	2.375853	-0.089400
N	0.217059	1.103690	-0.404973
B	-1.685311	-1.397306	-0.377826
C	-4.101223	-0.726717	-0.148581
H	-4.483559	-0.826991	-1.170406
H	-4.961273	-0.669117	0.522999
N	-1.906926	0.090828	-0.327879
C	-1.086178	1.157024	-0.262077
C	4.374613	-1.681858	-0.580389
H	4.378221	-0.908946	-1.369847
C	3.258812	-1.360773	0.409758
H	3.260818	-2.117253	1.198224
H	3.453820	-0.396373	0.890063
C	1.895850	-1.301399	-0.290230
H	1.929755	-0.573213	-1.103176
H	1.649422	-2.272469	-0.726263
C	0.818550	-0.887032	0.665564
C	-0.306247	-1.670922	0.917248
N	-1.880893	2.240378	0.027123
C	-1.116214	-1.961477	-1.766772
H	-0.225808	-1.417401	-2.088741
H	-0.878123	-3.028849	-1.733142
H	-1.869889	-1.825376	-2.549721
C	-3.157832	-1.930402	0.187519
C	0.027128	3.548924	-0.618339
H	-0.093783	3.417987	-1.696832
H	0.542250	4.496252	-0.444407
C	1.097001	2.540140	1.425040
H	1.854505	1.839823	1.782143
H	1.445307	3.550004	1.659515
H	0.172986	2.353505	1.976059
C	2.233369	2.394186	-0.799499
H	2.846798	1.556593	-0.459651
H	2.090113	2.296446	-1.876921
H	2.772364	3.322028	-0.592422
C	-3.214985	-2.134172	1.707079
H	-4.228055	-2.416631	2.013350
H	-2.539181	-2.927988	2.034339
H	-2.952175	-1.217761	2.243644
C	-3.651743	-3.207378	-0.492350
H	-4.664307	-3.466825	-0.163905
H	-3.664940	-3.104453	-1.579297
H	-3.000237	-4.051372	-0.248297
H	-0.222013	-2.713271	0.619256
H	-0.801007	-1.497761	1.863149
H	1.093891	-0.131225	1.386325
H	4.145987	-2.635324	-1.063852
N	5.667716	-1.807396	0.078064
H	6.306251	-2.281526	-0.546163
C	6.243280	-0.523615	0.451505
H	7.270113	-0.670865	0.786520
H	6.244242	0.212223	-0.368235
H	5.689251	-0.091957	1.286257

cat1_am1_cc

SCF energy in solution: –989.138471

Enthalpy in solution: –988.573386

Free energy in solution: –988.65101

Cartesian coordinates

Atom	X	Y	Z
C	-2.482990	1.213305	-1.834789
H	-3.182900	1.826110	-2.374166
C	-2.511853	-0.085968	-1.449677
C	-0.918671	3.151868	-1.244694
H	-1.680099	3.699635	-0.682789
H	-0.871047	3.570081	-2.251284
C	0.544342	2.351714	0.693067
N	0.387074	0.951579	0.226859
B	-1.465882	-1.587746	0.269737
C	-3.492860	-1.188853	-1.196025
H	-3.319716	-2.033655	-1.868750
H	-4.527027	-0.856842	-1.321297
N	-1.347053	-0.351035	-0.750420

C	-0.677488	0.776840	-0.604841
C	4.101805	-1.479269	-0.218355
H	3.721613	-1.909492	-1.161485
C	3.086235	-0.486909	0.333843
H	3.452775	-0.115199	1.295347
H	3.021778	0.371159	-0.343871
C	1.702605	-1.112769	0.476112
H	1.338574	-1.397639	-0.512111
H	1.772729	-2.033723	1.063647
C	0.654239	-0.211374	1.136114
C	-0.627887	-0.983765	1.548789
N	-1.292836	1.752510	-1.316447
C	-0.906553	-2.988040	-0.340698
H	0.155323	-3.006660	-0.585805
H	-1.067793	-3.783908	0.394855
H	-1.442328	-3.290897	-1.247030
C	-3.149275	-1.598341	0.278713
C	0.439095	3.243976	-0.558663
H	1.223832	2.933622	-1.252912
H	0.626722	4.281341	-0.276469
C	-0.537503	2.699282	1.724312
H	-0.397492	2.102926	2.627660
H	-0.479625	3.755310	1.999176
H	-1.537997	2.490258	1.340230
C	1.927060	2.591354	1.297463
H	2.098317	1.993050	2.191097
H	2.713193	2.371211	0.576347
H	2.001628	3.641795	1.585436
C	-3.729487	-0.532264	1.214318
H	-4.816672	-0.446415	1.097208
H	-3.526970	-0.785595	2.257781
H	-3.298607	0.456933	1.025051
C	-3.796384	-2.940586	0.613800
H	-4.890349	-2.879872	0.566737
H	-3.473455	-3.725762	-0.072007
H	-3.527429	-3.253526	1.626661
H	-0.305758	-1.771398	2.237144
H	-1.244725	-0.292441	2.134673
H	1.101965	0.227746	2.029996
H	4.209192	-2.314657	0.481688
N	5.409146	-0.858197	-0.372953
H	5.316815	-0.067055	-0.999427
C	6.389951	-1.783553	-0.918418
H	7.334179	-1.264698	-1.085871
H	6.571326	-2.579777	-0.193216
H	6.078843	-2.257121	-1.862436

cat1_am1_ts_cc'

SCF energy in solution: –989.072236

Enthalpy in solution: –988.510573

Free energy in solution: –988.591051

Cartesian coordinates

Atom	X	Y	Z
C	-1.371698	0.816474	-2.340186
H	-1.443883	0.791696	-3.413288
C	-0.632388	1.582432	-1.502645
C	-3.149455	-1.011126	-1.898626
H	-2.720843	-1.887981	-2.391958
H	-3.841562	-0.534690	-2.596163
C	-2.876049	-1.749475	0.521377
N	-2.077716	-0.551534	0.842887
B	-0.076300	1.744251	0.869264
C	0.539664	2.528035	-1.495696
H	0.351728	3.436887	-2.073855
H	1.403542	2.036577	-1.952167
N	-0.966421	1.225713	-0.203940
C	-1.790278	0.163261	-0.221430
C	3.586913	-1.818247	-0.847967
H	3.931147	-0.946940	-1.433813
C	2.836363	-1.317083	0.381957
H	2.542016	-2.178019	0.988805
H	3.495473	-0.701599	1.002660
C	1.605150	-0.487867	0.007181
H	1.911142	0.324090	-0.654724
H	0.912375	-1.103963	-0.579861
C	0.861389	0.035805	1.222104
C	-0.085646	-0.820578	1.779026
N	-2.103215	-0.073685	-1.536754
C	-0.714006	2.146837	2.282052
H	-1.376844	1.374218	2.671288
H	0.053921	2.358148	3.033811
H	-1.313818	3.054564	2.179560
C	0.804471	2.851779	0.017164
C	-3.871595	-1.402859	-0.608098
H	-4.490686	-0.566863	-0.272526
H	-4.526048	-2.255613	-0.801071
C	-2.004750	-2.934488	0.068120
H	-1.464233	-3.367748	0.910369
H	-2.632593	-3.722749	-0.356276
H	-1.278047	-2.626343	-0.686994
C	-3.650196	-2.136056	1.778082
H	-2.950727	-2.308844	2.598336
H	-4.319865	-1.325792	2.069211

H	-4.233647	-3.046072	1.617921
C	2.297537	2.934199	0.340876
H	2.786164	3.721744	-0.243039
H	2.438077	3.178025	1.398025
H	2.825560	1.999076	0.144435
C	0.191469	4.236086	0.299687
H	0.677337	5.000131	-0.317103
H	-0.878399	4.249576	0.072980
H	0.316115	4.519060	1.346466
H	-0.166015	-1.833390	1.413170
H	-0.477384	-0.644868	2.770290
H	1.431054	0.630643	1.935466
H	2.886510	-2.373483	-1.478624
N	4.681358	-2.716245	-0.498563
H	4.982008	-3.199639	-1.334494
C	5.825346	-2.021328	0.073476
H	6.660459	-2.715769	0.168303
H	6.156413	-1.155090	-0.520964
H	5.583566	-1.664776	1.075373

cat1_am1_cc'

SCF energy in solution: –989.130792

Enthalpy in solution: –988.565267

Free energy in solution: –988.643258

Cartesian coordinates

Atom	X	Y	Z
C	-2.342859	1.943242	-1.359310
H	-2.841543	2.414710	-2.186769
C	-1.305703	2.326384	-0.570412
C	-3.680226	-0.283248	-1.457703
H	-3.311246	-0.697359	-2.399529
H	-4.619151	0.234127	-1.658674
C	-2.585886	-1.981293	0.143854
N	-1.810800	-0.871146	0.717981
B	0.347375	1.332570	1.049477
C	-0.181665	3.311415	-0.453502
H	-0.385354	4.018944	0.355879
H	-0.016517	3.880098	-1.371897
N	-1.074085	1.319583	0.342526
C	-1.882674	0.315749	0.089388
C	2.855409	-0.951852	0.194506
H	3.200826	-1.458138	1.101356
H	3.140171	0.097688	0.299907
C	1.333406	-1.089603	0.122213
H	0.975447	-0.770830	-0.861974
H	1.094608	-2.160364	0.198100
C	0.641559	-0.303280	1.244764
C	-0.675698	-1.007364	1.667294
N	-2.719536	0.657043	-0.914912
C	0.250604	2.029383	2.518120
H	-0.385072	1.464340	3.208770
H	1.243171	2.083572	2.977746
H	-0.146596	3.049714	2.494655
C	1.040777	2.393595	-0.080586
C	-3.894986	-1.380109	-0.414072
H	-4.459100	-0.964845	0.424992
H	-4.487398	-2.183060	-0.855881
C	-1.790667	-2.684086	-0.962176
H	-0.899587	-3.153399	-0.543374
H	-2.396916	-3.458215	-1.439046
H	-1.463100	-1.971823	-1.721832
C	-2.966923	-2.977671	1.239200
H	-2.093353	-3.492346	1.638129
H	-3.476107	-2.466151	2.057410
H	-3.636098	-3.733642	0.823983
C	1.494535	1.767461	-1.407996
H	1.767089	2.554243	-2.122535
H	2.370338	1.131490	-1.283990
H	0.700729	1.172369	-1.869940
C	2.183521	3.250837	0.461745
H	2.526460	3.977451	-0.284645
H	1.883505	3.801193	1.355216
H	3.041282	2.627017	0.728473
H	-0.500353	-2.077651	1.786619
H	-1.006522	-0.615553	2.632253
H	1.272828	-0.409887	2.137465
C	3.550760	-1.535378	-1.030274
H	3.252404	-2.594288	-1.139575
H	3.187186	-1.007788	-1.916904
N	4.999636	-1.374323	-0.977476
H	5.376487	-1.524291	-1.903814
C	5.642704	-2.300382	-0.058043
H	6.725219	-2.227498	-0.167633
H	5.401203	-2.032851	0.971171
H	5.345751	-3.350731	-0.210398

cat1_C_2H_4_ts_CH

SCF energy in solution: –776.434708

Enthalpy in solution: –776.017308

Free energy in solution: –776.081621

Cartesian coordinates

Atom	X	Y	Z

C	0.021796	2.480085	0.211743
H	0.101710	3.492606	0.564520
C	-1.045005	1.712791	-0.119101
C	2.565294	1.946851	0.281466
H	2.712191	1.987707	1.364547
H	2.857576	2.912333	-0.135798
C	2.810717	-0.582791	-0.073719
N	1.452186	-0.648553	-0.628115
B	-1.573222	-0.634373	-0.615741
C	-2.543623	1.635392	-0.106596
H	-2.932583	1.912444	-1.092298
H	-3.003924	2.292787	0.634107
N	-0.565682	0.496827	-0.566385
C	0.765553	0.465744	-0.457746
C	-0.703812	-2.111046	0.238163
C	-0.671944	-2.202619	1.580396
N	1.169422	1.688744	-0.020024
C	-1.836155	-1.266176	-2.066467
H	-0.907322	-1.616557	-2.522844
H	-2.540889	-2.101095	-2.037526
H	-2.262116	-0.504617	-2.728297
C	-2.836783	0.114835	0.174832
C	3.395037	0.821003	-0.346011
H	3.429117	0.964720	-1.429033
H	4.417144	0.876889	0.034940
C	2.782101	-0.872557	1.433276
H	2.401094	-1.880619	1.605736
H	3.783367	-0.800224	1.866254
H	2.125074	-0.173240	1.956093
C	3.661938	-1.629550	-0.785136
H	3.219891	-2.617222	-0.643582
H	3.693539	-1.421458	-1.855391
H	4.680596	-1.641092	-0.390543
C	-2.839978	-0.052162	1.697593
H	-3.659105	0.525144	2.141033
H	-2.972158	-1.097232	1.983598
H	-1.906619	0.308475	2.138907
C	-4.213980	-0.273656	-0.361902
H	-5.005853	0.316796	0.112054
H	-4.283392	-0.126166	-1.441508
H	-4.420192	-1.327661	-0.157635
H	-0.961872	-3.096404	2.127250
H	-1.001963	-3.014373	-0.289840
H	-0.334587	-1.368539	2.188874
H	0.378976	-1.507526	-0.217994

cat1_C_2H_4_CH

SCF energy in solution: –776.50874
Enthalpy in solution: –776.085098
Free energy in solution: –776.150622

Cartesian coordinates

Atom	X	Y	Z
C	-0.046475	2.397227	-0.188190
H	-0.131283	3.445409	-0.411351
C	1.023478	1.581664	-0.008877
C	-2.579820	1.956879	-0.173748
H	-2.802494	2.077674	-1.236757
H	-2.755176	2.912721	0.320802
C	-2.986484	-0.548069	0.051085
N	-1.610428	-0.690917	0.546314
B	1.750122	-0.750579	0.528944
C	2.520332	1.618561	0.033233
H	2.839691	1.942076	1.029644
H	2.942379	2.317621	-0.694399
N	0.557365	0.306276	0.257370
C	-0.761771	0.340080	0.262852
C	1.401240	-2.168892	-0.154380
C	0.560588	-2.412708	-1.168070
N	-1.180689	1.594914	-0.009582
C	1.924871	-0.893557	2.138841
H	1.019574	-1.291684	2.609786
H	2.740840	-1.580841	2.383394
H	2.148761	0.061187	2.627023
C	2.950633	0.144837	-0.214356
C	-3.445968	0.863233	0.450582
H	-3.395486	0.937635	1.539274
H	-4.483419	1.009194	0.145128
C	-3.050850	-0.751367	-1.467544
H	-2.768649	-1.775904	-1.716956
H	-4.062360	-0.571406	-1.838997
H	-2.362578	-0.081733	-1.987249
C	-3.845349	-1.588345	0.761493
H	-3.481696	-2.594018	0.539279
H	-3.807983	-1.437695	1.840758
H	-4.880791	-1.519235	0.423825
C	2.973934	-0.087922	-1.728647
H	3.697668	0.575506	-2.217622
H	3.242729	-1.119675	-1.960357
H	1.992220	0.096045	-2.175762
C	4.345395	-0.108161	0.352348
H	5.099219	0.520961	-0.135943
H	4.382500	0.090592	1.425852
H	4.637192	-1.150588	0.196767

H	0.395739	-3.406725	-1.573576
H	1.906307	-3.044209	0.259934
H	0.034761	-1.601865	-1.669615
H	-1.164527	-1.590837	0.393948

cat2_am1_a

SCF energy in solution: –1028.464253

Enthalpy in solution: –1027.868571

Free energy in solution: –1027.95128

Cartesian coordinates

Atom	X	Y	Z
C	3.414355	0.889666	-0.640704
H	4.353738	1.195138	-1.067321
C	2.924338	-0.339621	-0.368401
C	2.481525	3.260502	-0.328482
H	2.366092	3.590371	-1.365630
H	3.452269	3.611225	0.028537
C	0.029458	3.058566	0.297481
N	0.179982	1.628467	0.553917
B	0.652494	-1.331207	0.568446
C	2.347358	-2.681281	-0.952154
H	2.775619	-3.672427	-1.146456
H	1.860492	-2.361938	-1.879505
N	1.661115	-0.195971	0.205225
C	1.349432	1.138152	0.224969
N	2.440842	1.815342	-0.252201
C	1.315869	-2.785532	0.189178
C	1.354958	3.805544	0.547038
H	1.623184	3.673024	1.598526
H	1.232457	4.874525	0.359203
C	-1.030599	3.594612	1.257121
H	-1.960967	3.040718	1.116250
H	-0.704728	3.452523	2.288592
H	-1.223740	4.656317	1.083951
C	-0.442110	3.269880	-1.150041
H	-1.409279	2.780535	-1.286858
H	-0.552817	4.332090	-1.386939
H	0.259671	2.823841	-1.858560
C	0.263230	-3.829674	-0.204241
H	-0.219786	-3.596974	-1.156929
H	0.725650	-4.817471	-0.312160
H	-0.515490	-3.915246	0.558646
C	2.041136	-3.341531	1.430752
H	2.717335	-2.613807	1.883689
H	1.323981	-3.633035	2.199680
H	2.626041	-4.230238	1.164806
C	3.481849	-1.700883	-0.629339
H	4.191367	-1.640708	-1.456688
H	4.038540	-2.063018	0.238911
N	-0.663148	-0.855091	-0.370592
C	-0.432977	-0.753011	-1.824779
H	-1.229714	-0.177581	-2.298002
H	0.517676	-0.252820	-1.998168
H	-0.400791	-1.748730	-2.263223
C	-1.987011	-1.452391	-0.069280
H	-2.165697	-2.272747	-0.767448
H	-1.948351	-1.871948	0.933893
C	-3.108235	-0.419759	-0.144903
H	-3.155486	0.032956	-1.139111
H	-2.890298	0.385721	0.564233
C	-4.468962	-1.045819	0.181891
H	-4.696302	-1.838363	-0.536790
H	-4.412643	-1.512975	1.171410
C	-5.568982	-0.024555	0.168928
H	-5.470899	0.791100	0.881457
C	-6.611745	-0.050465	-0.654022
H	-6.736768	-0.849182	-1.377078
H	-7.372988	0.718850	-0.629886
C	0.142295	-1.198431	2.102669
H	-0.430644	-2.064194	2.450081
H	1.010907	-1.119462	2.760438
H	-0.455990	-0.298908	2.266299
H	-0.686728	0.135839	-0.020610

cat2_am1_bts

SCF energy in solution: –1028.454709

Enthalpy in solution: –1027.865891

Free energy in solution: –1027.948123

Cartesian coordinates

Atom	X	Y	Z
C	3.247331	1.543316	-0.389425
H	4.124747	2.067365	-0.724159
C	3.011398	0.220526	-0.201284
C	1.739295	3.627018	-0.148575
H	1.672561	3.923063	-1.199092
H	2.533523	4.212281	0.318187
C	-0.657496	2.811488	0.181326
N	-0.159473	1.474241	0.511848
B	0.870556	-1.253352	0.518574
C	2.877412	-2.121540	-0.987692
H	3.483198	-2.997282	-1.252214
H	2.382271	-1.789512	-1.906620

N	1.715106	0.073521	0.271530
C	1.144047	1.289376	0.298056
N	2.066300	2.216268	-0.051992
C	1.827184	-2.524621	0.069496
C	0.410474	3.851066	0.575040
H	0.573516	3.774671	1.653236
H	0.047581	4.857535	0.356950
C	-1.923884	3.063301	0.995273
H	-2.680706	2.317823	0.743994
H	-1.704434	2.984244	2.060810
H	-2.331904	4.054425	0.783932
C	-0.979262	2.908458	-1.317057
H	-1.785066	2.214028	-1.563847
H	-1.301078	3.918054	-1.586483
H	-0.112229	2.642501	-1.925589
C	0.997859	-3.690054	-0.484318
H	0.514934	-3.446057	-1.432865
H	1.631220	-4.568473	-0.657182
H	0.217024	-3.983887	0.222943
C	2.586303	-3.074111	1.292302
H	3.108103	-2.295678	1.852729
H	1.899171	-3.559134	1.987524
H	3.326298	-3.821442	0.979765
C	3.815076	-1.001423	-0.505860
H	4.555707	-0.758715	-1.270096
H	4.365443	-1.335697	0.376714
N	-0.445076	-0.916542	-0.360003
C	-0.255915	-0.720655	-1.800160
H	-1.135190	-0.243492	-2.242311
H	0.603732	-0.072513	-1.975939
H	-0.085771	-1.666005	-2.321860
C	-1.659770	-1.703113	-0.098300
H	-1.781456	-2.471060	-0.872368
H	-1.547775	-2.222999	0.852214
C	-2.911035	-0.827424	-0.033079
H	-2.999847	-0.215225	-0.936440
H	-2.806221	-0.138672	0.811451
C	-4.188325	-1.657206	0.134016
H	-4.319420	-2.316617	-0.728805
H	-4.077307	-2.298831	1.015857
C	-5.401787	-0.788715	0.294986
H	-5.398438	-0.121938	1.154615
C	-6.437146	-0.770729	-0.537689
H	-6.471157	-1.420811	-1.405268
H	-7.281918	-0.112420	-0.379228
C	0.402650	-1.300241	2.077702
H	-0.014927	-2.267813	2.373365
H	1.259070	-1.122528	2.732397
H	-0.341138	-0.532954	2.310834
H	-0.579357	0.339796	0.111760

cat2_am1_c

SCF energy in solution: –1028.463273

Enthalpy in solution: –1027.869792

Free energy in solution: –1027.952211

Cartesian coordinates

Atom	X	Y	Z
C	3.299562	1.326980	-0.496221
H	4.203157	1.775624	-0.868581
C	2.952004	0.026909	-0.307231
C	2.021169	3.534929	-0.207311
H	1.961132	3.816841	-1.261261
H	2.888161	4.031731	0.229725
C	-0.423138	2.975390	0.217360
N	-0.015869	1.635185	0.658357
B	0.720672	-1.315304	0.504210
C	2.673325	-2.347317	-0.984861
H	3.234579	-3.261445	-1.217461
H	2.141149	-2.061666	-1.897459
N	1.662850	-0.009247	0.207664
C	1.233094	1.246543	0.283914
N	2.203234	2.094909	-0.106416
C	1.672238	-2.628046	0.151792
C	0.744633	3.919958	0.539485
H	0.925143	3.877582	1.616161
H	0.471914	4.944077	0.279139
C	-1.651438	3.376636	1.027519
H	-2.462784	2.666505	0.852969
H	-1.417467	3.378866	2.092571
H	-1.995910	4.369174	0.731155
C	-0.754560	2.979531	-1.280806
H	-1.619965	2.340104	-1.466643
H	-0.991588	3.989552	-1.623685
H	0.076133	2.592331	-1.874348
C	0.785421	-3.804465	-0.272263
H	0.256308	-3.598473	-1.205142
H	1.382416	-4.713124	-0.419620
H	0.035804	-4.023576	0.493478
C	2.475071	-3.087996	1.382009
H	3.022432	-2.270893	1.858519
H	1.813443	-3.509418	2.140562
H	3.199194	-3.865219	1.105063
C	3.675610	-1.241231	-0.627800

H	4.363102	-1.052311	-1.454775
H	4.282811	-1.557312	0.223819
N	-0.527605	-1.027722	-0.387444
C	-0.351101	-0.864610	-1.818572
H	-1.206726	-0.345075	-2.266443
H	0.537488	-0.263389	-2.026828
H	-0.241396	-1.817878	-2.359791
C	-1.776369	-1.714818	-0.093240
H	-1.981507	-2.501823	-0.837568
H	-1.700311	-2.217439	0.872096
C	-2.974504	-0.760426	-0.040697
H	-3.008940	-0.145404	-0.945708
H	-2.835424	-0.078140	0.806706
C	-4.310147	-1.497157	0.111235
H	-4.477051	-2.141068	-0.756994
H	-4.252087	-2.150487	0.989506
C	-5.462411	-0.548295	0.264881
H	-5.435387	0.095621	1.141615
C	-6.469361	-0.430911	-0.594591
H	-6.526125	-1.055171	-1.479798
H	-7.267294	0.284915	-0.441874
C	0.285372	-1.272413	2.076088
H	-0.130501	-2.227610	2.411607
H	1.146326	-1.070495	2.718525
H	-0.463609	-0.504473	2.292395
H	-0.655069	0.858473	0.438062

cat2_am1_d$_S$

SCF energy in solution: –1028.466905

Enthalpy in solution: –1027.872863

Free energy in solution: –1027.952633

Cartesian coordinates

Atom	X	Y	Z
C	1.450506	3.039263	-0.257582
H	1.832682	4.013232	-0.505852
C	2.069104	1.838053	-0.124896
C	-0.999963	3.773367	-0.084533
H	-1.179330	4.044753	-1.127555
H	-0.716107	4.675434	0.458820
C	-2.451751	1.692827	0.045430
N	-1.271146	0.922328	0.461641
B	1.318998	-0.721307	0.464452
C	3.590969	-0.022192	-0.758039
H	4.651058	-0.276287	-0.887186
H	3.113648	-0.153973	-1.733813
N	1.112589	0.887284	0.212725
C	-0.064335	1.507411	0.238966
N	0.096697	2.820907	-0.014357
C	2.957413	-0.968007	0.280517
C	-2.235214	3.131192	0.540709
H	-2.120962	3.102049	1.626858
H	-3.114287	3.733311	0.305440
C	-3.674771	1.098847	0.735559
H	-3.806913	0.051850	0.457570
H	-3.556252	1.149654	1.818756
H	-4.572692	1.649155	0.447133
C	-2.627701	1.657898	-1.479124
H	-2.883408	0.648331	-1.804256
H	-3.432678	2.328805	-1.789157
H	-1.709694	1.950400	-1.992812
C	3.256748	-2.404340	-0.164688
H	2.887619	-2.603280	-1.173086
H	4.338425	-2.588956	-0.166184
H	2.799841	-3.131504	0.511748
C	3.701312	-0.759432	1.612876
H	3.453872	0.190351	2.092987
H	3.450251	-1.548832	2.323213
H	4.787644	-0.787264	1.456427
C	3.495559	1.450173	-0.346141
H	3.919767	2.101253	-1.113334
H	4.076431	1.614083	0.564488
C	0.824719	-1.044774	1.985557
H	1.124089	-2.046172	2.310252
H	1.262260	-0.344987	2.701654
H	-0.260527	-0.978806	2.106035
N	0.315227	-1.360579	-0.557898
C	0.506619	-1.044945	-1.963872
H	0.817017	-0.004359	-2.075173
H	1.266239	-1.675603	-2.454033
H	-0.422802	-1.166554	-2.533230
C	0.027384	-2.780833	-0.384842
H	0.855668	-3.411075	-0.741489
H	-0.077784	-2.979738	0.682476
C	-1.233850	-3.274969	-1.109053
H	-1.070492	-3.273441	-2.190138
H	-1.396024	-4.317614	-0.820978
C	-2.499195	-2.467677	-0.799614
H	-2.323335	-1.433423	-1.114405
H	-3.337108	-2.847390	-1.390492
C	-2.867806	-2.496895	0.655566
H	-2.136006	-2.092612	1.350383
C	-4.008176	-2.991407	1.129810
H	-4.758677	-3.407099	0.465656

H	-4.225244	-3.002614	2.190626
H	-1.210170	-0.065493	0.189986

cat2_am1_ets$_S$

SCF energy in solution: –1028.411486

Enthalpy in solution: –1027.819995

Free energy in solution: –1027.893638

Cartesian coordinates

Atom	X	Y	Z
C	1.236211	-2.605275	-1.094849
H	1.598690	-3.461301	-1.636349
C	-0.020247	-2.228673	-0.767784
C	3.549587	-1.656650	-0.608263
H	3.893257	-1.397308	-1.612428
H	3.897324	-2.665503	-0.380033
C	3.287731	0.666164	0.337510
N	1.871160	0.395480	0.617113
B	-1.213628	-0.270609	0.620379
C	-2.539939	-2.111183	-0.737527
H	-3.411608	-2.777471	-0.751568
H	-2.710966	-1.358705	-1.513552
N	0.049075	-1.046494	-0.020790
C	1.352027	-0.703798	0.054800
N	2.096599	-1.649666	-0.570409
C	-2.413642	-1.433967	0.637380
C	4.058106	-0.657334	0.423685
H	3.924833	-1.067353	1.427745
H	5.123204	-0.478503	0.264665
C	3.795589	1.624008	1.412101
H	3.221194	2.550321	1.385639
H	3.681913	1.174250	2.399386
H	4.848574	1.860038	1.243259
C	3.446080	1.307147	-1.049529
H	2.932338	2.268328	-1.060724
H	4.501617	1.463818	-1.287462
H	3.000011	0.683764	-1.827561
C	-3.826497	-0.998618	1.073921
H	-4.392250	-0.509175	0.282323
H	-4.399971	-1.886697	1.362599
H	-3.800801	-0.335401	1.942391
C	-2.017824	-2.511135	1.675269
H	-0.969512	-2.810810	1.616871
H	-2.194679	-2.141824	2.686517
H	-2.637253	-3.406776	1.541740
C	-1.303050	-2.940325	-1.079040
H	-1.304727	-3.225690	-2.133561
H	-1.331717	-3.869139	-0.504044
C	-0.871212	0.209061	2.130789
H	-1.770106	0.586825	2.631380
H	-0.519938	-0.639833	2.721034
H	-0.108940	0.980361	2.208102
N	-1.469470	1.034451	-0.368395
C	-0.799420	0.947738	-1.672738
H	0.261884	1.167398	-1.530228
H	-0.907836	-0.038502	-2.125299
H	-1.206545	1.686468	-2.362447
C	-2.881321	1.406534	-0.536556
H	-3.410308	0.704445	-1.183293
H	-3.338207	1.366316	0.450576
C	-2.958883	2.847493	-1.073229
H	-3.063491	2.863957	-2.159270
H	-3.844715	3.336513	-0.666468
C	-1.661990	3.536070	-0.625139
H	-1.006884	3.753192	-1.471705
H	-1.856596	4.487866	-0.128034
C	-0.915607	2.648025	0.357556
H	-1.476599	2.507154	1.278827
C	0.483612	2.829465	0.520218
H	0.959385	3.502886	-0.188975
H	0.814931	2.970841	1.545474
H	1.245217	1.323428	0.558502

cat2_am1_f$_S$

SCF energy in solution: –1028.468947

Enthalpy in solution: –1027.871079

Free energy in solution: –1027.947786

Cartesian coordinates

Atom	X	Y	Z
C	1.313240	-2.349123	-1.280370
H	1.690246	-3.173706	-1.861025
C	0.047979	-1.981076	-1.001996
C	3.601588	-1.468114	-0.582600
H	4.083796	-1.112827	-1.498639
H	3.894687	-2.510018	-0.433768
C	3.288046	0.746365	0.593916
N	1.838372	0.579994	0.601407
B	-1.129846	-0.329466	0.623534
C	-2.453189	-2.375542	-0.579405
H	-2.891703	-3.344746	-0.317601
H	-3.222381	-1.865808	-1.160911
N	0.073114	-0.812696	-0.227181
C	1.403169	-0.455082	-0.044273

N	2.160411	-1.399143	-0.709369
C	-2.185339	-1.606850	0.732941
C	4.011330	-0.613961	0.612597
H	3.733495	-1.130589	1.535410
H	5.094833	-0.475049	0.611784
C	3.665773	1.526010	1.852249
H	3.117641	2.469566	1.869290
H	3.384830	0.956670	2.739971
H	4.738077	1.736391	1.885231
C	3.701680	1.555048	-0.645737
H	3.233340	2.540306	-0.602437
H	4.786894	1.685897	-0.695078
H	3.363683	1.066201	-1.562048
C	-3.556962	-1.279395	1.342579
H	-4.199245	-0.715461	0.660026
H	-4.093376	-2.205757	1.577448
H	-3.464944	-0.711086	2.270719
C	-1.515101	-2.611080	1.700134
H	-0.511603	-2.889177	1.370060
H	-1.435613	-2.201833	2.707557
H	-2.116634	-3.525067	1.759435
C	-1.221644	-2.608693	-1.485837
H	-1.441650	-2.226378	-2.488435
H	-1.031865	-3.675631	-1.613471
C	-0.679279	0.195582	2.092932
H	-1.508783	0.182530	2.807483
H	0.088736	-0.476101	2.479962
H	-0.220040	1.183721	2.118031
N	-1.780048	1.050636	-0.221304
C	-2.518558	0.674551	-1.445343
H	-1.902628	0.003566	-2.038833
H	-3.438133	0.171737	-1.162563
H	-2.761912	1.555520	-2.040536
C	-2.686531	1.849407	0.661273
H	-3.640465	1.340107	0.768178
H	-2.212338	1.912759	1.636340
C	-2.770333	3.234239	0.031159
H	-3.506732	3.259840	-0.773140
H	-3.065825	3.981768	0.766446
C	-1.345751	3.453106	-0.504873
H	-1.355580	3.931914	-1.485304
H	-0.770532	4.093597	0.163922
C	-0.682610	2.053287	-0.576328
H	0.072810	1.934201	0.197718
C	0.003793	1.823808	-1.917892
H	-0.654070	2.045027	-2.760646
H	0.846877	2.514733	-1.967403
H	0.394583	0.814074	-2.016480

cat2_am1_d$_R$

SCF energy in solution: –1028.45805

Enthalpy in solution: –1027.864212

Free energy in solution: –1027.9454

Cartesian coordinates

Atom	X	Y	Z
C	1.415215	3.034370	-0.452319
H	1.756186	3.996941	-0.789378
C	2.061439	1.847669	-0.318118
C	-1.023290	3.745813	-0.092439
H	-1.299851	3.946592	-1.130196
H	-0.711962	4.685655	0.365177
C	-2.417724	1.656173	0.302270
N	-1.188401	0.927778	0.641894
C	3.505776	-0.034416	-1.049608
H	4.543150	-0.293348	-1.297542
H	2.916378	-0.185735	-1.958789
N	1.158523	0.909585	0.165476
C	-0.020339	1.517733	0.275491
N	0.095395	2.816960	-0.061954
C	3.003227	-0.957596	0.079582
C	-2.185470	3.126657	0.680533
H	-1.974362	3.171530	1.751670
H	-3.093894	3.699864	0.487739
C	-3.547573	1.081427	1.150347
H	-3.675353	0.019858	0.930975
H	-3.317353	1.196742	2.210255
H	-4.486166	1.593675	0.928718
C	-2.741715	1.504193	-1.189303
H	-2.953068	0.456306	-1.407060
H	-3.618341	2.098468	-1.458751
H	-1.900781	1.815158	-1.812827
C	3.243636	-2.405182	-0.370653
H	2.651789	-2.675368	-1.247297
H	4.300780	-2.555690	-0.623548
H	3.001532	-3.111002	0.427826
C	3.917357	-0.732059	1.298206
H	3.757537	0.237228	1.776272
H	3.739569	-1.493449	2.059433
H	4.973628	-0.793595	1.004976
C	3.458409	1.449519	-0.668139
H	3.804568	2.076971	-1.492092
H	4.129160	1.634146	0.174085
B	1.400048	-0.681580	0.465275

N	0.284610	-1.366227	-0.398010
C	0.348510	-1.147681	-1.834300
H	0.521480	-0.088546	-2.041247
H	1.141976	-1.712641	-2.344714
H	-0.595053	-1.420074	-2.320854
C	-0.004966	-2.764659	-0.057133
H	-0.186072	-3.326014	-0.982533
H	0.865191	-3.238176	0.402313
C	-1.214928	-2.971745	0.883859
H	-0.949002	-3.693549	1.661239
H	-1.436289	-2.034116	1.396015
C	-2.480520	-3.485202	0.180467
H	-2.229939	-4.419220	-0.336867
H	-3.247937	-3.727843	0.920720
C	-3.053483	-2.520956	-0.815504
C	-4.312514	-2.087941	-0.807213
H	-4.685392	-1.403553	-1.559937
H	-5.013882	-2.416321	-0.047307
H	-1.136587	-0.068144	0.386165
C	1.093380	-0.928321	2.047648
H	1.274315	-1.968474	2.341083
H	1.735213	-0.310324	2.678958
H	0.063173	-0.692946	2.324243
H	-2.382036	-2.176552	-1.597196

cat2_am1_ets$_R$

SCF energy in solution: –1028.407283

Enthalpy in solution: –1027.816082

Free energy in solution: –1027.889862

Cartesian coordinates

Atom	X	Y	Z
C	1.236211	-2.605275	-1.094849
H	1.598690	-3.461301	-1.636349
C	-0.020247	-2.228673	-0.767784
C	3.549587	-1.656650	-0.608263
H	3.893257	-1.397308	-1.612428
H	3.897324	-2.665503	-0.380033
C	3.287731	0.666164	0.337510
N	1.871160	0.395480	0.617113
B	-1.213628	-0.270609	0.620379
C	-2.539939	-2.111183	-0.737527
H	-3.411608	-2.777471	-0.751568
H	-2.710966	-1.358705	-1.513552
N	0.049075	-1.046494	-0.020790
C	1.352027	-0.703798	0.054800
N	2.096599	-1.649666	-0.570409
C	-2.413642	-1.433967	0.637380
C	4.058106	-0.657334	0.423685
H	3.924833	-1.067353	1.427745
H	5.123204	-0.478503	0.264665
C	3.795589	1.624008	1.412101
H	3.221194	2.550321	1.385639
H	3.681913	1.174250	2.399386
H	4.848574	1.860038	1.243259
C	3.446080	1.307147	-1.049529
H	2.932338	2.268328	-1.060724
H	4.501617	1.463818	-1.287462
H	3.000011	0.683764	-1.827561
C	-3.826497	-0.998618	1.073921
H	-4.392250	-0.509175	0.282323
H	-4.399971	-1.886697	1.362599
H	-3.800801	-0.335401	1.942391
C	-2.017824	-2.511135	1.675269
H	-0.969512	-2.810810	1.616871
H	-2.194679	-2.141824	2.686517
H	-2.637253	-3.406776	1.541740
C	-1.303050	-2.940325	-1.079040
H	-1.304727	-3.225690	-2.133561
H	-1.331717	-3.869139	-0.504044
C	-0.871212	0.209061	2.130789
H	-1.770106	0.586825	2.631380
H	-0.519938	-0.639833	2.721034
H	-0.108940	0.980361	2.208102
N	-1.469470	1.034451	-0.368395
C	-0.799420	0.947738	-1.672738
H	0.261884	1.167398	-1.530228
H	-0.907836	-0.038502	-2.125299
H	-1.206545	1.686468	-2.362447
C	-2.881321	1.406534	-0.536556
H	-3.410308	0.704445	-1.183293
H	-3.338207	1.366316	0.450576
C	-2.958883	2.847493	-1.073229
H	-3.063491	2.863957	-2.159270
H	-3.844715	3.336513	-0.666468
C	-1.661990	3.536070	-0.625139
H	-1.006884	3.753192	-1.471705
H	-1.856596	4.487866	-0.128034
C	-0.915607	2.648025	0.357556
H	-1.476599	2.507154	1.278827
C	0.483612	2.829465	0.520218
H	0.959385	3.502886	-0.188975
H	0.814931	2.970841	1.545474
H	1.245217	1.323428	0.558502

cat2_am1_f_R

SCF energy in solution: –1028.458745

Enthalpy in solution: –1027.861926

Free energy in solution: –1027.93813

Cartesian coordinates

Atom	X	Y	Z
C	1.096690	-2.545716	-1.030435
H	1.409488	-3.476697	-1.471523
C	-0.133126	-2.021595	-0.874480
C	3.435023	-1.794842	-0.339733
H	3.979258	-1.620153	-1.273087
H	3.622621	-2.826611	-0.032754
C	3.302054	0.587436	0.499825
N	1.843141	0.562199	0.443995
C	-2.614004	-2.289705	-0.340434
H	-2.953535	-3.234789	0.095230
H	-3.465709	-1.922070	-0.915011
N	-0.021066	-0.763385	-0.262749
C	1.330184	-0.515029	-0.059673
N	2.012147	-1.615524	-0.539778
C	-2.285687	-1.328279	0.831041
C	3.883078	-0.818462	0.742918
H	3.521836	-1.170092	1.713379
H	4.974409	-0.783050	0.778067
C	3.697628	1.494724	1.663876
H	3.253612	2.481186	1.518746
H	3.313317	1.085672	2.599940
H	4.783319	1.600564	1.737297
C	3.851560	1.176073	-0.808544
H	3.465609	2.189474	-0.934795
H	4.945050	1.214839	-0.801095
H	3.526561	0.588062	-1.669729
C	-3.625448	-0.902710	1.456470
H	-4.261835	-0.316620	0.788365
H	-4.200406	-1.792983	1.735583
H	-3.473022	-0.321815	2.369108
C	-1.602895	-2.206765	1.911767
H	-0.621876	-2.564359	1.591605
H	-1.477597	-1.665358	2.848749
H	-2.227995	-3.081910	2.119616
C	-1.446982	-2.575518	-1.315119
H	-1.687229	-2.165216	-2.301827
H	-1.323217	-3.648860	-1.468059
B	-1.181474	-0.111118	0.516833
N	-1.878871	1.179892	-0.541226
C	-2.780074	0.566611	-1.535526
H	-2.231681	-0.177299	-2.105607
H	-3.614271	0.093520	-1.033357
H	-3.162166	1.333672	-2.214758
C	-2.653319	2.143548	0.309258
H	-3.474570	2.532015	-0.300567
H	-3.071836	1.620652	1.162419
C	-1.684972	3.282218	0.691712
H	-2.169227	4.243725	0.519504
H	-1.409260	3.231133	1.742012
C	-0.463803	3.096647	-0.231310
H	-0.142439	4.032893	-0.689457
H	0.390827	2.646333	0.273618
C	-0.973018	2.139177	-1.296820
C	0.089729	1.544982	-2.204206
H	-0.285706	0.716228	-2.805806
H	0.412407	2.333337	-2.888220
C	-0.705129	0.590687	1.896466
H	-1.541854	0.799381	2.571468
H	-0.048302	-0.110304	2.414492
H	-0.109212	1.488373	1.788681
H	-1.679147	2.700425	-1.924805
H	0.948744	1.219135	-1.625601

cat3_am1_a

SCF energy in solution: –1183.312639

Enthalpy in solution: –1182.639742

Free energy in solution: –1182.725702

Cartesian coordinates

Atom	X	Y	Z
C	2.833584	1.505621	-1.590358
H	3.540132	1.922086	-2.287534
C	2.448344	0.226515	-1.384696
C	2.170523	3.742595	-0.521948
H	1.696056	4.244191	-1.371454
H	3.213004	4.066560	-0.481543
C	0.103048	3.332276	0.890810
N	0.286813	1.883662	0.807402
N	1.521135	0.212884	-0.332250
C	1.262571	1.512808	0.022399
N	2.123554	2.306125	-0.692549
C	1.450486	4.074291	0.783057
H	2.075360	3.763012	1.624535
H	1.299517	5.153804	0.853114
C	-0.528978	3.642320	2.245680
H	-1.456878	3.076968	2.348451

H	0.143127	3.335213	3.048320
H	-0.748716	4.708065	2.349088
C	-0.845851	3.788559	-0.228968
H	-1.818883	3.311156	-0.092860
H	-0.988881	4.873132	-0.218581
H	-0.463432	3.495057	-1.209514
B	0.633334	-0.992567	0.070154
C	1.327586	-2.326400	-0.531663
C	0.369688	-1.264511	1.648694
H	-0.193313	-0.446687	2.109819
C	0.310770	-3.468978	-0.460103
H	-0.559920	-3.199171	-1.071711
H	0.725973	-4.376911	-0.918689
C	-0.397335	-2.596024	1.912449
H	-1.470857	-2.408962	1.901172
H	-0.185663	-2.917139	2.939617
C	-0.122108	-3.803540	0.975197
H	-1.018591	-4.430349	0.941203
H	0.652679	-4.435227	1.409543
C	1.743773	-1.320812	2.333614
H	2.302620	-0.407736	2.107164
H	1.627430	-1.365594	3.422492
C	2.595990	-2.635530	0.325985
H	3.368189	-1.921321	0.036034
H	2.971985	-3.625447	0.030715
C	2.525446	-2.545550	1.859417
H	3.549641	-2.507409	2.242871
H	2.081978	-3.441543	2.293218
C	1.827701	-2.165206	-1.976777
H	0.980972	-2.009362	-2.649839
H	2.310266	-3.093678	-2.308113
C	2.840808	-1.015544	-2.137063
H	2.950228	-0.757491	-3.192910
H	3.825706	-1.353104	-1.807836
N	-0.853542	-0.401564	-0.596254
C	-0.859395	-0.201496	-2.059294
H	-1.578948	0.566673	-2.342469
H	0.130429	0.110523	-2.382163
H	-1.126047	-1.139111	-2.547744
C	-2.155522	-0.918740	-0.111925
H	-2.254518	-1.966055	-0.404449
H	-2.114755	-0.870063	0.972556
C	-3.362142	-0.110763	-0.585020
H	-3.542816	-0.246771	-1.653123
H	-3.172799	0.956161	-0.417794
C	-4.623402	-0.531114	0.181253
H	-4.809176	-1.598520	0.030927
H	-4.452152	-0.380504	1.252702
C	-5.826381	0.254576	-0.253872
H	-5.774260	1.330440	-0.103029
C	-6.909261	-0.273806	-0.813356
H	-6.991482	-1.342618	-0.978318
H	-7.746954	0.339928	-1.119145
H	-0.768287	0.533620	-0.150993

cat3_am1_bts

SCF energy in solution: –1183.300427

Enthalpy in solution: –1182.633202

Free energy in solution: –1182.716677

Cartesian coordinates

Atom	X	Y	Z
C	2.385928	2.477437	-1.174671
H	2.973748	3.177075	-1.742330
C	2.426785	1.121386	-1.112811
C	0.816827	4.226536	-0.104007
H	0.384200	4.611384	-1.031197
H	1.623215	4.897016	0.198537
C	-1.199954	2.938617	0.765678
N	-0.426524	1.691574	0.770522
N	1.471598	0.706318	-0.184297
C	0.769901	1.789628	0.183776
N	1.355195	2.896864	-0.327599
C	-0.239247	4.120674	0.997492
H	0.256726	3.969968	1.959782
H	-0.801691	5.055135	1.047659
C	-2.209234	2.872158	1.907832
H	-2.848120	1.995028	1.784161
H	-1.689242	2.779782	2.862031
H	-2.840176	3.763815	1.925203
C	-1.936582	3.110254	-0.571952
H	-2.687056	2.326451	-0.688329
H	-2.444546	4.077385	-0.618173
H	-1.246006	3.036404	-1.414780
B	0.915179	-0.763803	0.057091
C	2.025598	-1.739579	-0.635857
C	0.795573	-1.261981	1.605406
H	0.012675	-0.715768	2.144797
C	1.376334	-3.121148	-0.756100
H	0.463985	-3.029161	-1.358000
H	2.033953	-3.813007	-1.301307
C	0.448171	-2.781414	1.681817
H	-0.632717	-2.907078	1.651923
H	0.744380	-3.154589	2.670244

C	1.057213	-3.736180	0.616828
H	0.376244	-4.581935	0.480493
H	1.981879	-4.168845	1.000045
C	2.121042	-1.004693	2.333402
H	2.413584	0.044142	2.214463
H	2.012127	-1.188061	3.408710
C	3.315730	-1.800244	0.245401
H	3.873568	-0.877786	0.078413
H	3.952493	-2.608533	-0.142778
C	3.212607	-1.912944	1.774092
H	4.184059	-1.643734	2.200566
H	3.022790	-2.937515	2.093491
C	2.506252	-1.246983	-2.013326
H	1.669026	-1.214463	-2.714300
H	3.229491	-1.958494	-2.432543
C	3.188964	0.138650	-1.959051
H	3.266903	0.553473	-2.966418
H	4.213010	0.034436	-1.597149
N	-0.594733	-0.530740	-0.534141
C	-0.678428	-0.212002	-1.962023
H	-1.578386	0.365365	-2.186961
H	0.180943	0.389543	-2.254935
H	-0.694186	-1.120176	-2.575829
C	-1.694920	-1.411847	-0.123286
H	-1.546430	-2.432185	-0.500795
H	-1.680801	-1.456338	0.963850
C	-3.085520	-0.927590	-0.537632
H	-3.230286	-0.993766	-1.617991
H	-3.203001	0.125552	-0.257657
C	-4.174604	-1.759990	0.151369
H	-4.048520	-2.816170	-0.104015
H	-4.050345	-1.674300	1.236791
C	-5.553584	-1.310357	-0.235289
H	-5.807234	-0.281795	0.012448
C	-6.447259	-2.066878	-0.863206
H	-6.224795	-3.095314	-1.126277
H	-7.425542	-1.688115	-1.130610
H	-0.770095	0.617019	0.188625

cat3_am1_c

SCF energy in solution: –1183.311924

Enthalpy in solution: –1182.639265

Free energy in solution: –1182.724977

Cartesian coordinates

Atom	X	Y	Z
C	2.499073	2.132300	-1.436208
H	3.132919	2.728376	-2.068664
C	2.368533	0.784609	-1.307242
C	1.273390	4.120906	-0.373669
H	0.793579	4.501388	-1.278234
H	2.200412	4.674180	-0.219704
C	-0.770119	3.210571	0.827784
N	-0.118425	1.893641	0.911012
N	1.410095	0.537572	-0.328899
C	0.930151	1.711323	0.056248
N	1.588874	2.712491	-0.555777
C	0.353343	4.257525	0.838153
H	0.932451	4.124387	1.754868
H	-0.079885	5.258887	0.850065
C	-1.641802	3.374416	2.067823
H	-2.393735	2.583110	2.105290
H	-1.032449	3.312313	2.969782
H	-2.158334	4.335738	2.045947
C	-1.624154	3.321986	-0.442421
H	-2.464809	2.628392	-0.387734
H	-2.021371	4.333866	-0.552976
H	-1.047822	3.070017	-1.334692
B	0.716877	-0.912323	0.010928
C	1.853440	-1.973663	-0.522318
C	0.570574	-1.239007	1.609970
H	-0.220315	-0.642997	2.086479
C	1.180388	-3.349438	-0.490643
H	0.269181	-3.298903	-1.098712
H	1.825316	-4.108149	-0.956852
C	0.193056	-2.733683	1.845315
H	-0.886600	-2.847186	1.756067
H	0.422114	-2.991594	2.887487
C	0.841612	-3.806983	0.933822
H	0.169541	-4.669111	0.884633
H	1.758660	-4.180777	1.390156
C	1.880641	-0.914986	2.340741
H	2.175779	0.120459	2.138014
H	1.746086	-0.998462	3.425805
C	3.130718	-1.936031	0.371675
H	3.701634	-1.044969	0.099684
H	3.768977	-2.790187	0.101275
C	2.992929	-1.865711	1.901533
H	3.951123	-1.539025	2.318027
H	2.804906	-2.849295	2.331037
C	2.339321	-1.683520	-1.951045
H	1.501206	-1.747511	-2.646453
H	3.058897	-2.451027	-2.266177
C	3.032912	-0.312995	-2.093204

H	3.054560	-0.011167	-3.143016
H	4.075886	-0.394103	-1.781005
N	-0.673716	-0.719132	-0.671951
C	-0.717477	-0.515420	-2.108387
H	-1.570667	0.105595	-2.401997
H	0.179319	0.005185	-2.444627
H	-0.794985	-1.457071	-2.678498
C	-1.852037	-1.431168	-0.212268
H	-1.883180	-2.479496	-0.565291
H	-1.826673	-1.464916	0.875229
C	-3.183061	-0.775048	-0.597567
H	-3.373562	-0.849351	-1.670191
H	-3.133847	0.293348	-0.353228
C	-4.355742	-1.424535	0.147620
H	-4.383874	-2.495188	-0.074820
H	-4.188265	-1.326483	1.226470
C	-5.671728	-0.801433	-0.215315
H	-5.772409	0.260387	0.000506
C	-6.683054	-1.443839	-0.790332
H	-6.614885	-2.500961	-1.023016
H	-7.606975	-0.939596	-1.044385
H	-0.745504	1.094470	0.807743

cat3_am1_d$_S$

SCF energy in solution: –1183.31753

Enthalpy in solution: –1182.645736

Free energy in solution: –1182.728402

Cartesian coordinates

Atom	X	Y	Z
C	0.163244	-3.113991	-1.230875
H	0.218375	-4.063080	-1.733884
C	-0.843959	-2.207458	-1.128171
C	2.560918	-3.181612	-0.322421
H	3.153564	-3.089969	-1.235422
H	2.435124	-4.241777	-0.100618
C	3.129219	-0.932684	0.705603
N	1.696470	-0.600154	0.697998
N	-0.393210	-1.146836	-0.346895
C	0.872950	-1.396508	-0.038151
N	1.247323	-2.593044	-0.530190
C	3.225028	-2.458864	0.845548
H	2.735797	-2.749736	1.778441
H	4.274978	-2.749820	0.904135
C	3.754538	-0.266583	1.927333
H	3.640576	0.816858	1.860654
H	3.270993	-0.618306	2.839308
H	4.821352	-0.493942	1.973988
C	3.824043	-0.449147	-0.573746
H	3.861704	0.641105	-0.583308
H	4.848160	-0.828339	-0.617634
H	3.288465	-0.780239	-1.465861
B	-1.223924	0.244631	-0.062252
C	-2.784024	-0.249284	-0.237097
C	-1.138275	0.757718	1.495371
H	-0.160687	1.199936	1.741068
C	-3.635161	1.024396	-0.199691
H	-3.272675	1.699177	-0.984250
H	-4.682159	0.795392	-0.445490
C	-2.191489	1.866695	1.796456
H	-1.792397	2.832633	1.488583
H	-2.316462	1.942497	2.884599
C	-3.597396	1.729157	1.160760
H	-4.030536	2.729054	1.061078
H	-4.263264	1.190962	1.836094
C	-1.352320	-0.425305	2.451608
H	-0.631155	-1.220261	2.235102
H	-1.174207	-0.114987	3.488473
C	-3.192918	-1.251106	0.882700
H	-2.756954	-2.223772	0.637359
H	-4.282516	-1.396811	0.839878
C	-2.776291	-0.970239	2.336651
H	-2.865236	-1.900467	2.906862
H	-3.459089	-0.267385	2.812908
C	-3.047187	-0.970960	-1.565577
H	-2.852001	-0.291329	-2.395324
H	-4.108053	-1.246109	-1.639062
C	-2.220186	-2.261076	-1.737677
H	-2.116107	-2.499356	-2.799195
H	-2.755807	-3.101470	-1.290757
N	-0.539232	1.222567	-1.057187
C	-0.609394	0.936088	-2.477147
H	-0.665634	-0.138439	-2.648206
H	-1.477651	1.404420	-2.972192
H	0.283139	1.289529	-3.007306
C	-0.519836	2.654536	-0.827149
H	-1.465358	3.145451	-1.122589
H	-0.399511	2.828028	0.238407
C	0.620177	3.395687	-1.547371
H	0.446888	3.410476	-2.625528
H	0.608783	4.438340	-1.217053
C	1.996260	2.779819	-1.266790
H	1.922180	1.707423	-1.477361
H	2.753061	3.202097	-1.933091

C	2.431949	2.976392	0.157127
H	1.719866	2.690690	0.929940
C	3.603102	3.488733	0.529988
H	4.336640	3.804391	-0.204500
H	3.859867	3.620937	1.573997
H	1.450160	0.378886	0.609232

cat3_am1_ets$_S$

SCF energy in solution: –1183.271282

Enthalpy in solution: –1182.602316

Free energy in solution: –1182.679649

Cartesian coordinates

Atom	X	Y	Z
C	1.641636	-2.115478	-1.821102
H	2.063999	-2.838021	-2.497286
C	0.358076	-1.749674	-1.598472
C	3.873155	-1.446803	-0.770278
H	4.389391	-0.961368	-1.601737
H	4.159136	-2.499729	-0.759568
C	3.508668	0.581666	0.688619
N	2.057025	0.359952	0.641264
N	0.344529	-0.790276	-0.579087
C	1.624729	-0.549665	-0.242735
N	2.435004	-1.360828	-0.964555
C	4.209610	-0.777084	0.557529
H	3.879754	-1.415561	1.381282
H	5.290303	-0.645047	0.637379
C	3.835113	1.198254	2.046108
H	3.291766	2.136211	2.167448
H	3.536834	0.520845	2.847389
H	4.905038	1.402972	2.126295
C	3.947428	1.531601	-0.436195
H	3.503987	2.513962	-0.278142
H	5.036052	1.632145	-0.453555
H	3.612184	1.171786	-1.411325
B	-0.999592	-0.188291	0.057849
C	-2.102946	-1.385053	-0.217169
C	-0.958681	-0.024976	1.677975
H	-0.274860	0.766359	1.997252
C	-3.509641	-1.024636	0.292167
H	-3.973836	-0.320945	-0.400220
H	-4.136918	-1.925069	0.241920
C	-2.360444	0.357726	2.218943
H	-2.553586	1.409094	1.992028
H	-2.341787	0.307037	3.314631
C	-3.576272	-0.469751	1.732115
H	-4.473437	0.150701	1.826439
H	-3.738060	-1.299819	2.417471
C	-0.456624	-1.322877	2.333759
H	0.568334	-1.513663	2.000394
H	-0.406505	-1.192609	3.421591
C	-1.633922	-2.673174	0.521218
H	-0.724442	-3.056200	0.053146
H	-2.399724	-3.447221	0.370788
C	-1.328321	-2.541328	2.018122
H	-0.818232	-3.451488	2.349444
H	-2.249381	-2.495694	2.597395
C	-2.198826	-1.727673	-1.708472
H	-2.496412	-0.836733	-2.267944
H	-2.983754	-2.474673	-1.882873
C	-0.878680	-2.276501	-2.277640
H	-0.814901	-2.060882	-3.347457
H	-0.865648	-3.364530	-2.184724
N	-1.201131	1.264319	-0.720343
C	-0.443755	1.359943	-1.977636
H	0.612285	1.507011	-1.738886
H	-0.553517	0.464475	-2.589837
H	-0.782589	2.213010	-2.564344
C	-2.585272	1.710986	-0.948225
H	-3.062634	1.147208	-1.752525
H	-3.145371	1.528969	-0.035331
C	-2.577609	3.224509	-1.248027
H	-2.620958	3.418051	-2.320968
H	-3.467010	3.681081	-0.812429
C	-1.287968	3.783966	-0.631941
H	-0.569294	4.084499	-1.397407
H	-1.481086	4.669024	-0.023061
C	-0.644630	2.743915	0.270888
H	-1.277482	2.513995	1.121590
C	0.738413	2.836146	0.572593
H	1.310747	3.541280	-0.025225
H	0.971067	2.870959	1.633793
H	1.471094	1.313645	0.604100

cat3_am1_f$_S$

SCF energy in solution: –1183.326879

Enthalpy in solution: –1182.652663

Free energy in solution: –1182.732644

Cartesian coordinates

Atom	X	Y	Z
C	1.729228	-1.263311	-2.340228
H	2.151161	-1.687002	-3.235672

C	0.455073	-1.227556	-1.908157
C	3.969712	-0.674565	-1.295815
H	4.412532	0.142786	-1.872824
H	4.318791	-1.615442	-1.727100
C	3.560426	0.537873	0.878431
N	2.125007	0.284294	0.793967
N	0.423430	-0.570426	-0.662861
C	1.728320	-0.248139	-0.318993
N	2.522066	-0.628537	-1.384776
C	4.360817	-0.573415	0.174403
H	4.136559	-1.519574	0.674594
H	5.434194	-0.388443	0.257507
C	3.931299	0.558174	2.359735
H	3.320636	1.302746	2.872959
H	3.724563	-0.414936	2.808725
H	4.987249	0.802460	2.502475
C	3.890120	1.904473	0.255359
H	3.409343	2.695416	0.833556
H	4.968803	2.087549	0.248338
H	3.516813	1.967189	-0.769452
B	-0.882303	-0.340652	0.109861
C	-1.887533	-1.568295	-0.287716
C	-0.815796	-0.289493	1.720251
H	-0.177274	0.518788	2.086215
C	-3.277735	-1.502656	0.374478
H	-3.917478	-0.830478	-0.200368
H	-3.751702	-2.488139	0.274138
C	-2.215777	-0.127600	2.353355
H	-2.568390	0.898105	2.208049
H	-2.128209	-0.240015	3.440332
C	-3.313460	-1.101542	1.867652
H	-4.291879	-0.661283	2.087003
H	-3.270611	-2.003013	2.475239
C	-0.138289	-1.594579	2.194593
H	0.897798	-1.568290	1.851708
H	-0.103780	-1.606506	3.290901
C	-1.164208	-2.853308	0.213492
H	-0.235111	-2.987543	-0.344590
H	-1.801064	-3.715061	-0.030032
C	-0.812716	-2.884023	1.705749
H	-0.137636	-3.726676	1.884465
H	-1.703378	-3.097210	2.296271
C	-2.072386	-1.721033	-1.801384
H	-2.633157	-0.868239	-2.193196
H	-2.692260	-2.600820	-2.015767
C	-0.743107	-1.867478	-2.565586
H	-0.853849	-1.475616	-3.580523
H	-0.517574	-2.930142	-2.678656
N	-1.449883	1.333467	-0.533180
C	-0.899285	1.568250	-1.890020
H	0.182763	1.492317	-1.866576
H	-1.283871	0.806342	-2.563899
H	-1.189470	2.553510	-2.259376
C	-2.934856	1.473592	-0.607820
H	-3.324012	0.872855	-1.425385
H	-3.342923	1.097719	0.324554
C	-3.239759	2.970767	-0.748476
H	-3.328768	3.261352	-1.795444
H	-4.185222	3.212555	-0.264603
C	-2.033729	3.653381	-0.078321
H	-1.520405	4.324530	-0.769669
H	-2.318598	4.246369	0.790566
C	-1.094102	2.510312	0.355774
H	-1.368390	2.189535	1.357661
C	0.364646	2.918907	0.363463
H	0.682642	3.302108	-0.608806
H	0.474808	3.733809	1.083292
H	1.012092	2.095646	0.666722

cat3_am1_d_R

SCF energy in solution: –1183.29846

Enthalpy in solution: –1182.626149

Free energy in solution: –1182.708522

Cartesian coordinates

Atom	X	Y	Z
C	1.677098	-2.725787	-1.194177
H	2.144986	-3.535652	-1.725487
C	0.379789	-2.324379	-1.125094
C	3.858483	-1.786892	-0.217525
H	4.335211	-1.497220	-1.156586
H	4.216082	-2.780188	0.055804
C	3.363140	0.521770	0.724494
N	1.941042	0.155345	0.816027
N	0.319478	-1.228066	-0.272478
C	1.558867	-0.934299	0.090800
N	2.417060	-1.841821	-0.409857
C	4.160432	-0.780399	0.890928
H	3.901038	-1.215061	1.859217
H	5.228261	-0.556217	0.892396
C	3.673016	1.464715	1.882362
H	3.059284	2.365602	1.813623
H	3.461362	0.977094	2.834248
H	4.721729	1.766021	1.855670

C	3.671865	1.201482	-0.615307
H	3.114938	2.136532	-0.696407
H	4.738313	1.424828	-0.695591
H	3.378592	0.574947	-1.459128
B	-0.978359	-0.285989	-0.069020
C	-2.213559	-1.329729	-0.335262
C	-1.139888	0.120881	1.522583
H	-0.417463	0.882392	1.845397
C	-3.522018	-0.536199	-0.244534
H	-3.513248	0.243464	-1.009178
H	-4.374215	-1.187580	-0.486787
C	-2.541162	0.693366	1.868111
H	-2.525215	1.768860	1.708467
H	-2.706095	0.577077	2.947180
C	-3.773690	0.089712	1.139990
H	-4.537807	0.867870	1.039773
H	-4.229601	-0.671197	1.773532
C	-0.905197	-1.123412	2.400389
H	0.072791	-1.567779	2.193924
H	-0.898046	-0.837171	3.459155
C	-2.217920	-2.497907	0.693474
H	-1.420781	-3.197890	0.432355
H	-3.155920	-3.060681	0.577862
C	-2.002359	-2.166737	2.179765
H	-1.746910	-3.091458	2.707092
H	-2.923306	-1.810415	2.640379
C	-2.072990	-1.943029	-1.733771
H	-2.022865	-1.132409	-2.466402
H	-2.949432	-2.551889	-1.992603
C	-0.824324	-2.840191	-1.868419
H	-0.551649	-2.944451	-2.921228
H	-1.054300	-3.846068	-1.510933
N	-0.637916	0.906550	-1.085100
C	0.197183	0.631612	-2.257457
H	0.984573	-0.094831	-2.077561
H	-0.375232	0.266312	-3.128581
H	0.690332	1.558377	-2.576105
C	-1.609413	1.879519	-1.595905
H	-1.057548	2.541882	-2.273766
H	-2.372972	1.401025	-2.233295
C	-2.302489	2.817848	-0.615467
H	-2.858127	3.545390	-1.218724
H	-3.042510	2.296372	-0.014681
C	-1.310946	3.568226	0.280545
H	-1.867394	4.218336	0.965221
H	-0.748728	2.852931	0.882503
C	-0.350189	4.398681	-0.519333
C	0.973501	4.307660	-0.437484
H	1.632936	4.930011	-1.029738
H	1.432274	3.602790	0.248207
H	1.278266	0.914951	0.677602
H	-0.790840	5.111907	-1.214094

cat3_am1_ets$_R$

SCF energy in solution: –1183.259595

Enthalpy in solution: –1182.590767

Free energy in solution: –1182.667662

Cartesian coordinates

Atom	X	Y	Z
C	1.729818	-2.412737	-1.331537
H	2.182201	-3.259700	-1.816716
C	0.436570	-2.022884	-1.244244
C	3.912966	-1.500813	-0.354103
H	4.473744	-1.201665	-1.242737
H	4.197458	-2.522835	-0.099204
C	3.476896	0.795155	0.607162
N	2.031348	0.555039	0.529638
N	0.380857	-0.865010	-0.462700
C	1.644464	-0.533100	-0.143666
N	2.486997	-1.473894	-0.636316
C	4.178964	-0.554737	0.812728
H	3.801184	-1.001212	1.736297
H	5.254147	-0.399755	0.920702
C	3.725672	1.696639	1.813316
H	3.165986	2.626436	1.700253
H	3.390207	1.202268	2.726029
H	4.787705	1.936109	1.901482
C	3.987628	1.478651	-0.670913
H	3.561571	2.477737	-0.750037
H	5.077685	1.562922	-0.653175
H	3.693772	0.921168	-1.562888
B	-0.979361	-0.134142	-0.051587
C	-2.076422	-1.361266	-0.086907
C	-0.979619	0.363922	1.510231
H	-0.364811	1.253583	1.664328
C	-3.487526	-0.884104	0.292666
H	-3.875626	-0.203270	-0.465155
H	-4.166547	-1.747890	0.278822
C	-2.393085	0.702020	2.060066
H	-2.652067	1.718994	1.777724
H	-2.333570	0.724666	3.155486
C	-3.576065	-0.220208	1.675982
H	-4.501848	0.362272	1.727893

H	-3.693999	-1.002501	2.424077
C	-0.381868	-0.757475	2.384528
H	0.637661	-0.983948	2.067960
H	-0.307309	-0.408656	3.421440
C	-1.641978	-2.461096	0.935858
H	-0.787992	-3.004726	0.528040
H	-2.458123	-3.194528	1.002192
C	-1.233669	-2.029529	2.355968
H	-0.678974	-2.853347	2.816294
H	-2.110834	-1.884421	2.984562
C	-2.120526	-2.037267	-1.463145
H	-2.412929	-1.306923	-2.222682
H	-2.888965	-2.820589	-1.481571
C	-0.774004	-2.676816	-1.859369
H	-0.664846	-2.666663	-2.947193
H	-0.765670	-3.728345	-1.565492
N	-1.101521	1.085336	-1.229684
C	-0.245443	0.807521	-2.397048
H	0.801837	0.896297	-2.107362
H	-0.417956	-0.182614	-2.819920
H	-0.438638	1.547389	-3.176759
C	-2.436953	1.492813	-1.708480
H	-2.297183	2.023276	-2.654861
H	-3.084923	0.645657	-1.919458
C	-3.031064	2.479800	-0.702586
H	-3.747698	3.128043	-1.209018
H	-3.574579	1.954824	0.080039
C	-1.838726	3.266973	-0.128801
H	-1.931921	4.335827	-0.334087
H	-1.757614	3.162218	0.952073
C	-0.539410	2.798205	-0.761007
C	0.692263	2.934012	-0.067308
H	1.488933	3.413061	-0.627508
H	0.614179	3.277659	0.961869
H	1.414833	1.480528	0.312136
H	-0.488745	3.100994	-1.808846

cat3_am1_f$_R$

SCF energy in solution: –1183.327331

Enthalpy in solution: –1182.655654

Free energy in solution: –1182.73902

Cartesian coordinates

Atom	X	Y	Z
C	-1.861975	-0.744826	2.499174
H	-2.269851	-0.805631	3.494037
C	-0.675349	-1.151395	2.027306
C	-4.011968	0.117927	1.435510
H	-4.187110	1.148447	1.756820
H	-4.515609	-0.543782	2.143574
C	-3.601003	0.527353	-1.029476
N	-2.240278	-0.002976	-0.918121
N	-0.627477	-0.851743	0.642101
C	-1.869939	-0.300378	0.271842
N	-2.591264	-0.180534	1.445698
C	-4.532877	-0.109193	0.019362
H	-4.580955	-1.183846	-0.177092
H	-5.541976	0.298429	-0.070458
C	-4.107470	0.175165	-2.426731
H	-3.423890	0.584930	-3.171540
H	-4.135228	-0.908595	-2.552126
H	-5.107827	0.580420	-2.598551
C	-3.577161	2.052672	-0.868789
H	-2.954956	2.489492	-1.650890
H	-4.585361	2.469075	-0.947270
H	-3.153689	2.341099	0.096001
B	0.533579	-1.089310	-0.172149
C	1.767706	-1.801835	0.502714
C	0.593663	-1.067715	-1.736859
H	-0.216482	-0.492577	-2.182541
C	3.084529	-1.228424	-0.057265
H	3.174768	-0.213294	0.341466
H	3.930143	-1.804424	0.341297
C	1.945575	-0.536264	-2.245653
H	1.959695	0.541192	-2.056571
H	2.013159	-0.666456	-3.331612
C	3.193113	-1.141760	-1.584721
H	4.057458	-0.517616	-1.833622
H	3.413057	-2.121055	-2.006546
C	0.329057	-2.566054	-2.064217
H	-0.699577	-2.788736	-1.758830
H	0.369120	-2.716192	-3.148533
C	1.540171	-3.291563	0.112501
H	0.668556	-3.656370	0.666347
H	2.396550	-3.886102	0.456268
C	1.285790	-3.565214	-1.384156
H	0.865581	-4.570520	-1.480810
H	2.230915	-3.592039	-1.921862
C	1.791530	-1.642846	2.029649
H	2.100672	-0.618427	2.258233
H	2.542775	-2.308390	2.471213
C	0.434175	-1.907046	2.689530
H	0.463998	-1.642089	3.748358
H	0.210349	-2.977263	2.644216

N	1.576541	2.095141	0.784752
C	0.614876	2.083569	1.872670
H	-0.374468	1.811790	1.504737
H	0.904948	1.340281	2.616453
H	0.552525	3.067087	2.370242
C	2.925080	2.403155	1.252660
H	2.915918	3.296577	1.902479
H	3.338165	1.572277	1.828988
C	3.695691	2.697886	-0.038623
H	4.520183	3.389571	0.132077
H	4.110238	1.775979	-0.447834
C	2.613727	3.269222	-0.985249
H	2.806705	4.305109	-1.265462
H	2.550573	2.687312	-1.905886
C	1.300720	3.156847	-0.191062
C	0.075722	2.874486	-1.043096
H	-0.016695	3.628152	-1.828339
H	0.149514	1.887999	-1.503625
H	1.145810	4.106539	0.356180
H	-0.838540	2.896372	-0.451361

am2

SCF energy in solution: –369.849059

Enthalpy in solution: –369.593609

Free energy in solution: –369.642591

Cartesian coordinates

Atom	X	Y	Z
C	-1.258291	0.187470	-0.867264
H	-1.415120	-0.728758	-1.447044
H	-0.974144	0.975534	-1.575968
C	-0.077717	-0.035961	0.102467
C	1.148528	-0.397155	-0.755770
H	1.299223	0.391052	-1.507534
H	0.913763	-1.314634	-1.307333
N	2.366241	-0.586452	0.030858
H	2.757378	-1.498456	-0.150544
C	3.382013	0.430170	-0.197595
H	4.266579	0.202628	0.398613
H	3.686285	0.526314	-1.250497
H	3.004403	1.400449	0.128501
C	-2.548972	0.568710	-0.201227
H	-2.583861	1.544842	0.274850
C	-3.628722	-0.206188	-0.162439
H	-3.632134	-1.185020	-0.630013
H	-4.538799	0.109342	0.332150
C	-0.380834	-1.192547	1.055208
H	-1.229856	-0.954807	1.697986
H	-0.627720	-2.100343	0.495766
H	0.493892	-1.393401	1.675354
C	0.218398	1.229295	0.909986
H	1.104768	1.066988	1.525465
H	0.398020	2.084701	0.250786
H	-0.612783	1.475959	1.573259

cat1_am2_a

SCF energy in solution: –1067.772559

Enthalpy in solution: –1067.148706

Free energy in solution: –1067.233923

Cartesian coordinates

Atom	X	Y	Z
C	3.861882	0.544651	-0.033068
H	4.925749	0.670982	0.060473
C	2.847619	1.431842	-0.153915
C	3.904909	-2.039144	-0.035557
H	4.184566	-2.311474	0.986993
H	4.817550	-2.006547	-0.634522
C	1.498290	-2.888162	-0.028328
N	0.987392	-1.538247	-0.256033
B	0.414640	1.585578	-0.418304
C	2.544078	2.898703	-0.281303
H	2.689041	3.205185	-1.323065
H	3.188849	3.528551	0.337014
N	1.669856	0.720653	-0.254634
C	1.910241	-0.610613	-0.208447
N	-0.688847	0.711089	0.490119
C	-0.342844	0.504928	1.919139
H	-0.889442	-0.347590	2.314693
H	0.723628	0.311771	1.993596
H	-0.595340	1.394721	2.486854
C	-2.125432	1.057255	0.309542
H	-2.471702	1.525631	1.234753
H	-2.193261	1.800339	-0.484227
C	-3.042779	-0.129112	-0.041669
N	3.271449	-0.737217	-0.060928
C	-0.087055	1.574466	-1.957041
H	-0.273833	0.559087	-2.315290
H	-0.966082	2.186138	-2.179385
H	0.727775	1.971670	-2.570582
C	1.028911	3.044895	0.102499
C	2.915656	-3.049787	-0.620080
H	2.847179	-2.893916	-1.700207
H	3.286769	-4.062287	-0.445438

C	1.514195	-3.181470	1.479799
H	0.496035	-3.115894	1.869223
H	1.906500	-4.180527	1.692433
H	2.121209	-2.445706	2.012487
C	0.556485	-3.867429	-0.724943
H	-0.457369	-3.729635	-0.342502
H	0.542936	-3.670699	-1.798367
H	0.859258	-4.903614	-0.554028
C	0.971423	3.311545	1.612852
H	1.478127	4.255304	1.843232
H	-0.058709	3.409002	1.966824
H	1.466784	2.527244	2.188783
C	0.425302	4.260847	-0.604206
H	0.943610	5.182243	-0.315983
H	0.483027	4.168456	-1.689862
H	-0.629088	4.382189	-0.336813
C	-2.970778	-1.239405	1.010795
H	-3.179567	-0.854254	2.013151
H	-3.714163	-2.005573	0.785419
H	-1.987957	-1.718756	1.010218
C	-4.474445	0.461810	-0.078773
H	-4.469552	1.331080	-0.746956
H	-4.728644	0.823799	0.922991
C	-5.536419	-0.497405	-0.535674
H	-5.537179	-0.762430	-1.588957
C	-6.458555	-1.023158	0.265142
H	-6.491379	-0.774667	1.320704
H	-7.208746	-1.710306	-0.105323
C	-2.667321	-0.717894	-1.406780
H	-2.752996	0.031021	-2.198013
H	-1.645226	-1.106051	-1.407436
H	-3.327352	-1.553585	-1.645966
H	-0.503351	-0.216897	0.065041

cat1_am2_bts

SCF energy in solution: –1067.758565

Enthalpy in solution: –1067.14023

Free energy in solution: –1067.222601

Cartesian coordinates

Atom	X	Y	Z
C	-3.897650	0.156535	-0.125374
H	-4.958243	0.279846	-0.000997
C	-3.107986	-0.942186	-0.263146
C	-3.291321	2.692907	-0.038748
H	-3.497165	2.928466	1.008936
H	-4.168990	2.966836	-0.626294
C	-0.725344	2.895904	0.021161
N	-0.607073	1.480166	-0.346045
B	-0.690462	-1.564653	-0.404792
C	-3.084126	-2.446368	-0.287233
H	-3.241347	-2.789463	-1.315329
H	-3.861307	-2.898756	0.333537
N	-1.818861	-0.503902	-0.423455
C	-1.764548	0.817858	-0.350405
N	0.450106	-0.760572	0.436401
C	0.151942	-0.526359	1.859860
H	0.789899	0.262582	2.259862
H	-0.885168	-0.208545	1.966953
H	0.303210	-1.425692	2.456720
C	1.830773	-1.261531	0.272913
H	2.126878	-1.782758	1.192745
H	1.835826	-2.003454	-0.525524
C	2.915561	-0.218584	-0.064477
N	-3.031313	1.273382	-0.192321
C	-0.177311	-1.816645	-1.923367
H	0.280085	-0.918784	-2.348010
H	0.530693	-2.641768	-2.040825
H	-1.039977	-2.057999	-2.552677
C	-1.633249	-2.840456	0.187981
C	-2.055369	3.444253	-0.546017
H	-2.015151	3.359700	-1.635180
H	-2.151042	4.501958	-0.292103
C	-0.689618	3.067859	1.545993
H	0.281828	2.756892	1.934634
H	-0.852473	4.111849	1.827330
H	-1.453033	2.452169	2.026739
C	0.428759	3.664013	-0.618382
H	1.384782	3.274107	-0.265239
H	0.395881	3.550798	-1.703082
H	0.374539	4.725671	-0.366596
C	-1.698761	-3.007172	1.712606
H	-2.389716	-3.818849	1.968961
H	-0.724053	-3.271580	2.128451
H	-2.056070	-2.106061	2.215184
C	-1.257011	-4.202623	-0.400864
H	-1.949586	-4.984269	-0.067430
H	-1.265432	-4.189777	-1.491707
H	-0.253090	-4.496648	-0.080562
C	2.982002	0.895907	0.980841
H	3.143408	0.488668	1.983266
H	3.808978	1.572186	0.755383
H	2.058985	1.478258	0.986934
C	4.254640	-0.997639	-0.064528

H	4.142064	-1.866916	-0.723520
H	4.438493	-1.377918	0.945734
C	5.444456	-0.197977	-0.510745
H	5.490703	0.063157	-1.564300
C	6.424470	0.198479	0.296055
H	6.414411	-0.048974	1.352383
H	7.265147	0.774792	-0.069475
C	2.656579	0.390308	-1.446479
H	2.716805	-0.375002	-2.225274
H	1.666364	0.846792	-1.494975
H	3.393603	1.165836	-1.667605
H	0.180223	0.503497	-0.011020

cat1_am2_c

SCF energy in solution: –1067.775771

Enthalpy in solution: –1067.15311

Free energy in solution: –1067.238279

Cartesian coordinates

Atom	X	Y	Z
C	3.822856	0.827144	-0.163278
H	4.870261	1.052819	-0.076673
C	2.716126	1.612819	-0.239018
C	4.109086	-1.740578	-0.089201
H	4.419395	-1.861935	0.951527
H	5.005949	-1.688833	-0.707394
C	1.794757	-2.822846	0.040965
N	1.222835	-1.560658	-0.441361
B	0.202849	1.549782	-0.371437
C	2.282331	3.048684	-0.271848
H	2.343574	3.411733	-1.303118
H	2.917796	3.693416	0.341841
N	1.616296	0.789442	-0.341105
C	2.019563	-0.463408	-0.338775
N	-0.759074	0.645511	0.449628
C	-0.389914	0.308907	1.819237
H	-0.796958	-0.659339	2.126003
H	0.695994	0.247069	1.911484
H	-0.739218	1.044144	2.556438
C	-2.184432	0.920740	0.333336
H	-2.571158	1.322896	1.285209
H	-2.339568	1.702501	-0.415004
C	-3.095862	-0.264257	-0.071959
H	0.259101	-1.323424	-0.203151
N	3.364311	-0.499060	-0.232359
C	-0.225385	1.648588	-1.938569
H	-0.357856	0.656317	-2.378026
H	-1.145471	2.211566	-2.117901
H	0.559478	2.149527	-2.515824
C	0.793353	3.028866	0.201828
C	3.217784	-2.900639	-0.539632
H	3.136180	-2.890728	-1.628980
H	3.680773	-3.842561	-0.240615
C	1.811887	-2.870539	1.573502
H	0.789591	-2.851371	1.956115
H	2.297078	-3.783303	1.926990
H	2.337752	-2.009279	1.990631
C	0.946532	-3.960730	-0.516010
H	-0.084193	-3.867633	-0.165827
H	0.943358	-3.932190	-1.606098
H	1.334616	-4.924393	-0.181745
C	0.798075	3.168333	1.729520
H	1.236014	4.130065	2.024083
H	-0.217691	3.133687	2.129123
H	1.379506	2.381172	2.215866
C	0.050004	4.238290	-0.368715
H	0.485139	5.180411	-0.013639
H	0.069201	4.249221	-1.460007
H	-0.998236	4.224125	-0.055342
C	-2.960631	-1.443347	0.892530
H	-3.134748	-1.131659	1.926422
H	-3.685076	-2.222123	0.645226
H	-1.958836	-1.875708	0.826304
C	-4.546073	0.273680	-0.024097
H	-4.586150	1.190609	-0.624577
H	-4.781544	0.553526	1.008166
C	-5.590086	-0.682336	-0.524076
H	-5.592520	-0.888511	-1.590993
C	-6.492369	-1.279768	0.249235
H	-6.523145	-1.093979	1.317671
H	-7.226847	-1.964757	-0.155950
C	-2.744816	-0.736465	-1.483483
H	-2.918741	0.053548	-2.219141
H	-1.688727	-1.007448	-1.530500
H	-3.335620	-1.611561	-1.763985

cat1_am2_d_S

SCF energy in solution: –1067.774546

Enthalpy in solution: –1067.152532

Free energy in solution: –1067.237218

Cartesian coordinates

Atom	X	Y	Z
C	3.535571	1.105816	-0.046849

H	4.560510	1.399398	0.089805
C	2.394445	1.816755	-0.249753
C	3.957160	-1.433843	0.212209
H	4.190971	-1.488006	1.278262
H	4.895396	-1.356803	-0.338140
C	1.706132	-2.653794	0.230961
N	1.099120	-1.445417	-0.334745
B	-0.098590	1.583682	-0.524558
N	1.352306	0.923534	-0.364820
C	1.823320	-0.300707	-0.248147
N	-1.032951	0.685060	0.339305
C	-0.704227	0.526487	1.747511
H	-0.959451	-0.473785	2.116830
H	0.368775	0.652126	1.897901
H	-1.218059	1.246579	2.399755
C	-2.459098	0.861958	0.116809
H	-2.842536	1.761892	0.634997
H	-2.593972	1.042518	-0.949993
C	-3.410660	-0.306549	0.503429
C	-2.786681	-1.682923	0.200427
H	-1.900350	-1.801315	0.835362
H	-3.495274	-2.463791	0.498298
C	-2.396967	-1.890983	-1.234520
H	-1.737531	-1.142351	-1.663167
C	-2.800708	-2.916171	-1.980406
H	-3.467264	-3.673971	-1.581847
H	-2.484464	-3.027561	-3.010146
H	0.108452	-1.259676	-0.179990
N	3.156942	-0.247708	-0.051500
C	1.885412	3.217869	-0.423297
H	2.433204	3.942475	0.185692
H	2.010949	3.508965	-1.471593
C	-0.467598	1.520407	-2.109410
H	-1.376331	2.064304	-2.379153
H	0.342658	1.963334	-2.698950
H	-0.580467	0.490532	-2.463801
C	0.365469	3.146548	-0.065086
C	3.170262	-2.664913	-0.244842
H	3.665090	-3.563585	0.127430
H	3.167007	-2.704400	-1.336596
C	1.615116	-2.648986	1.761394
H	0.568516	-2.693089	2.069690
H	2.135507	-3.511809	2.183528
H	2.046702	-1.737821	2.180772
C	0.966594	-3.857388	-0.343940
H	-0.097535	-3.797509	-0.105088
H	1.065658	-3.878139	-1.429814
H	1.365581	-4.783828	0.072904
C	0.235308	3.445901	1.434707
H	0.560984	4.471805	1.646379
H	-0.800887	3.354145	1.767234
H	0.846995	2.778584	2.046007
C	-0.393681	4.244196	-0.815574
H	-0.044734	5.242092	-0.523542
H	-0.278370	4.151339	-1.896881
H	-1.463229	4.192470	-0.591124
C	-3.822349	-0.268331	1.983192
H	-4.239159	0.709831	2.235603
H	-4.593451	-1.019948	2.174098
H	-2.991529	-0.465462	2.659017
C	-4.689623	-0.129283	-0.325791
H	-5.437265	-0.877531	-0.049203
H	-5.120134	0.860599	-0.150651
H	-4.485112	-0.231707	-1.392933

cat1_am2_ets$_S$

SCF energy in solution: –1067.735051

Enthalpy in solution: –1067.11633

Free energy in solution: –1067.196127

Cartesian coordinates

Atom	X	Y	Z
C	2.590487	2.444494	0.098478
H	3.284622	3.253514	0.238105
C	1.255695	2.419256	-0.100201
C	4.361078	0.594942	0.216247
H	4.658603	0.576248	1.267956
H	5.036422	1.268093	-0.313863
C	3.243828	-1.679913	0.100981
N	1.989234	-1.009442	-0.219333
B	-0.739144	1.031106	-0.534460
N	0.836382	1.095349	-0.207203
C	1.923839	0.313694	-0.117626
N	-1.446786	-0.230825	0.159174
C	-0.863023	-0.623989	1.452274
H	-0.175383	-1.456750	1.275677
H	-0.308446	0.195708	1.901546
H	-1.636371	-0.943792	2.149428
C	-2.903214	-0.002927	0.242099
H	-3.157525	0.586262	1.125269
H	-3.185732	0.581764	-0.633474
C	-3.674706	-1.353654	0.228648
C	-2.609487	-2.409835	-0.085828
H	-2.205739	-2.859336	0.827066

H	-3.026829	-3.225382	-0.682681
C	-1.477375	-1.770338	-0.863155
H	-1.832316	-1.273686	-1.762748
C	-0.246719	-2.470200	-0.985726
H	-0.189262	-3.409643	-0.439891
H	0.164838	-2.523215	-1.989616
H	1.056832	-1.589088	-0.469018
N	3.008158	1.108203	0.091201
C	0.119782	3.371159	-0.271523
H	0.227143	4.270216	0.342352
H	0.060909	3.690085	-1.317022
C	-0.900116	0.976209	-2.148696
H	-1.934723	0.881232	-2.494603
H	-0.504727	1.888215	-2.605724
H	-0.333784	0.142060	-2.571884
C	-1.132802	2.537838	0.108403
C	4.407521	-0.803921	-0.392727
H	5.360222	-1.276488	-0.145625
H	4.335803	-0.725466	-1.480369
C	3.337488	-1.918186	1.614623
H	2.532117	-2.585269	1.926041
H	4.294150	-2.374568	1.882435
H	3.226452	-0.982927	2.166775
C	3.264912	-3.017050	-0.636417
H	2.409135	-3.623307	-0.337091
H	3.208050	-2.856348	-1.714180
H	4.181899	-3.562093	-0.403749
C	-1.226208	2.610608	1.642851
H	-1.447204	3.638998	1.951691
H	-2.009773	1.974707	2.057189
H	-0.281110	2.329171	2.115142
C	-2.372091	3.213304	-0.486273
H	-2.397745	4.274675	-0.212367
H	-2.381001	3.150083	-1.576622
H	-3.296654	2.767555	-0.113479
C	-4.379558	-1.630639	1.558910
H	-5.130864	-0.864252	1.767641
H	-4.886048	-2.598423	1.524675
H	-3.676157	-1.651057	2.393809
C	-4.729587	-1.313747	-0.883716
H	-5.318497	-2.233946	-0.890190
H	-5.414239	-0.473549	-0.739523
H	-4.258739	-1.201153	-1.863396

cat1_am2_f$_S$

SCF energy in solution: –1067.785461

Enthalpy in solution: –1067.159823

Free energy in solution: –1067.240737

Cartesian coordinates

Atom	X	Y	Z
C	-2.331102	2.274906	-1.023441
H	-2.962348	2.992207	-1.517626
C	-1.017230	2.288283	-0.728952
C	-4.210494	0.619079	-0.505551
H	-4.542235	0.247208	-1.480301
H	-4.835392	1.476941	-0.245807
C	-3.186887	-1.505007	0.418273
N	-1.875216	-0.874273	0.533086
B	0.728616	1.095317	0.552200
C	0.175830	3.163755	-0.907625
H	-0.058691	4.224455	-0.781067
H	0.576293	3.052628	-1.922395
N	-0.683951	1.105055	-0.077138
C	-1.807871	0.317742	0.021436
N	-2.827248	1.043469	-0.568687
C	0.601271	0.698079	2.117513
H	-0.046442	-0.173885	2.228097
H	1.526853	0.517938	2.666386
H	0.085513	1.509959	2.632532
C	1.211328	2.672187	0.151041
C	-4.321383	-0.471026	0.557276
H	-4.240473	-0.015741	1.548127
H	-5.297291	-0.956562	0.483703
C	-3.286828	-2.229712	-0.933314
H	-2.513071	-2.998288	-0.986195
H	-4.263386	-2.706074	-1.062753
H	-3.122648	-1.535307	-1.760069
C	-3.306220	-2.526630	1.547432
H	-2.474583	-3.230821	1.484964
H	-3.248888	-2.021250	2.513018
H	-4.246744	-3.080708	1.488021
C	2.610271	2.993429	-0.395183
H	2.682895	4.069842	-0.587452
H	3.408532	2.745305	0.306425
H	2.820656	2.496747	-1.345625
C	1.016947	3.550484	1.400060
H	1.254075	4.594901	1.168821
H	-0.016313	3.513331	1.752528
H	1.662058	3.230173	2.221476
C	3.109544	-0.170252	-0.219770
C	3.487055	-1.592323	-0.687704
H	4.407759	-1.915076	-0.198078
H	3.672985	-1.623298	-1.763039

C	2.289052	-2.504640	-0.308769
C	1.230745	-1.507190	0.208307
H	1.274777	-1.458072	1.292773
H	0.195180	-1.723884	-0.053720
N	1.599057	-0.143424	-0.298595
C	1.231037	-0.025793	-1.736579
H	0.199881	-0.342003	-1.866951
H	1.324631	1.014683	-2.036129
H	1.886895	-0.634078	-2.354610
H	3.483186	0.588969	-0.902699
C	3.654322	0.109830	1.174913
H	3.311471	1.064433	1.564420
H	3.374231	-0.670215	1.883080
H	4.744040	0.128585	1.111609
C	2.662060	-3.482575	0.812033
H	1.780732	-4.034836	1.146597
H	3.401367	-4.205605	0.459729
H	3.080742	-2.959412	1.674070
C	1.788324	-3.328198	-1.502184
H	2.583472	-3.980968	-1.870859
H	0.948642	-3.957157	-1.197947
H	1.451449	-2.704024	-2.329986

am3

SCF energy in solution: –753.393365
Enthalpy in solution: –753.023456
Free energy in solution: –753.08733

Cartesian coordinates

Atom	X	Y	Z
C	-0.218486	-0.839820	-1.931932
H	0.585096	-0.687439	-2.661560
H	-1.143370	-0.510941	-2.412488
C	0.029039	0.112829	-0.721655
C	0.351336	1.487505	-1.351687
H	-0.475937	1.781054	-2.008076
H	1.231090	1.346311	-2.002934
N	0.553593	2.537189	-0.374556
H	1.288185	2.253616	0.262684
C	0.908823	3.797807	-1.005876
H	1.127003	4.542295	-0.240323
H	1.774730	3.726547	-1.681925
H	0.060613	4.160569	-1.591784
C	-0.320793	-2.305031	-1.622734
H	0.543008	-2.768152	-1.154165
C	-1.386623	-3.047178	-1.905736
H	-2.269592	-2.611661	-2.359954
H	-1.413750	-4.107037	-1.685483
C	1.255911	-0.287866	0.103161
C	2.387778	-0.834449	-0.511546
C	1.329074	-0.000283	1.470714
C	3.542345	-1.105440	0.215834
H	2.375892	-1.054477	-1.571957
C	2.485376	-0.265521	2.199611
H	0.469737	0.434251	1.965322
C	3.596216	-0.824052	1.577113
H	4.400722	-1.536642	-0.284425
H	2.513573	-0.034326	3.257395
H	4.493991	-1.035815	2.144045
C	-1.249659	0.130877	0.116394
C	-2.157029	1.191175	0.072761
C	-1.577753	-0.982964	0.898792
C	-3.358523	1.133410	0.775135
H	-1.914471	2.087116	-0.479550
C	-2.773771	-1.040728	1.604401
H	-0.883962	-1.811172	0.960475
C	-3.674392	0.018346	1.541583
H	-4.042771	1.971748	0.728090
H	-3.000972	-1.914822	2.202317
H	-4.607186	-0.023038	2.090192

cat1_am3_a

SCF energy in solution: –1451.310074
Enthalpy in solution: –1450.571655
Free energy in solution: –1450.672495

Cartesian coordinates

Atom	X	Y	Z
C	-0.218486	-0.839820	-1.931932
H	0.585096	-0.687439	-2.661560
H	-1.143370	-0.510941	-2.412488
C	0.029039	0.112829	-0.721655
C	0.351336	1.487505	-1.351687
H	-0.475937	1.781054	-2.008076
H	1.231090	1.346311	-2.002934
N	0.553593	2.537189	-0.374556
H	1.288185	2.253616	0.262684
C	0.908823	3.797807	-1.005876
H	1.127003	4.542295	-0.240323
H	1.774730	3.726547	-1.681925
H	0.060613	4.160569	-1.591784
C	-0.320793	-2.305031	-1.622734
H	0.543008	-2.768152	-1.154165
C	-1.386623	-3.047178	-1.905736

H	-2.269592	-2.611661	-2.359954
H	-1.413750	-4.107037	-1.685483
C	1.255911	-0.287866	0.103161
C	2.387778	-0.834449	-0.511546
C	1.329074	-0.000283	1.470714
C	3.542345	-1.105440	0.215834
H	2.375892	-1.054477	-1.571957
C	2.485376	-0.265521	2.199611
H	0.469737	0.434251	1.965322
C	3.596216	-0.824052	1.577113
H	4.400722	-1.536642	-0.284425
H	2.513573	-0.034326	3.257395
H	4.493991	-1.035815	2.144045
C	-1.249659	0.130877	0.116394
C	-2.157029	1.191175	0.072761
C	-1.577753	-0.982964	0.898792
C	-3.358523	1.133410	0.775135
H	-1.914471	2.087116	-0.479550
C	-2.773771	-1.040728	1.604401
H	-0.883962	-1.811172	0.960475
C	-3.674392	0.018346	1.541583
H	-4.042771	1.971748	0.728090
H	-3.000972	-1.914822	2.202317
H	-4.607186	-0.023038	2.090192

cat1_am3_bts

SCF energy in solution: –1451.296286

Enthalpy in solution: –1450.563416

Free energy in solution: –1450.661303

Cartesian coordinates

Atom	X	Y	Z
C	4.921224	0.460099	0.160861
H	5.951984	0.478586	0.465707
C	4.007350	1.443468	-0.052868
C	4.697150	-2.135064	0.005130
H	4.721206	-2.420478	1.060607
H	5.705371	-2.241438	-0.398340
C	2.227903	-2.709286	-0.465204
N	1.955529	-1.288246	-0.719178
B	1.573074	1.711023	-0.544989
C	3.757853	2.925390	0.013344
H	4.037630	3.376918	-0.944470
H	4.336732	3.424170	0.794386
N	2.849452	0.843487	-0.478530
C	2.986110	-0.475997	-0.490331
N	0.492276	0.685010	0.122549
C	0.698591	0.349324	1.542021
H	0.255498	-0.619517	1.774885
H	1.767492	0.292380	1.745774
H	0.251160	1.090608	2.205002
C	-0.897742	1.076248	-0.152096
H	-1.168515	1.918092	0.495233
H	-0.919141	1.446681	-1.169238
C	-1.991071	-0.029746	-0.043303
C	-1.456297	-1.282192	-0.776395
H	-0.927170	-0.964958	-1.679467
N	4.263699	-0.758098	-0.134189
C	1.175197	1.968294	-2.098037
H	0.880183	1.036376	-2.595182
H	0.378769	2.701715	-2.252589
H	2.052831	2.343273	-2.633627
C	2.203075	3.072078	0.234011
C	3.712616	-3.002486	-0.785240
H	3.868511	-2.822269	-1.852247
H	3.922978	-4.055380	-0.587019
C	1.919103	-3.070818	0.994178
H	0.855309	-2.929751	1.197831
H	2.169448	-4.115247	1.198687
H	2.474934	-2.433863	1.685582
C	1.366789	-3.556719	-1.401363
H	0.305407	-3.391418	-1.212605
H	1.574106	-3.289463	-2.438728
H	1.576932	-4.619392	-1.258061
C	1.969257	3.159109	1.748738
H	2.426411	4.073254	2.145297
H	0.903765	3.199696	1.987626
H	2.409033	2.317724	2.287186
C	1.725997	4.393622	-0.374598
H	2.228918	5.248745	0.091798
H	1.914097	4.437885	-1.448465
H	0.650437	4.522412	-0.221177
C	-2.325687	-0.313644	1.425806
C	-2.264900	-1.588119	1.994315
C	-2.707464	0.747114	2.258437
C	-2.550520	-1.792318	3.343635
H	-1.981590	-2.443338	1.395673
C	-2.994009	0.548984	3.603040
H	-2.800410	1.743129	1.842439
C	-2.911747	-0.726266	4.156529
H	-2.487777	-2.792545	3.754354
H	-3.283645	1.391975	4.218279
H	-3.131336	-0.884752	5.204729
C	-3.240134	0.463442	-0.802891

C	-3.118820	0.860843	-2.141521
C	-4.520153	0.450136	-0.245749
C	-4.224774	1.262281	-2.879189
H	-2.152017	0.843381	-2.630563
C	-5.632217	0.850632	-0.984189
H	-4.660618	0.121556	0.774654
C	-5.490891	1.266376	-2.301090
H	-4.095919	1.567015	-3.910375
H	-6.611275	0.832276	-0.521236
H	-6.354328	1.580868	-2.873886
H	0.986644	-0.465945	-0.415692
C	-2.505371	-2.292285	-1.156554
H	-3.300189	-2.479690	-0.440290
C	-2.505722	-2.948678	-2.312656
H	-1.742921	-2.766360	-3.062400
H	-3.269211	-3.678943	-2.548792
H	-0.695966	-1.747094	-0.141523

cat1_am3_c

SCF energy in solution: –1451.321339

Enthalpy in solution: –1450.584397

Free energy in solution: –1450.682772

Cartesian coordinates

Atom	X	Y	Z
C	-4.744134	1.446987	-0.027429
H	-5.757052	1.764094	-0.197502
C	-3.560921	2.114757	-0.022989
C	-5.316246	-1.048786	0.290952
H	-5.590611	-1.316253	-0.732266
H	-6.227545	-0.792363	0.832090
C	-3.143590	-2.383687	0.487860
N	-2.440981	-1.124177	0.763664
B	-1.084177	1.826588	0.254153
C	-2.980763	3.488395	-0.188646
H	-3.049042	4.017988	0.767472
H	-3.517550	4.083291	-0.933148
N	-2.561375	1.207669	0.259463
C	-3.101472	0.019575	0.438613
N	-0.169636	0.743630	-0.388877
C	-0.572876	0.161346	-1.668925
H	-0.295554	-0.893492	-1.749276
H	-1.655828	0.228357	-1.783709
H	-0.123547	0.673539	-2.530623
C	1.246911	1.062167	-0.356981
H	1.610542	1.334580	-1.360540
H	1.381732	1.936988	0.280233
C	2.203408	-0.047098	0.200132
C	1.892664	-0.198365	1.710457
H	2.037414	0.782217	2.170549
H	-1.449508	-1.056852	0.535387
N	-4.437853	0.110053	0.271846
C	-0.712190	2.106780	1.815142
H	-0.714285	1.177556	2.392762
H	0.256925	2.588404	1.973117
H	-1.459396	2.765427	2.271529
C	-1.485162	3.247507	-0.561572
C	-4.587135	-2.198484	0.987197
H	-4.549381	-2.002470	2.061364
H	-5.143888	-3.123609	0.828620
C	-3.100339	-2.719214	-1.007423
H	-2.065942	-2.872597	-1.322258
H	-3.667278	-3.629682	-1.215880
H	-3.511869	-1.905110	-1.607839
C	-2.467363	-3.483144	1.299813
H	-1.421156	-3.576644	1.004178
H	-2.506821	-3.247854	2.363892
H	-2.958790	-4.441736	1.124452
C	-1.401056	3.131393	-2.088424
H	-1.696408	4.075240	-2.563201
H	-0.381118	2.905652	-2.408040
H	-2.055780	2.348819	-2.479394
C	-0.640717	4.451527	-0.139127
H	-0.964473	5.366996	-0.649059
H	-0.694870	4.628577	0.936610
H	0.410720	4.291075	-0.397481
C	1.943833	-1.322663	-0.594000
C	1.165270	-2.375439	-0.108805
C	2.412349	-1.409454	-1.911491
C	0.857908	-3.472795	-0.914437
H	0.791362	-2.349306	0.906563
C	2.098923	-2.493471	-2.720202
H	3.025282	-0.606294	-2.303400
C	1.314264	-3.533304	-2.225657
H	0.266896	-4.287274	-0.511248
H	2.467841	-2.528525	-3.737914
H	1.073901	-4.384267	-2.850754
C	3.665933	0.387609	0.055862
C	4.041894	1.729678	-0.043607
C	4.685859	-0.571367	0.091755
C	5.384332	2.098186	-0.114325
H	3.294721	2.510524	-0.071540
C	6.024454	-0.208153	0.023350
H	4.422841	-1.619245	0.165811

C	6.382013	1.133139	-0.082705
H	5.643965	3.146570	-0.197410
H	6.789175	-0.974852	0.052601
H	7.424733	1.420098	-0.140138
C	2.719120	-1.203126	2.461136
H	2.696870	-2.232594	2.114765
C	3.467127	-0.900160	3.517657
H	3.531163	0.117504	3.886432
H	4.042376	-1.653992	4.040626
H	0.825241	-0.423668	1.801029

cat1_am3_d$_S$

SCF energy in solution: –1451.316366

Enthalpy in solution: –1450.579471

Free energy in solution: –1450.679365

Cartesian coordinates

Atom	X	Y	Z
C	4.779789	1.209408	0.453813
H	5.769935	1.468737	0.782083
C	3.616802	1.911221	0.398303
C	5.332478	-1.252322	-0.110180
H	5.499513	-1.631472	0.900935
H	6.298852	-0.976977	-0.533990
C	3.150838	-2.472592	-0.662011
N	2.530395	-1.165055	-0.902217
B	1.177457	1.728033	-0.189375
N	2.643623	1.081622	-0.114813
C	3.179069	-0.091213	-0.376610
N	0.204756	0.562061	0.168187
C	0.399946	-0.118160	1.443332
H	0.111347	-1.171871	1.383289
H	1.454001	-0.081784	1.723465
H	-0.180022	0.313135	2.269186
C	-1.187760	0.872952	-0.100013
H	-1.598285	1.569869	0.652473
H	-1.204798	1.382809	-1.061090
C	-2.187706	-0.313150	-0.227060
C	-1.626782	-1.333957	-1.245266
H	-0.650598	-1.684033	-0.898077
H	-2.297568	-2.198685	-1.278778
C	-1.501072	-0.788731	-2.639132
H	-2.409776	-0.381565	-3.073685
C	-0.384200	-0.805069	-3.359202
H	0.548145	-1.185495	-2.955422
H	-0.359632	-0.417264	-4.369984
H	1.522363	-1.053782	-0.782194
N	4.487705	-0.069204	-0.050185
C	3.035558	3.264948	0.680586
H	3.494867	3.746522	1.548407
H	3.209254	3.911228	-0.186310
C	0.972156	2.250009	-1.716390
H	0.084451	2.873261	-1.857183
H	1.826373	2.860814	-2.028746
H	0.896115	1.411270	-2.413532
C	1.504098	3.013840	0.862185
C	4.645816	-2.302389	-0.987926
H	5.155940	-3.259041	-0.862700
H	4.728659	-2.006295	-2.036230
C	2.943653	-2.929733	0.786831
H	1.880101	-3.081403	0.980916
H	3.466809	-3.870502	0.973179
H	3.305070	-2.181669	1.495107
C	2.523087	-3.472051	-1.627280
H	1.447516	-3.544073	-1.448246
H	2.679435	-3.153434	-2.658600
H	2.959143	-4.462567	-1.486790
C	1.265294	2.711592	2.347204
H	1.533968	3.580346	2.960981
H	0.214810	2.484616	2.540293
H	1.861966	1.866562	2.698688
C	0.731310	4.289774	0.519912
H	1.005063	5.114443	1.189302
H	0.918431	4.612635	-0.505696
H	-0.345696	4.127357	0.625287
C	-2.484111	-0.965708	1.130870
C	-3.076603	-0.186239	2.131368
C	-2.230638	-2.308277	1.416983
C	-3.376028	-0.717555	3.378772
H	-3.323280	0.847423	1.918366
C	-2.534652	-2.847783	2.665920
H	-1.776032	-2.948641	0.672336
C	-3.102702	-2.055158	3.654933
H	-3.831559	-0.088495	4.133779
H	-2.324566	-3.892503	2.861270
H	-3.338162	-2.473751	4.625403
C	-3.544304	0.195432	-0.754687
C	-4.598816	-0.721405	-0.859955
C	-3.786271	1.512907	-1.147773
C	-5.838574	-0.345738	-1.357259
H	-4.446364	-1.741553	-0.526383
C	-5.034575	1.895663	-1.639857
H	-3.010995	2.262317	-1.075089
C	-6.063393	0.971173	-1.752830

H	-6.632873	-1.078768	-1.428356
H	-5.194499	2.925297	-1.935750
H	-7.030305	1.270719	-2.137330

cat1_am3_ets$_S$

SCF energy in solution: –1451.276191

Enthalpy in solution: –1450.542699

Free energy in solution: –1450.638629

Cartesian coordinates

Atom	X	Y	Z
C	4.435585	1.870628	0.794882
H	5.255701	2.428193	1.209900
C	3.148003	2.195977	0.551762
C	5.790137	-0.268381	0.382777
H	5.955231	-0.678582	1.382399
H	6.640119	0.368590	0.134457
C	4.275890	-2.094062	-0.524240
N	3.217742	-1.098393	-0.653065
B	0.977412	1.454881	-0.363588
N	2.496313	1.090661	0.010989
C	3.397253	0.106987	-0.121301
N	-0.012404	0.222684	-0.092625
C	0.367987	-0.639323	1.039442
H	0.889912	-1.512390	0.633254
H	1.037200	-0.122231	1.721858
H	-0.509197	-0.971006	1.594149
C	-1.391135	0.718103	-0.008847
H	-1.568824	1.243674	0.925841
H	-1.493481	1.433810	-0.822244
C	-2.395957	-0.449678	-0.227834
C	-1.544150	-1.513168	-0.959343
H	-1.229035	-2.304018	-0.277549
H	-2.085805	-1.986624	-1.777558
C	-0.282596	-0.890114	-1.528099
H	-0.495773	-0.086489	-2.228724
C	0.784698	-1.758310	-1.873567
H	0.631344	-2.811127	-1.647567
H	1.253686	-1.578113	-2.836101
H	2.222791	-1.360349	-1.077942
N	4.586667	0.544422	0.371124
C	2.238335	3.375903	0.643785
H	2.452918	4.007826	1.510355
H	2.350112	3.994400	-0.252649
C	0.959041	1.904998	-1.922876
H	-0.030127	2.161554	-2.314760
H	1.585343	2.791081	-2.065026
H	1.373308	1.121406	-2.562964
C	0.817116	2.754351	0.696198
C	5.633341	-1.381454	-0.650345
H	6.443441	-2.103693	-0.531876
H	5.700626	-0.952374	-1.653065
C	4.154173	-2.814457	0.825852
H	3.206025	-3.353239	0.863966
H	4.969588	-3.529037	0.965319
H	4.164414	-2.102123	1.653273
C	4.118383	-3.097417	-1.664346
H	3.133690	-3.564150	-1.617613
H	4.211481	-2.594026	-2.627786
H	4.881262	-3.875038	-1.590834
C	0.582822	2.396710	2.175617
H	0.517836	3.315277	2.770365
H	-0.335019	1.833536	2.351478
H	1.412642	1.811022	2.580088
C	-0.203856	3.816715	0.278796
H	-0.080880	4.726715	0.877770
H	-0.090220	4.089976	-0.772275
H	-1.231344	3.475608	0.428095
C	-3.001754	-0.952850	1.094536
C	-3.499441	-0.032423	2.024412
C	-3.162809	-2.311297	1.374669
C	-4.094049	-0.450799	3.207890
H	-3.443776	1.028815	1.812286
C	-3.763699	-2.735115	2.558446
H	-2.826897	-3.057537	0.666779
C	-4.222761	-1.808909	3.485850
H	-4.464053	0.285861	3.910399
H	-3.871228	-3.795617	2.750709
H	-4.685120	-2.138310	4.407749
C	-3.604852	0.004919	-1.063176
C	-4.446177	-0.958472	-1.630389
C	-3.963967	1.346824	-1.203566
C	-5.579610	-0.595933	-2.345685
H	-4.220392	-2.009409	-1.494409
C	-5.103192	1.714951	-1.917283
H	-3.366112	2.128555	-0.752163
C	-5.911404	0.747744	-2.499316
H	-6.207609	-1.364376	-2.779421
H	-5.353511	2.764110	-2.015417
H	-6.793686	1.033929	-3.057782

cat1_am3_f$_S$

SCF energy in solution: –1451.328943

Enthalpy in solution: –1450.588848

Free energy in solution: –1450.685752

Cartesian coordinates

Atom	X	Y	Z
C	-4.474115	0.437898	0.645106
H	-5.463708	0.610321	1.029904
C	-3.691797	-0.658162	0.636281
C	-4.176694	2.787701	-0.324930
H	-4.163455	3.455929	0.542059
H	-5.207029	2.725118	-0.682983
C	-1.773480	3.065123	-1.064209
N	-1.500848	1.644273	-0.855487
B	-1.632949	-1.597220	-0.350777
C	-3.703043	-2.063306	1.131348
H	-4.686710	-2.533942	1.050662
H	-3.432037	-2.078975	2.193874
N	-2.485672	-0.352998	0.015129
C	-2.488146	0.976995	-0.329805
N	-3.725243	1.462681	0.046602
C	-1.366276	-1.589204	-1.948458
H	-1.013917	-0.606202	-2.268125
H	-0.682222	-2.344108	-2.341448
H	-2.321360	-1.738022	-2.454462
C	-2.629382	-2.814231	0.284994
C	-3.252783	3.303989	-1.424272
H	-3.465669	2.767400	-2.352945
H	-3.440742	4.366681	-1.593458
C	-1.405737	3.857843	0.201476
H	-0.329348	3.789695	0.372487
H	-1.670747	4.914863	0.101350
H	-1.913567	3.449683	1.078090
C	-0.896092	3.535040	-2.222600
H	0.148564	3.311776	-1.995841
H	-1.165197	2.999747	-3.134624
H	-1.000401	4.609856	-2.392828
C	-2.074263	-3.947611	1.161729
H	-2.900329	-4.594207	1.478577
H	-1.360975	-4.583603	0.634908
H	-1.601071	-3.581774	2.076224
C	-3.372494	-3.485148	-0.883787
H	-4.061140	-4.249145	-0.506414
H	-3.960265	-2.757660	-1.448015
H	-2.681207	-3.966625	-1.579704
C	0.766608	-2.578031	0.718624
C	2.123894	-1.943440	1.086555
H	2.937862	-2.611140	0.814354
H	2.204439	-1.789182	2.161586
C	2.175460	-0.563835	0.356060
C	0.769113	-0.483640	-0.288040
H	0.836722	-0.897398	-1.288632
H	0.309948	0.498095	-0.388544
N	-0.135465	-1.389676	0.485892
C	-0.453289	-0.793757	1.814024
H	-0.856733	0.202154	1.664259
H	-1.205471	-1.414642	2.296213
H	0.434558	-0.732360	2.438593
H	0.358663	-3.143874	1.552770
C	0.895519	-3.492938	-0.493227
H	-0.071748	-3.839247	-0.847516
H	1.413564	-3.002771	-1.318037
H	1.488252	-4.360963	-0.196699
C	3.194945	-0.459651	-0.789599
C	3.330476	0.783587	-1.420923
C	3.936117	-1.530416	-1.288420
C	4.176168	0.950004	-2.508827
H	2.768218	1.630744	-1.045592
C	4.793191	-1.363478	-2.376329
H	3.859778	-2.515035	-0.848361
C	4.917282	-0.125878	-2.991718
H	4.258680	1.922306	-2.978395
H	5.361051	-2.211232	-2.739562
H	5.581715	0.001493	-3.836932
C	2.489658	0.555740	1.354892
C	3.671823	0.457501	2.097115
C	1.687101	1.683098	1.530775
C	4.033845	1.444931	3.003472
H	4.319887	-0.399419	1.945271
C	2.050077	2.676332	2.440401
H	0.769859	1.802230	0.967338
C	3.219274	2.561494	3.181010
H	4.953956	1.347505	3.566407
H	1.408513	3.540576	2.564607
H	3.498405	3.334214	3.886207

am4

SCF energy in solution: –522.306742

Enthalpy in solution: –522.023508

Free energy in solution: –522.079776

Cartesian coordinates

Atom	X	Y	Z
C	-4.010651	-0.358097	-0.341095
H	-4.161113	-1.269586	0.244529
H	-4.059330	-0.642844	-1.398405

C	-2.624141	0.227140	-0.052859
H	-2.476214	1.148666	-0.622042
H	-2.564523	0.494841	1.007194
C	-1.502031	-0.741624	-0.401449
H	-1.558252	-0.994265	-1.465822
H	-1.641362	-1.685652	0.153390
N	-0.203128	-0.133798	-0.155659
C	-5.105386	0.622347	-0.034672
H	-5.081378	1.554098	-0.595321
C	-6.057708	0.433194	0.872374
H	-6.107740	-0.482872	1.450938
H	-6.816601	1.181301	1.063585
H	-0.141191	0.146720	0.817323
C	0.901985	-1.033206	-0.452762
H	0.844000	-1.280710	-1.518808
H	0.837819	-1.989222	0.092125
C	2.235014	-0.384231	-0.158815
C	3.287794	-1.131722	0.366854
C	2.433996	0.971423	-0.426738
C	4.523585	-0.540942	0.613983
H	3.136831	-2.182817	0.587754
C	3.666489	1.564465	-0.175543
H	1.607702	1.548534	-0.822022
C	4.715589	0.810095	0.343582
H	5.332162	-1.133518	1.023990
H	3.809308	2.617456	-0.385555
H	5.674558	1.273414	0.539602

cat1_am4_a

SCF energy in solution: –1220.230117

Enthalpy in solution: –1219.578447

Free energy in solution: –1219.670396

Cartesian coordinates

Atom	X	Y	Z
C	4.077468	1.013747	0.341494
H	5.105124	1.242889	0.561494
C	2.956944	1.766210	0.363877
C	4.525031	-1.402062	-0.407288
H	4.808472	-1.959197	0.490873
H	5.440795	-1.032725	-0.874242
C	2.299881	-2.529731	-0.892163
N	1.575907	-1.266702	-0.737521
B	0.608075	1.774862	-0.265382
C	2.499942	3.186255	0.537771
H	2.772740	3.762033	-0.353098
H	2.955073	3.684219	1.398502
N	1.889755	0.968478	-0.015040
C	2.326540	-0.283721	-0.318186
N	-0.629739	0.768326	0.186283
C	-0.518664	0.018625	1.478034
H	0.496743	-0.369433	1.522266
H	-0.672633	0.722800	2.290420
C	-1.970026	1.410324	0.023518
H	-2.487358	1.363714	0.983114
H	-1.809253	2.459750	-0.222010
N	3.681914	-0.275388	-0.065387
C	0.383849	2.045994	-1.847847
H	0.374904	1.106603	-2.411545
H	-0.520317	2.607654	-2.103252
H	1.229793	2.626799	-2.227926
C	0.942140	3.113880	0.656095
C	3.745257	-2.288033	-1.377565
H	3.695821	-1.793197	-2.351538
H	4.268207	-3.238717	-1.504409
C	2.317704	-3.288095	0.445307
H	1.297061	-3.529279	0.747749
H	2.886141	-4.219992	0.367894
H	2.758818	-2.674018	1.233342
C	1.568257	-3.366196	-1.940199
H	0.536034	-3.536351	-1.626128
H	1.548013	-2.834487	-2.892851
H	2.051731	-4.336210	-2.080958
C	0.599207	2.963528	2.143927
H	0.937908	3.842722	2.703099
H	-0.481010	2.881653	2.302514
H	1.084771	2.087822	2.581761
C	0.332232	4.424164	0.152674
H	0.733571	5.280199	0.706923
H	0.539999	4.583059	-0.907056
H	-0.753692	4.437947	0.286729
C	-2.813320	0.738558	-1.052028
H	-2.983137	-0.308231	-0.787488
H	-2.264903	0.756811	-1.998961
C	-4.159614	1.451323	-1.221086
H	-4.721650	1.407414	-0.283813
H	-3.974167	2.509108	-1.440663
C	-4.977002	0.845955	-2.325519
H	-4.534207	0.875293	-3.318315
C	-6.165992	0.277980	-2.157064
H	-6.631227	0.229485	-1.178643
H	-6.710995	-0.153904	-2.986724
C	-1.527719	-1.101563	1.541843
C	-2.611892	-1.049194	2.415949

C	-1.388925	-2.198848	0.686754
C	-3.552734	-2.076667	2.435470
H	-2.717794	-0.204438	3.088708
C	-2.329123	-3.222151	0.704059
H	-0.535328	-2.223971	0.016077
C	-3.413445	-3.162749	1.578249
H	-4.391150	-2.027693	3.119093
H	-2.214841	-4.069053	0.038360
H	-4.144561	-3.961455	1.591689
H	-0.514714	0.041877	-0.528896

cat1_am4_bts

SCF energy in solution: –1220.201132

Enthalpy in solution: –1219.55532

Free energy in solution: –1219.645213

Cartesian coordinates

Atom	X	Y	Z
C	3.992045	0.925374	0.592895
H	4.992485	1.020071	0.973987
C	2.941163	1.787239	0.536117
C	4.241954	-1.522270	-0.285245
H	4.348834	-2.124013	0.621086
H	5.240339	-1.290200	-0.659646
C	1.918385	-2.336459	-1.021267
N	1.398159	-0.962800	-0.942046
B	0.628004	1.904189	-0.361396
C	2.468943	3.191750	0.818119
H	2.830696	3.854520	0.025487
H	2.837063	3.587389	1.767998
N	1.907584	1.122623	-0.065566
C	2.252780	-0.115052	-0.380813
N	-0.504687	0.715907	-0.286793
C	-0.733053	0.180644	1.061728
H	0.235100	0.155152	1.566471
H	-1.370889	0.857798	1.637575
C	-1.741313	1.269482	-0.900801
H	-1.888172	2.271238	-0.472216
H	-1.537445	1.412902	-1.960846
H	0.262040	-0.289103	-0.816309
N	3.541336	-0.284883	0.007969
C	0.694951	2.458613	-1.888645
H	0.713261	1.633918	-2.609599
H	-0.118735	3.132841	-2.166669
H	1.626565	3.016817	-2.026211
C	0.889931	3.126851	0.777474
C	3.429522	-2.264713	-1.352330
H	3.543328	-1.748922	-2.309483
H	3.825618	-3.276414	-1.460872
C	1.726081	-3.082520	0.308563
H	0.669135	-3.257169	0.501438
H	2.241902	-4.047097	0.284504
H	2.123457	-2.496857	1.140588
C	1.210652	-3.077672	-2.150958
H	0.140735	-3.137639	-1.950281
H	1.359787	-2.554190	-3.096595
H	1.597145	-4.095319	-2.240423
C	0.424817	2.853142	2.215155
H	0.742151	3.671170	2.872288
H	-0.663845	2.791731	2.283114
H	0.847639	1.930742	2.619780
C	0.343383	4.497399	0.369997
H	0.660348	5.275242	1.074545
H	0.681826	4.788298	-0.625629
H	-0.750661	4.493169	0.361202
C	-3.071175	0.527973	-0.763638
H	-3.295600	0.282485	0.276059
H	-3.060159	-0.413114	-1.315149
C	-4.198129	1.413276	-1.316869
H	-4.264672	2.338207	-0.736914
H	-3.951765	1.697426	-2.346755
C	-5.523336	0.709091	-1.294188
H	-5.586578	-0.208895	-1.874178
C	-6.584975	1.119163	-0.608523
H	-6.554016	2.027579	-0.016750
H	-7.515302	0.565628	-0.617413
C	-1.321878	-1.218970	1.144979
C	-1.628264	-1.718838	2.413022
C	-1.545406	-2.037758	0.040864
C	-2.141368	-3.000345	2.575338
H	-1.457805	-1.092966	3.283246
C	-2.071079	-3.318699	0.195709
H	-1.302233	-1.676566	-0.949121
C	-2.367405	-3.807435	1.463139
H	-2.368801	-3.367429	3.568526
H	-2.240397	-3.936794	-0.678172
H	-2.772484	-4.804114	1.584438

cat1_am4_c

SCF energy in solution: –1220.234562

Enthalpy in solution: –1219.584804

Free energy in solution: –1219.677354

Cartesian coordinates

Atom	X	Y	Z
C	3.575311	1.936809	0.463856
H	4.488772	2.385369	0.810424
C	2.316306	2.419174	0.322217
C	4.603003	-0.377337	0.023590
H	4.761913	-0.744352	1.040390
H	5.521217	0.105643	-0.311977
C	2.777602	-2.001962	-0.689870
N	1.902782	-0.844321	-0.925483
B	-0.008719	1.912437	-0.458200
C	1.558335	3.702720	0.451800
H	1.733581	4.306000	-0.445326
H	1.878706	4.293977	1.314942
N	1.510459	1.405287	-0.170644
C	2.268734	0.338496	-0.365464
N	-1.012362	0.778432	-0.110333
C	-0.821211	-0.010581	1.088571
H	0.186181	0.158884	1.482395
H	-1.507929	0.290402	1.897025
C	-2.396569	1.224679	-0.244903
H	-2.727217	1.755591	0.667182
H	-2.442799	1.953694	-1.055734
H	0.904257	-1.010678	-0.911479
N	3.533770	0.608917	0.023265
C	-0.054530	2.266825	-2.046552
H	0.087807	1.357535	-2.639803
H	-0.992890	2.721992	-2.373554
H	0.741500	2.965960	-2.325747
C	0.068471	3.273367	0.523150
C	4.216236	-1.513338	-0.919706
H	4.297090	-1.168473	-1.953211
H	4.906669	-2.347092	-0.781762
C	2.586298	-2.556247	0.726545
H	1.582084	-2.970012	0.832612
H	3.312942	-3.346979	0.929659
H	2.705326	-1.771615	1.477482
C	2.430656	-3.066835	-1.724587
H	1.393277	-3.382540	-1.601206
H	2.564203	-2.674299	-2.733415
H	3.071117	-3.940711	-1.591481
C	-0.247133	2.971601	1.994434
H	-0.146916	3.877632	2.604669
H	-1.267202	2.603001	2.117058
H	0.432064	2.221750	2.410254
C	-0.823771	4.426172	0.060572
H	-0.675378	5.318727	0.680866
H	-0.616700	4.699096	-0.976440
H	-1.880101	4.153707	0.129211
C	-3.432411	0.137456	-0.536476
H	-3.425455	-0.628907	0.242763
H	-3.179901	-0.361163	-1.477094
C	-4.841589	0.735119	-0.636328
H	-5.114336	1.207221	0.312038
H	-4.835361	1.524929	-1.397212
C	-5.868051	-0.297995	-0.997635
H	-5.710932	-0.812997	-1.943010
C	-6.912696	-0.628541	-0.245611
H	-7.097011	-0.139335	0.704664
H	-7.614354	-1.393955	-0.552579
C	-0.963082	-1.520922	0.917198
C	-0.902950	-2.342709	2.046914
C	-1.109427	-2.121510	-0.332263
C	-0.973105	-3.726084	1.931137
H	-0.798068	-1.887244	3.026684
C	-1.185314	-3.509170	-0.453704
H	-1.184346	-1.475136	-1.199780
C	-1.109818	-4.317484	0.675557
H	-0.924263	-4.345048	2.819020
H	-1.312006	-3.956443	-1.432931
H	-1.170260	-5.394744	0.583113

cat1_am4_d$_S$

SCF energy in solution: –1220.23231

Enthalpy in solution: –1219.5822

Free energy in solution: –1219.671999

Cartesian coordinates

Atom	X	Y	Z
C	-2.544313	2.896545	0.101336
H	-3.154898	3.762713	0.281895
C	-2.804835	1.566212	0.150935
C	-0.407537	4.222801	-0.445375
H	-0.121572	4.605415	0.537202
H	-1.017189	4.978435	-0.941803
C	1.530651	2.609441	-0.803598
N	0.546978	1.522626	-0.913282
B	-1.865829	-0.717143	-0.259209
N	-1.645810	0.883576	-0.175454
C	-0.707757	1.771498	-0.458077
N	-0.586071	-1.440342	0.258446
C	0.026924	-0.946942	1.481234
H	-0.379567	0.041709	1.715633
H	-0.229209	-1.578668	2.346385
C	-0.783628	-2.892636	0.309055

H	-1.181434	-3.175976	1.297616
H	-1.557857	-3.159315	-0.414103
C	0.437479	-3.786009	0.034122
H	1.327609	-3.374616	0.513024
H	0.248369	-4.753743	0.509269
C	0.708333	-4.063110	-1.455244
H	1.509029	-4.802260	-1.549945
H	-0.196999	-4.517963	-1.876288
C	1.056503	-2.856285	-2.277015
H	0.330489	-2.050055	-2.266522
C	2.174685	-2.732214	-2.988495
H	2.919955	-3.520671	-3.008240
H	0.866256	0.579141	-0.726089
N	-1.203674	3.015653	-0.286630
C	-3.947065	0.619058	0.353961
H	-4.628597	0.945382	1.145189
H	-4.524537	0.562091	-0.574709
C	-2.135396	-1.013585	-1.839929
H	-2.253844	-2.071247	-2.091594
H	-3.041499	-0.507513	-2.190659
H	-1.309160	-0.626055	-2.445508
C	-3.279238	-0.752024	0.654243
C	0.821726	3.885535	-1.286535
H	1.521647	4.722012	-1.251394
H	0.518550	3.734982	-2.325389
C	2.033677	2.756194	0.637130
H	2.606428	1.873943	0.926018
H	2.676217	3.635629	0.729020
H	1.201187	2.857232	1.337340
C	2.690007	2.282292	-1.738406
H	3.159156	1.344843	-1.434382
H	2.334688	2.183288	-2.764876
H	3.442274	3.071869	-1.692730
C	-3.036211	-0.812628	2.168628
H	-3.989328	-0.794304	2.711189
H	-2.514336	-1.728069	2.453660
H	-2.444161	0.036077	2.522006
C	-4.237221	-1.884382	0.279146
H	-5.191049	-1.791334	0.812846
H	-4.450369	-1.892418	-0.791859
H	-3.812920	-2.856643	0.542641
H	2.377164	-1.845084	-3.576813
C	1.544347	-0.786063	1.488987
C	2.339956	-0.996627	0.365359
C	2.164491	-0.366013	2.670542
C	3.719931	-0.795346	0.416897
H	1.877574	-1.349582	-0.547256
C	3.537312	-0.156473	2.725629
H	1.557996	-0.201160	3.555888
C	4.324678	-0.368332	1.593602
H	4.316588	-0.985812	-0.468201
H	3.996138	0.169454	3.651403
H	5.395404	-0.212033	1.635839

cat1_am4_ets$_S$

SCF energy in solution: –1220.184098

Enthalpy in solution: –1219.536964

Free energy in solution: –1219.621784

Cartesian coordinates

Atom	X	Y	Z
C	-3.247707	1.515416	-1.357525
H	-4.009869	1.927449	-1.993994
C	-2.135869	2.051331	-0.810777
C	-4.307454	-0.812254	-1.206099
H	-4.138011	-1.236388	-2.199113
H	-5.283530	-0.325094	-1.208936
C	-2.806647	-2.357545	0.134577
N	-2.013149	-1.194872	0.516673
B	-0.186276	1.704629	0.671669
N	-1.478197	1.074786	-0.066292
C	-2.222702	-0.041458	-0.112703
N	1.043825	0.654885	0.747717
C	1.048194	-0.267630	-0.418659
H	0.361553	-1.071768	-0.142617
H	0.623309	0.255423	-1.273339
C	2.299600	1.387731	0.998961
H	2.705225	1.826997	0.088310
H	2.039831	2.207955	1.668683
C	3.320277	0.467845	1.690041
H	4.017772	0.048424	0.965960
H	3.902463	1.051369	2.404986
C	2.518588	-0.645268	2.374811
H	2.729760	-1.612780	1.922666
H	2.770054	-0.729632	3.434424
C	1.026264	-0.362187	2.295593
H	0.759907	0.477315	2.928204
C	0.107757	-1.448630	2.315057
H	0.549545	-2.440573	2.242104
H	-1.117219	-1.302728	1.178803
N	-3.294479	0.188260	-0.916949
C	-1.451111	3.372994	-0.718207
H	-1.532802	3.955662	-1.640215
H	-1.905326	3.962413	0.084506

C	-0.681683	2.173366	2.146402
H	0.107343	2.582086	2.785479
H	-1.437670	2.958788	2.052878
H	-1.155213	1.350961	2.689285
C	0.018327	3.021858	-0.365316
C	-4.248653	-1.893860	-0.129999
H	-4.862712	-2.743226	-0.435695
H	-4.653645	-1.496390	0.803634
C	-2.199824	-3.019174	-1.110695
H	-1.196878	-3.380696	-0.876145
H	-2.808344	-3.864328	-1.443115
H	-2.110439	-2.304787	-1.931616
C	-2.790273	-3.338396	1.304648
H	-1.762708	-3.615631	1.543982
H	-3.234494	-2.879822	2.189452
H	-3.349457	-4.240878	1.050233
C	0.706362	2.748693	-1.712856
H	0.720646	3.666923	-2.311323
H	1.741551	2.428231	-1.598978
H	0.175002	1.992654	-2.297263
C	0.682472	4.250014	0.265570
H	0.564500	5.125138	-0.384345
H	0.242756	4.492993	1.234916
H	1.754798	4.100981	0.408495
H	-0.671099	-1.381630	3.070563
C	2.350420	-0.904152	-0.853139
C	2.622024	-2.230781	-0.510377
C	3.260029	-0.233412	-1.675557
C	3.795417	-2.852964	-0.924076
H	1.900665	-2.771215	0.092547
C	4.437559	-0.848428	-2.088391
H	3.041731	0.775156	-2.004457
C	4.713945	-2.157749	-1.704762
H	3.990086	-3.880047	-0.640682
H	5.134297	-0.308624	-2.717812
H	5.630124	-2.637395	-2.025998

cat1_am4_f$_S$

SCF energy in solution: –1220.23405

Enthalpy in solution: –1219.58083

Free energy in solution: –1219.66729

Cartesian coordinates

Atom	X	Y	Z
C	-2.573526	0.937486	-2.217489
H	-3.049044	1.114849	-3.166014
C	-1.505379	1.508093	-1.628786
C	-4.232274	-0.852588	-1.448290
H	-4.074004	-1.695088	-2.129525
H	-5.032229	-0.234169	-1.862616
C	-3.363666	-1.894917	0.689877
N	-2.320652	-0.880167	0.812439
B	-0.262336	1.628805	0.504448
C	-0.471568	2.543100	-1.912360
H	-0.879641	3.415843	-2.429913
H	0.304453	2.127788	-2.566552
N	-1.296392	0.911993	-0.389236
C	-2.235802	-0.076354	-0.203640
N	-3.027698	-0.056820	-1.337734
C	-0.963053	1.942198	1.931487
H	-1.491163	1.055470	2.287607
H	-0.337497	2.323016	2.738564
H	-1.739572	2.689632	1.759667
C	0.125964	2.927002	-0.522384
C	-4.599144	-1.346536	-0.051549
H	-4.997443	-0.511456	0.531327
H	-5.375778	-2.111361	-0.126098
C	-2.796507	-3.117821	-0.048948
H	-1.964669	-3.528762	0.526992
H	-3.552434	-3.898701	-0.176090
H	-2.414148	-2.836742	-1.032744
C	-3.775251	-2.307383	2.101587
H	-2.894838	-2.650562	2.647754
H	-4.189725	-1.449241	2.633349
H	-4.517535	-3.109850	2.082034
C	1.567857	3.398618	-0.767893
H	1.555327	4.219557	-1.493571
H	2.053302	3.780269	0.131245
H	2.204495	2.619937	-1.195638
C	-0.657365	4.158307	-0.030841
H	-0.484990	5.008026	-0.700756
H	-1.731583	3.961372	-0.012313
H	-0.354438	4.454226	0.976220
C	2.379639	1.030236	1.243991
C	3.116242	-0.165340	1.883800
H	3.692334	0.180855	2.742699
H	3.810453	-0.629141	1.187164
C	2.009932	-1.157191	2.294718
H	2.207359	-2.142910	1.879846
H	1.944937	-1.264041	3.377564
C	0.704236	-0.555079	1.756165
H	0.183885	-0.031634	2.550391
H	-0.015371	-1.249970	1.327754
N	1.068860	0.477469	0.725593

C	1.250072	-0.152537	-0.633194
H	0.317274	-0.670567	-0.838495
H	1.327056	0.675887	-1.334322
H	2.924179	1.432565	0.393052
C	2.201596	2.122568	2.293410
H	1.575276	2.940895	1.953267
H	1.773343	1.714641	3.210402
H	3.191947	2.514121	2.534313
C	2.400905	-1.099374	-0.874958
C	3.602728	-0.636469	-1.416549
C	2.248317	-2.470013	-0.655704
C	4.651454	-1.513075	-1.673995
H	3.715671	0.419190	-1.639621
C	3.295013	-3.350493	-0.908503
H	1.298676	-2.844673	-0.288387
C	4.502740	-2.871703	-1.408707
H	5.579034	-1.138572	-2.088506
H	3.164032	-4.409953	-0.727422
H	5.316941	-3.556514	-1.609784

am5

SCF energy in solution: –330.528708

Enthalpy in solution: –330.302236

Free energy in solution: –330.350074

Cartesian coordinates

Atom	X	Y	Z
C	-0.714621	-0.487718	-0.129202
H	-0.814468	-1.569774	0.011649
H	-0.799217	-0.303783	-1.204875
C	0.654090	-0.031815	0.371483
H	0.731725	1.053345	0.252576
H	0.759783	-0.244953	1.439020
C	1.794621	-0.721987	-0.370885
H	1.720492	-0.475403	-1.445030
H	1.663541	-1.803782	-0.278421
N	3.098130	-0.380834	0.186202
H	3.783379	-1.031214	-0.174840
C	3.521271	0.972413	-0.143353
H	4.562911	1.106942	0.148872
H	3.423938	1.215450	-1.213352
H	2.930640	1.697284	0.418343
C	-1.866662	0.224826	0.589001
H	-1.768958	0.048711	1.666250
H	-1.786959	1.304380	0.431872
C	-3.209569	-0.253451	0.119169
H	-3.417770	-1.311273	0.264355
C	-4.122333	0.513481	-0.467664
H	-5.072153	0.114455	-0.800553
H	-3.944571	1.570966	-0.630568

cat1_am5_a

SCF energy in solution: –1028.4526

Enthalpy in solution: –1027.856623

Free energy in solution: –1027.9412

Cartesian coordinates

Atom	X	Y	Z
C	-3.876085	0.955989	-0.308722
H	-4.878411	1.240480	-0.575253
C	-2.763879	1.680569	-0.051970
C	-4.338045	-1.582478	-0.241221
H	-4.506567	-1.857757	-1.287180
H	-5.310794	-1.377053	0.210945
C	-2.126589	-2.794296	0.139016
N	-1.440839	-1.532924	0.410806
B	-0.400352	1.476079	0.558160
C	-2.252816	3.088262	0.063118
H	-2.488092	3.476480	1.060076
H	-2.696789	3.770005	-0.666975
N	-1.743160	0.803407	0.258886
C	-2.183347	-0.478049	0.204217
N	0.671374	0.417380	-0.164633
C	0.467822	0.109316	-1.601051
H	0.825558	-0.896527	-1.815028
H	-0.594136	0.158299	-1.820633
H	1.006695	0.831595	-2.209570
C	2.094871	0.683786	0.145244
H	2.365058	1.621201	-0.348569
H	2.164273	0.843097	1.219387
N	-3.510930	-0.397877	-0.152676
C	-0.063471	1.464624	2.141812
H	0.033598	0.445314	2.531614
H	0.825933	2.031230	2.431159
H	-0.906786	1.917589	2.671639
C	-0.697112	2.974818	-0.099578
C	-3.622851	-2.706057	0.511419
H	-3.689988	-2.511638	1.585260
H	-4.122427	-3.655600	0.305797
C	-1.969486	-3.153067	-1.347174
H	-0.908661	-3.268585	-1.578439
H	-2.484588	-4.086328	-1.593768
H	-2.363364	-2.356878	-1.983023
C	-1.468550	-3.876912	0.991546

H	-0.400309	-3.910925	0.769074
H	-1.586434	-3.640082	2.050203
H	-1.902296	-4.860394	0.793506
C	-0.386516	3.114272	-1.596380
H	-0.681433	4.108805	-1.948884
H	0.682507	3.007316	-1.801844
H	-0.930300	2.381895	-2.196592
C	-0.009866	4.128119	0.634279
H	-0.324589	5.096871	0.230421
H	-0.238209	4.118346	1.701434
H	1.077671	4.066938	0.527768
C	3.042139	-0.438367	-0.266661
H	3.081992	-0.531555	-1.355046
H	2.665901	-1.390483	0.124699
C	4.452752	-0.187472	0.265385
H	4.818868	0.779380	-0.093102
H	4.425707	-0.127297	1.358287
C	5.437519	-1.282664	-0.159783
H	5.055157	-2.250393	0.183859
H	5.491765	-1.327180	-1.251180
C	6.809924	-1.053177	0.403343
H	6.885251	-1.037460	1.488243
C	7.901035	-0.852602	-0.327820
H	7.859592	-0.859956	-1.411615
H	8.867026	-0.679204	0.129066
H	0.363573	-0.447510	0.312650

cat1_am5_bts

SCF energy in solution: –1028.435412

Enthalpy in solution: –1027.847603

Free energy in solution: –1027.929439

Cartesian coordinates

Atom	X	Y	Z
C	-3.999669	0.088628	0.091222
H	-5.042788	0.182560	0.332914
C	-3.202183	-0.987578	-0.142866
C	-3.447508	2.639175	0.146447
H	-3.539420	2.848675	1.215973
H	-4.391352	2.904066	-0.332916
C	-0.898387	2.905091	-0.068652
N	-0.790556	1.501443	-0.475399
B	-0.791405	-1.545568	-0.510105
C	-3.139182	-2.490520	-0.164174
H	-3.378605	-2.843960	-1.172750
H	-3.842597	-2.961133	0.527003
N	-1.950887	-0.515586	-0.448507
C	-1.923192	0.808002	-0.366492
N	0.380325	-0.699287	0.224035
C	0.236917	-0.478701	1.667574
H	0.787038	0.413677	1.974925
H	-0.813499	-0.319034	1.906015
H	0.603975	-1.327880	2.248457
C	1.755171	-1.092694	-0.108884
H	1.981144	-2.071146	0.339049
H	1.815050	-1.212010	-1.189569
H	0.041199	0.550018	-0.206032
N	-3.176103	1.229287	-0.066526
C	-0.378321	-1.806635	-2.055341
H	-0.002329	-0.894287	-2.530778
H	0.370292	-2.592451	-2.190877
H	-1.264177	-2.112860	-2.620361
C	-1.640087	-2.839022	0.177564
C	-2.292679	3.432155	-0.477256
H	-2.369821	3.367900	-1.565845
H	-2.386244	4.482273	-0.192554
C	-0.695439	3.053735	1.445455
H	0.322506	2.762856	1.711606
H	-0.850265	4.088781	1.762322
H	-1.382359	2.410627	1.999845
C	0.171756	3.701074	-0.810787
H	1.159712	3.302131	-0.571271
H	0.022137	3.616587	-1.887818
H	0.145346	4.754926	-0.524309
C	-1.561229	-2.994151	1.703401
H	-2.180529	-3.840560	2.022754
H	-0.541035	-3.197273	2.036135
H	-1.926134	-2.111296	2.232315
C	-1.280160	-4.196045	-0.433522
H	-1.926682	-4.990961	-0.043672
H	-1.373384	-4.189151	-1.520424
H	-0.247794	-4.465519	-0.191649
C	2.814591	-0.079617	0.324647
H	2.904868	-0.051318	1.414284
H	2.505764	0.921965	0.001335
C	4.178927	-0.414060	-0.275660
H	4.463876	-1.434529	-0.001111
H	4.111770	-0.391902	-1.368535
C	5.276530	0.551025	0.186349
H	4.973248	1.573300	-0.067772
H	5.374315	0.506036	1.274891
C	6.601376	0.246126	-0.450184
H	6.634959	0.306383	-1.535843
C	7.696092	-0.106004	0.215543

H	7.694874	-0.179425	1.297735
H	8.624571	-0.329140	-0.294463

cat1_am5_c

SCF energy in solution: –1028.45356

Enthalpy in solution: –1027.859406

Free energy in solution: –1027.945914

Cartesian coordinates

Atom	X	Y	Z
C	3.949946	0.676241	-0.021073
H	4.995842	0.864818	0.141091
C	2.877667	1.499994	-0.157244
C	4.149247	-1.898920	0.020724
H	4.389367	-2.047207	1.076318
H	5.084406	-1.865881	-0.539123
C	1.797921	-2.903841	-0.014984
N	1.300598	-1.618905	-0.517985
B	0.376485	1.528838	-0.450922
C	2.496607	2.950451	-0.189670
H	2.637934	3.328986	-1.207529
H	3.111245	3.561326	0.477598
N	1.760022	0.716675	-0.349305
C	2.120959	-0.549355	-0.341177
N	-0.658026	0.646797	0.291885
C	-0.422204	0.240987	1.666946
H	-0.859701	-0.744005	1.875071
H	0.648640	0.165199	1.862757
H	-0.844288	0.936545	2.407498
C	-2.061554	0.953571	0.078744
H	-2.422176	1.708543	0.802096
H	-2.175408	1.390543	-0.913634
H	0.327733	-1.354156	-0.359638
N	3.453933	-0.632198	-0.145523
C	0.016102	1.654949	-2.033273
H	-0.261291	0.681103	-2.450998
H	-0.800868	2.349380	-2.245789
H	0.881863	2.016065	-2.598957
C	0.980299	2.972969	0.181472
C	3.252483	-3.022626	-0.504619
H	3.241784	-2.995574	-1.596540
H	3.664231	-3.983298	-0.190698
C	1.717488	-2.971540	1.515123
H	0.674599	-2.932435	1.834411
H	2.157444	-3.900907	1.884247
H	2.236926	-2.129945	1.977670
C	0.953423	-4.009418	-0.638768
H	-0.093484	-3.890746	-0.350730
H	1.019221	-3.968699	-1.726382
H	1.292816	-4.987557	-0.293846
C	0.878482	3.067589	1.708463
H	1.310635	4.010113	2.066671
H	-0.163987	3.036986	2.032491
H	1.410281	2.253577	2.207544
C	0.318014	4.217794	-0.410958
H	0.750645	5.137868	0.000380
H	0.423908	4.252099	-1.496942
H	-0.751836	4.227403	-0.182112
C	-2.984317	-0.265820	0.162556
H	-2.968438	-0.692981	1.170155
H	-2.600675	-1.033903	-0.518987
C	-4.425904	0.080917	-0.202555
H	-4.793975	0.875104	0.454342
H	-4.457705	0.480554	-1.222070
C	-5.367286	-1.125101	-0.101385
H	-4.982422	-1.923265	-0.746637
H	-5.364646	-1.510966	0.922209
C	-6.771526	-0.784560	-0.506542
H	-6.900076	-0.425036	-1.525227
C	-7.831879	-0.868910	0.290151
H	-7.737933	-1.218018	1.312813
H	-8.822531	-0.594632	-0.050006

cat1_am5_d_S

SCF energy in solution: –1028.451935

Enthalpy in solution: –1027.858509

Free energy in solution: –1027.939983

Cartesian coordinates

Atom	X	Y	Z
C	0.825607	-3.361910	0.193202
H	1.121938	-4.393631	0.134879
C	-0.383545	-2.760928	0.336072
C	3.203428	-2.406723	-0.104875
H	3.385855	-2.668268	-1.150111
H	3.619613	-3.197300	0.520516
C	3.055442	0.134168	-0.330890
N	1.709173	0.060330	0.244994
B	-1.536953	-0.534741	0.468350
N	-0.185422	-1.395008	0.348355
C	1.106075	-1.154411	0.233905
N	-1.337770	0.715456	-0.437198
C	-0.932444	0.497360	-1.819466
H	-0.336980	-0.413053	-1.901373

H	-1.778869	0.396221	-2.514011
H	-0.315038	1.322603	-2.197236
C	-2.467335	1.640269	-0.374617
H	-3.360315	1.174549	-0.830304
H	-2.711777	1.819409	0.674946
C	-1.444600	4.064346	-0.359451
H	-1.530180	4.987251	-0.939977
H	-1.874721	4.279856	0.623926
C	0.052067	3.737724	-0.183376
H	0.371940	3.094512	-1.012330
H	0.645541	4.654166	-0.245042
C	0.337773	3.066338	1.128844
H	-0.268973	2.192527	1.342463
C	1.247606	3.482945	2.005669
H	1.860915	4.357298	1.811309
H	1.403976	2.967073	2.945215
H	1.056489	0.824678	0.092692
N	1.770514	-2.325551	0.132071
C	-1.837895	-3.076441	0.515181
H	-2.143460	-3.972441	-0.032818
H	-2.030887	-3.259168	1.577552
C	-1.689798	-0.140943	2.042403
H	-2.616327	0.385639	2.284629
H	-1.679133	-1.044167	2.662194
H	-0.857107	0.479555	2.388870
C	-2.587668	-1.790910	0.046903
C	3.837084	-1.059059	0.245489
H	4.861324	-1.037946	-0.130717
H	3.869284	-0.945043	1.331372
C	2.999355	0.079127	-1.862638
H	2.473172	0.956395	-2.243963
H	4.005984	0.067598	-2.287026
H	2.462512	-0.806464	-2.209024
C	3.695984	1.438985	0.128198
H	3.106151	2.291548	-0.213889
H	3.740126	1.478421	1.216966
H	4.704420	1.526341	-0.280322
C	-2.832691	-1.933134	-1.460854
H	-3.471774	-2.801397	-1.664573
H	-3.337585	-1.053369	-1.864971
H	-1.902546	-2.072442	-2.017223
C	-3.951041	-1.710910	0.737308
H	-4.575368	-2.577687	0.487935
H	-3.851269	-1.669758	1.823428
H	-4.492831	-0.815300	0.420631
C	-2.292222	3.001258	-1.066620
H	-1.914291	2.858052	-2.083196
H	-3.297589	3.417949	-1.183061

cat1_am5_ets$_S$

SCF energy in solution: –1028.409757

Enthalpy in solution: –1027.819367

Free energy in solution: –1027.895285

Cartesian coordinates

Atom	X	Y	Z
C	2.069244	2.639222	-0.040070
H	2.664007	3.532434	0.025833
C	0.742823	2.444546	-0.192969
C	4.048800	1.020079	0.104524
H	4.406689	1.090434	1.134865
H	4.605949	1.740169	-0.496191
C	3.218180	-1.372960	0.176507
N	1.866692	-0.872426	-0.048384
B	-1.109857	0.835617	-0.502369
N	0.473245	1.076795	-0.194722
C	1.649513	0.439906	-0.071069
N	-1.705194	-0.479310	0.216375
C	-1.037303	-0.796140	1.484170
H	-0.187488	-1.446474	1.261859
H	-0.666819	0.100373	1.978271
H	-1.703875	-1.317664	2.168296
C	-3.165926	-0.275638	0.362656
H	-3.356404	0.593781	0.989656
H	-3.544630	-0.036914	-0.635641
C	-3.803204	-2.704333	0.057212
H	-4.340328	-3.542621	0.508656
H	-4.255194	-2.527817	-0.924999
C	-2.334619	-3.062264	-0.136260
H	-1.854483	-3.280050	0.823805
H	-2.259885	-3.979666	-0.725919
C	-1.520726	-2.022377	-0.889156
H	-2.087866	-1.557669	-1.691857
C	-0.175839	-2.372845	-1.159286
H	0.127735	-3.351835	-0.795021
H	0.194830	-2.139208	-2.152847
H	1.028490	-1.505208	-0.430625
N	2.639357	1.364984	0.039830
C	-0.490695	3.260148	-0.368611
H	-0.456433	4.195044	0.198665
H	-0.619959	3.520283	-1.423251
C	-1.282608	0.755756	-2.114810
H	-2.314496	0.582117	-2.436496
H	-0.968705	1.690709	-2.587735

H	-0.665725	-0.035154	-2.545403
C	-1.635405	2.325579	0.102063
C	4.226980	-0.392133	-0.445562
H	5.245842	-0.732882	-0.251326
H	4.069940	-0.378370	-1.527099
C	3.466608	-1.528029	1.683175
H	2.775680	-2.267921	2.089643
H	4.490330	-1.857782	1.879461
H	3.291768	-0.587924	2.209280
C	3.336891	-2.732117	-0.508777
H	2.597883	-3.422434	-0.099909
H	3.157213	-2.635905	-1.580758
H	4.332412	-3.150495	-0.348479
C	-1.664898	2.472165	1.635917
H	-1.947184	3.497458	1.902292
H	-2.373545	1.807338	2.131973
H	-0.678451	2.285977	2.069460
C	-2.946714	2.869005	-0.478067
H	-3.054595	3.933060	-0.236099
H	-2.970052	2.772207	-1.565650
H	-3.825837	2.361982	-0.077729
C	-3.959114	-1.456723	0.912666
H	-3.670721	-1.675085	1.944269
H	-5.007433	-1.147767	0.951395

cat1_am5_f$_S$

SCF energy in solution: –1028.465958

Enthalpy in solution: –1027.869608

Free energy in solution: –1027.945367

Cartesian coordinates

Atom	X	Y	Z
C	2.182221	2.519006	-0.186250
H	2.793405	3.404314	-0.167339
C	0.851273	2.355582	-0.269858
C	4.133706	0.888128	-0.096855
H	4.579526	1.051359	0.889524
H	4.651979	1.536152	-0.807882
C	3.236756	-1.442447	0.251858
N	1.871241	-0.995072	0.005505
B	-1.024041	0.857430	-0.516819
N	0.536314	0.991667	-0.232383
C	1.719961	0.291831	-0.108540
N	-1.719654	-0.552425	0.146005
C	-0.971397	-0.959876	1.366297
H	0.046658	-1.226970	1.079834
H	-0.944556	-0.110375	2.043911
H	-1.462388	-1.796861	1.858866
C	-3.127913	-0.172426	0.501472
H	-3.068735	0.633545	1.221031
H	-3.574499	0.224199	-0.412656
C	-4.077643	-2.450940	0.058284
H	-4.637329	-3.290840	0.474297
H	-4.608350	-2.118148	-0.840250
C	-2.663048	-2.870275	-0.319679
H	-2.160985	-3.339061	0.531652
H	-2.683993	-3.622105	-1.112125
C	-1.823822	-1.701921	-0.850531
H	-2.364643	-1.264839	-1.690348
C	-0.488330	-2.231015	-1.344478
H	0.011125	-2.831495	-0.585317
H	-0.691075	-2.863736	-2.211994
N	2.728932	1.238087	-0.082801
C	-0.360186	3.218308	-0.349097
H	-0.252881	4.136986	0.234974
H	-0.569877	3.513526	-1.381101
C	-1.345706	0.875550	-2.110349
H	-2.414592	0.823416	-2.345312
H	-0.989883	1.814256	-2.539705
H	-0.847414	0.082359	-2.669446
C	-1.498469	2.314857	0.197854
C	4.254761	-0.574174	-0.509807
H	5.274162	-0.923826	-0.330568
H	4.044567	-0.666247	-1.579042
C	3.526357	-1.406306	1.760830
H	2.840700	-2.083113	2.273835
H	4.553072	-1.715512	1.979489
H	3.366229	-0.404508	2.163921
C	3.342622	-2.883319	-0.245336
H	2.595494	-3.496802	0.262313
H	3.141953	-2.922478	-1.317862
H	4.333697	-3.301809	-0.051286
C	-1.371122	2.415254	1.731775
H	-1.491887	3.459916	2.039186
H	-2.122506	1.847572	2.285439
H	-0.384508	2.086620	2.066590
C	-2.832080	2.935946	-0.233593
H	-2.852191	3.998256	0.035374
H	-2.974175	2.867525	-1.314230
H	-3.695356	2.474602	0.250419
C	-3.996626	-1.298820	1.049563
H	-3.611016	-1.650318	2.009755
H	-4.984839	-0.876614	1.247013
H	0.209600	-1.449552	-1.622506