Supporting Information

Mechanism and chemoselectivity origins of bioconjugation of cysteine with Au(III)-aryl reagents

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Contents

1. Additional computational results

(a) The LAu(I) with counteranion

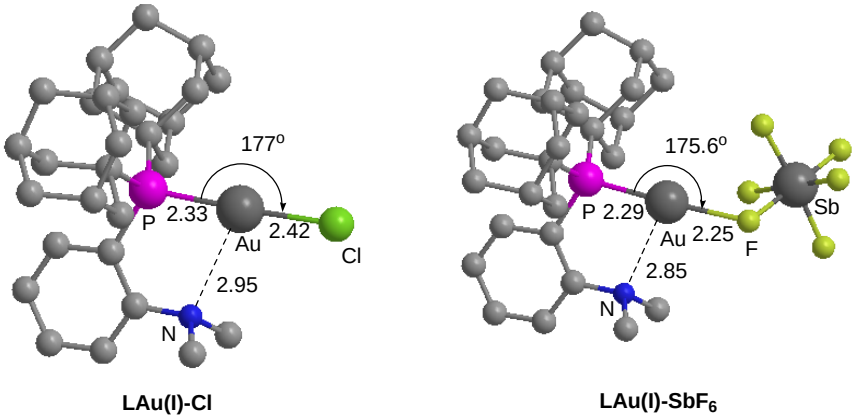
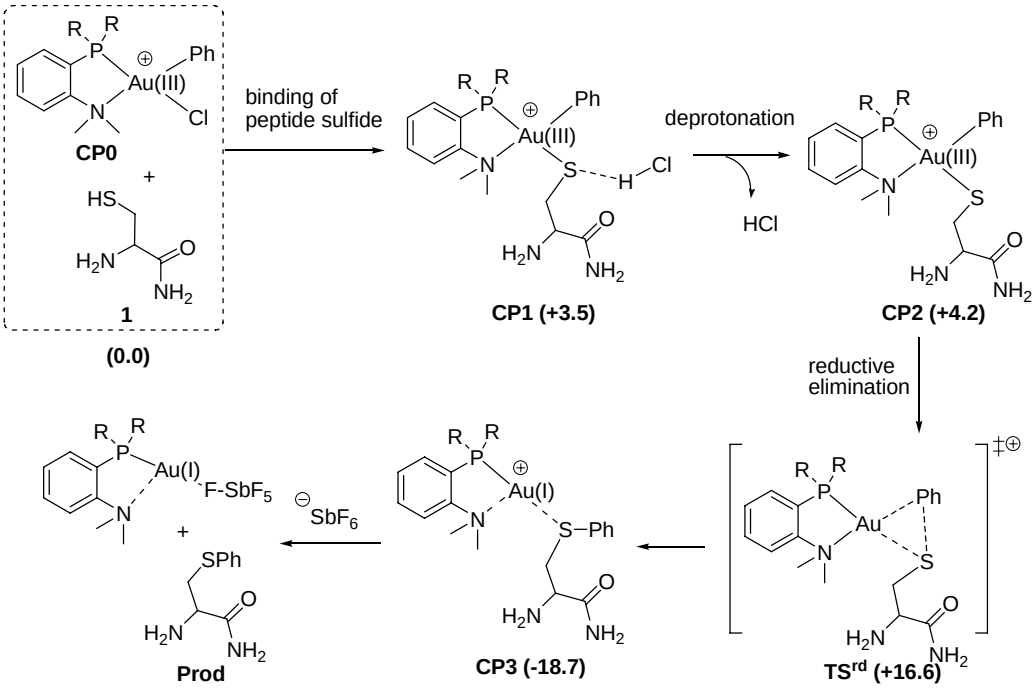


Figure S1. The LAu(I) with a counteranion of Cl^- or SbF_6^-. Both show a linear geometry around the Au(I) center with a bystanding dimethylamino group.

(b) ωb97xd-predicted reaction energy profile of the favored pathway in Scheme 2

Scheme S1. ωb97xd/SDD for Au and 6-311+g(d,p) for the other atoms predicted reaction energy profile



(c) Comparison of b3lyp and ωb97xd optimized key intermediate and transition state

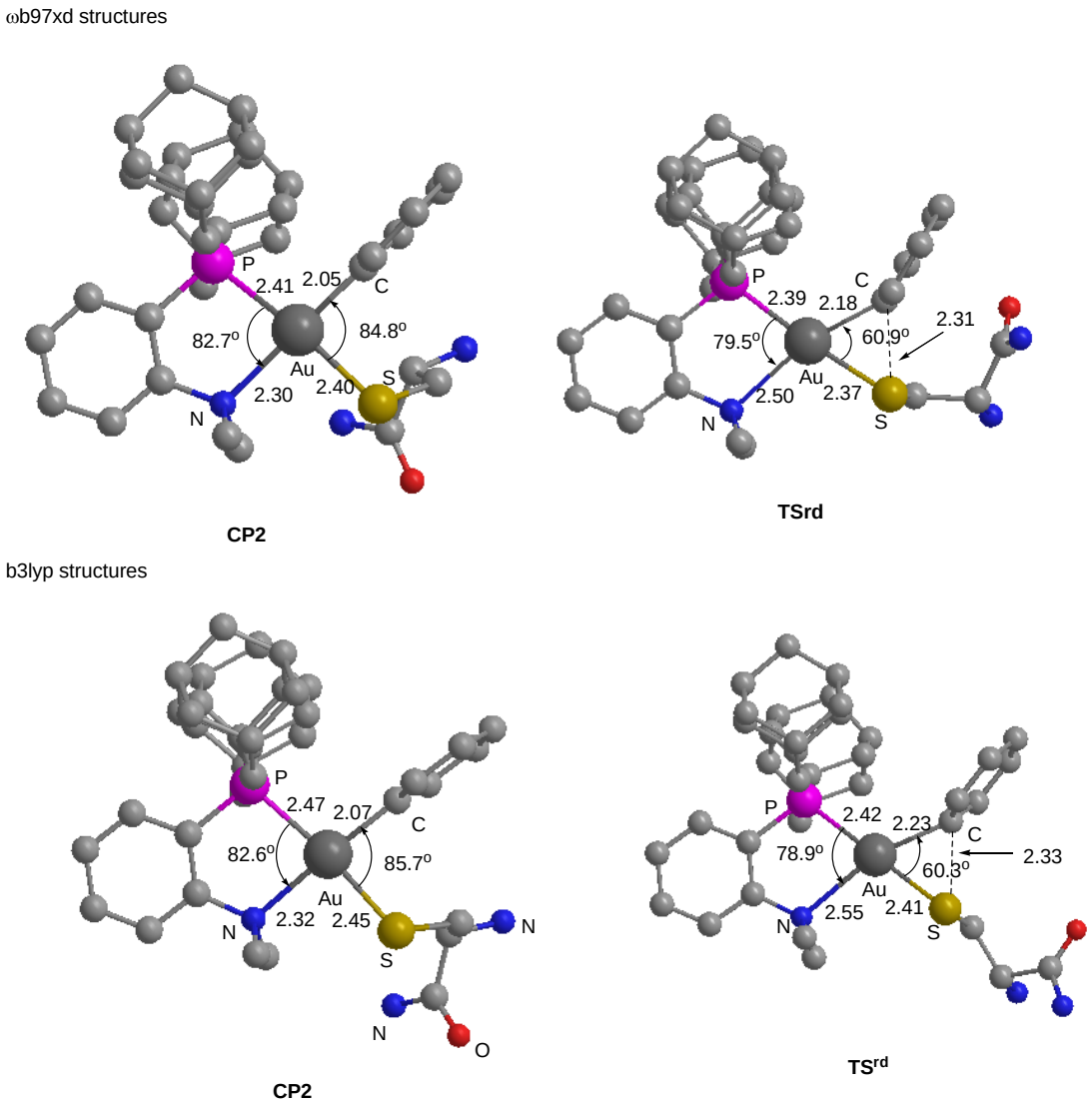


Figure S2. Comparison of key structures of **CP2** and **TSrd** using ωb97xd and b3lyp methods with the same basis set of LANL2DZ+ECP for Au and 6-31g* for the other atoms.

As can be seen, very similar structures are obtained using ωb97xd and b3lyp.

2. Optimized Cartesian Coordinates of Stationary Points

CP0

SCF Done: E(RB3LYP) = -2314.37728692 A.U.; No imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.005845	3.056803	2.597921
2	6	0	-1.468609	3.112684	2.525374
3	6	0	-1.030720	4.281451	1.623162
4	6	0	-1.599643	4.068183	0.208098
5	6	0	-3.138332	4.008086	0.268203
6	6	0	-3.567175	2.843285	1.180961
7	6	0	-0.927886	1.781113	1.953706
8	6	0	-1.484779	1.551740	0.524086
9	6	0	-1.054750	2.744146	-0.377957
10	6	0	-3.036228	1.508776	0.601567
11	15	0	-0.743710	-0.038003	-0.256405
12	6	0	-1.227081	-0.045450	-2.037060
13	6	0	-0.262616	0.011030	-3.057844
14	6	0	-0.662823	0.005189	-4.399650
15	6	0	-2.010075	-0.048333	-4.743692
16	6	0	-2.977960	-0.098874	-3.742148
17	6	0	-2.587106	-0.099820	-2.406792
18	7	0	1.177175	0.080365	-2.759399
19	6	0	1.762934	1.337748	-3.325989
20	79	0	1.645405	0.101678	-0.515107
21	17	0	4.059546	0.202299	-0.971932
22	6	0	2.225918	0.132849	1.470314
23	6	0	2.439930	-1.059596	2.158902
24	6	0	2.967274	-1.016989	3.456930
25	6	0	3.282505	0.205562	4.050619
26	6	0	3.082709	1.392005	3.341398
27	6	0	2.558470	1.360802	2.044113
28	6	0	-1.275012	-1.730176	0.480830
29	6	0	-0.335332	-2.811335	-0.126051
30	6	0	-0.679233	-4.199866	0.461092
31	6	0	-2.133891	-4.562131	0.108485
32	6	0	-3.077557	-3.504698	0.711310
33	6	0	-2.737499	-2.114477	0.117002
34	6	0	-0.507461	-4.168926	1.992317
35	6	0	-1.464426	-3.121394	2.593234
36	6	0	-1.138722	-1.718994	2.026268
37	6	0	-2.920096	-3.480860	2.242443
38	6	0	1.880854	-1.114430	-3.327943
39	1	0	0.079307	0.043147	-5.188713
40	1	0	-2.297185	-0.050574	-5.790382
41	1	0	-4.033067	-0.140635	-3.992061
42	1	0	-3.356796	-0.149853	-1.650553
43	1	0	0.039580	2.798245	-0.443187
44	1	0	-1.437465	2.612017	-1.396125
45	1	0	-1.283361	4.886126	-0.450896
46	1	0	1.229568	2.196200	-2.915215
47	1	0	1.681230	1.345393	-4.417127
48	1	0	2.814003	1.386074	-3.042354
49	1	0	0.065180	4.344243	1.586580

50	1	0	-1.393647	5.232201	2.035361
51	1	0	-1.051027	3.241511	3.531622
52	1	0	-3.325733	2.241575	3.260751
53	1	0	-3.399150	3.990292	3.021319
54	1	0	-4.661770	2.779998	1.216250
55	1	0	-3.473965	1.367098	-0.389304
56	1	0	-3.366809	0.680696	1.238004
57	1	0	-3.536713	4.954352	0.656641
58	1	0	-3.552493	3.873479	-0.740007
59	1	0	-1.216899	0.963525	2.619969
60	1	0	0.161985	1.810218	1.933757
61	1	0	-0.447241	-2.838028	-1.216974
62	1	0	0.714746	-2.579723	0.085320
63	1	0	0.007078	-4.934278	0.022116
64	1	0	2.934490	-1.053911	-3.056761
65	1	0	1.785252	-1.136301	-4.417745
66	1	0	1.444663	-2.021351	-2.905867
67	1	0	-2.380207	-5.555892	0.504346
68	1	0	-2.260329	-4.607986	-0.981431
69	1	0	-4.116317	-3.735330	0.444573
70	1	0	-3.608545	-2.749088	2.686004
71	1	0	-3.179127	-4.462001	2.661277
72	1	0	-1.339924	-3.083728	3.682342
73	1	0	-1.840928	-0.997977	2.457612
74	1	0	-0.130980	-1.417819	2.327462
75	1	0	-3.446051	-1.372639	0.500621
76	1	0	-2.860465	-2.166440	-0.967913
77	1	0	-0.724959	-5.159402	2.412632
78	1	0	0.532012	-3.931580	2.255363
79	1	0	2.426736	2.288672	1.496883
80	1	0	3.338518	2.348902	3.788073
81	1	0	3.131452	-1.947358	3.993533
82	1	0	2.223428	-2.021018	1.705997
83	1	0	3.689698	0.234196	5.057138

Cysteinamide (**1**)
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.010443	0.847701	-0.321393
2	6	0	-0.383791	0.734588	0.299558
3	6	0	-1.065324	-0.581417	-0.124799
4	8	0	-0.800772	-1.152003	-1.182978
5	16	0	2.218804	-0.397126	0.293789
6	7	0	-1.212571	1.839967	-0.221380
7	7	0	-2.011199	-1.030189	0.735234
8	1	0	1.447568	1.817572	-0.066802
9	1	0	0.938217	0.773847	-1.407493
10	1	0	-0.283637	0.745472	1.396777
11	1	0	-2.147743	1.778946	0.180673
12	1	0	-0.828377	2.721915	0.117888
13	1	0	-2.518368	-1.877558	0.515244
14	1	0	-2.172892	-0.602413	1.635907
15	1	0	1.668963	-1.461409	-0.326167

CP1

SCF Done: E(RB3LYP) = -3016.42775083 A.U.; No imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.847958	-3.763819	-2.714779
2	6	0	2.864989	-4.073923	-1.206440
3	6	0	1.627350	-4.913876	-0.837342
4	6	0	0.356302	-4.111784	-1.173199
5	6	0	0.328050	-3.790390	-2.680342
6	6	0	1.574931	-2.964501	-3.050088
7	6	0	2.856804	-2.757427	-0.390210
8	6	0	1.585241	-1.931860	-0.731620
9	6	0	0.344638	-2.794496	-0.364899
10	6	0	1.585719	-1.637342	-2.255092
11	15	0	1.426853	-0.303422	0.271996
12	79	0	-0.910849	0.422830	0.441790
13	17	0	-3.615804	4.430597	0.279536
14	6	0	2.635585	1.125969	-0.165547
15	6	0	2.320835	1.697541	-1.573679
16	6	0	3.215990	2.925155	-1.863343
17	6	0	4.695354	2.499655	-1.832378
18	6	0	5.025575	1.938657	-0.437238
19	6	0	4.131543	0.710438	-0.134630
20	6	0	4.782548	3.022391	0.630701
21	6	0	3.304842	3.457074	0.589083
22	6	0	2.966375	4.016945	-0.805814
23	6	0	2.397907	2.242200	0.891531
24	6	0	1.735788	-0.736785	2.038887
25	6	0	0.730587	-0.600106	3.011653
26	6	0	1.004213	-0.919716	4.348587
27	6	0	2.261962	-1.370815	4.735924
28	6	0	3.267662	-1.514347	3.781957
29	6	0	3.001657	-1.202260	2.452597
30	7	0	-0.627685	-0.136661	2.673832
31	6	0	-1.618237	-1.213874	2.990724
32	6	0	-0.952488	1.102366	3.448263
33	16	0	-3.236859	1.103324	0.874904
34	6	0	-4.360207	0.369654	-0.388457
35	6	0	-5.038045	-0.926019	0.067695
36	6	0	-4.031293	-2.090097	0.144751
37	8	0	-3.109671	-2.224912	-0.662544
38	6	0	-1.219137	1.037326	-1.507631
39	6	0	-1.602720	0.122232	-2.488032
40	6	0	-1.831529	0.571846	-3.796465
41	6	0	-1.691378	1.922894	-4.115008
42	6	0	-1.333859	2.833919	-3.118302
43	6	0	-1.099684	2.395639	-1.809636
44	7	0	-6.041936	-1.292117	-0.950882
45	7	0	-4.270634	-2.980536	1.135294
46	1	0	0.231651	-0.819764	5.102098
47	1	0	2.449056	-1.610351	5.777944
48	1	0	4.253921	-1.868430	4.064169
49	1	0	3.794334	-1.332231	1.730275
50	1	0	1.347692	2.562074	0.878247
51	1	0	2.612848	1.866230	1.898595

52	1	0	3.119035	4.221041	1.354385
53	1	0	-0.228955	1.879749	3.198806
54	1	0	-0.925404	0.911001	4.525134
55	1	0	-1.956627	1.431774	3.179209
56	1	0	1.918956	4.346086	-0.838087
57	1	0	3.587093	4.897172	-1.019311
58	1	0	2.956713	3.305222	-2.859449
59	1	0	4.888957	1.741242	-2.603011
60	1	0	5.342508	3.358230	-2.055599
61	1	0	6.071690	1.609636	-0.403268
62	1	0	4.410806	0.322818	0.847936
63	1	0	4.326544	-0.074626	-0.873916
64	1	0	5.433465	3.886550	0.443203
65	1	0	5.037565	2.637837	1.627546
66	1	0	2.498068	0.942146	-2.344038
67	1	0	1.271297	1.985934	-1.641150
68	1	0	0.357690	-3.026152	0.708380
69	1	0	-0.587478	-2.256200	-0.566974
70	1	0	-0.535990	-4.687908	-0.898131
71	1	0	-2.611973	-0.864318	2.713841
72	1	0	-1.602614	-1.454568	4.058218
73	1	0	-1.370750	-2.105101	2.412489
74	1	0	1.635394	-5.859733	-1.394919
75	1	0	1.645061	-5.167974	0.231044
76	1	0	3.779017	-4.623274	-0.948076
77	1	0	3.741263	-3.190457	-2.997153
78	1	0	2.870384	-4.699152	-3.289448
79	1	0	1.557297	-2.720653	-4.119612
80	1	0	2.486066	-1.076370	-2.526368
81	1	0	0.721970	-1.026775	-2.536326
82	1	0	3.766434	-2.187206	-0.609893
83	1	0	2.871682	-3.011660	0.673246
84	1	0	0.309704	-4.721571	-3.261888
85	1	0	-0.585520	-3.236440	-2.934014
86	1	0	-0.834334	3.117256	-1.044096
87	1	0	-1.240360	3.891593	-3.349437
88	1	0	-2.124882	-0.144191	-4.559525
89	1	0	-1.766452	-0.920723	-2.241545
90	1	0	-1.870568	2.266718	-5.129746
91	1	0	-5.125591	1.129408	-0.577108
92	1	0	-3.811169	0.197160	-1.313559
93	1	0	-5.476527	-0.766015	1.065786
94	1	0	-6.521106	-2.144430	-0.660314
95	1	0	-6.762267	-0.570123	-0.968787
96	1	0	-3.690428	-3.805973	1.213885
97	1	0	-5.021260	-2.862871	1.800804
98	1	0	-3.403035	3.096489	0.467130

CP2

SCF Done: E(RB3LYP) = -2555.62089144 A.U.; No imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.629938	-1.231909	2.350117
2	6	0	1.095628	-1.732017	1.160604
3	6	0	0.699056	-3.068822	1.078490

4	6	0	0.805622	-3.895821	2.203619
5	6	0	1.316740	-3.395307	3.402854
6	6	0	1.732952	-2.064949	3.471851
7	79	0	0.977620	-0.526852	-0.515468
8	16	0	3.145721	-1.478672	-1.128585
9	6	0	4.298031	-1.413225	0.300169
10	6	0	4.744552	-0.004945	0.700331
11	7	0	5.579575	-0.112040	1.911851
12	15	0	-1.285844	0.418300	-0.232268
13	6	0	-1.410550	1.387602	-1.795874
14	6	0	-0.333797	1.451751	-2.697629
15	6	0	-0.441208	2.228008	-3.859769
16	6	0	-1.600901	2.943023	-4.141239
17	6	0	-2.675728	2.891032	-3.255482
18	6	0	-2.575447	2.122904	-2.099825
19	7	0	0.931209	0.730307	-2.463144
20	6	0	2.063300	1.704624	-2.359230
21	6	0	-2.638363	-0.939895	-0.296239
22	6	0	-4.044426	-0.423859	-0.709782
23	6	0	-5.049421	-1.601640	-0.750917
24	6	0	-5.134596	-2.274352	0.631770
25	6	0	-3.743209	-2.809231	1.019454
26	6	0	-2.747602	-1.628794	1.089754
27	6	0	-3.268267	-3.834982	-0.028038
28	6	0	-3.194581	-3.157035	-1.410558
29	6	0	-4.587766	-2.629211	-1.801238
30	6	0	-2.189562	-1.982970	-1.359281
31	6	0	-1.431056	1.697778	1.194771
32	6	0	-1.015596	1.055296	2.544638
33	6	0	-1.017397	2.119669	3.666841
34	6	0	-2.431287	2.711300	3.816119
35	6	0	-2.844367	3.366305	2.485405
36	6	0	-2.851571	2.303043	1.358857
37	6	0	-0.019265	3.240677	3.321168
38	6	0	-0.437331	3.897886	1.992274
39	6	0	-0.427496	2.838880	0.866115
40	6	0	-1.853386	4.490572	2.127855
41	6	0	1.182007	-0.224244	-3.588915
42	6	0	5.623192	0.613755	-0.405706
43	7	0	5.421509	1.937887	-0.620389
44	8	0	6.466886	-0.038665	-1.017291
45	1	0	0.387311	2.282667	-4.556408
46	1	0	-1.658597	3.537574	-5.047568
47	1	0	-3.587887	3.443418	-3.457164
48	1	0	-3.421629	2.098936	-1.428595
49	1	0	0.586147	2.429616	0.761855
50	1	0	-0.688135	3.316187	-0.084889
51	1	0	0.274611	4.688759	1.724956
52	1	0	1.857635	2.404017	-1.547387
53	1	0	2.187009	2.259623	-3.294584
54	1	0	2.976604	1.151615	-2.141609
55	1	0	0.997195	2.832192	3.239049
56	1	0	-0.002116	3.990218	4.123391
57	1	0	-0.717197	1.628659	4.601070
58	1	0	-3.146768	1.924463	4.091086
59	1	0	-2.445856	3.456209	4.622819
60	1	0	-3.858616	3.776411	2.568811
61	1	0	-3.184566	2.782066	0.434216

62	1	0	-3.574880	1.518850	1.607607
63	1	0	-1.864675	5.262112	2.908884
64	1	0	-2.153144	4.976723	1.189628
65	1	0	-1.698326	0.245548	2.818236
66	1	0	-0.019585	0.619294	2.459323
67	1	0	-2.125513	-1.508353	-2.346815
68	1	0	-1.192294	-2.368761	-1.121187
69	1	0	-2.842975	-3.876341	-2.160765
70	1	0	2.121730	-0.745348	-3.404125
71	1	0	1.257633	0.306016	-4.542990
72	1	0	0.362655	-0.943103	-3.636626
73	1	0	-5.302780	-3.460794	-1.856018
74	1	0	-4.554191	-2.166492	-2.796798
75	1	0	-6.030235	-1.197335	-1.030946
76	1	0	-5.487041	-1.555228	1.383640
77	1	0	-5.862701	-3.095778	0.605483
78	1	0	-3.786050	-3.280205	2.009412
79	1	0	-3.106904	-0.912310	1.836159
80	1	0	-1.767444	-1.986782	1.421470
81	1	0	-4.406604	0.337378	-0.011053
82	1	0	-4.003651	0.028111	-1.704770
83	1	0	-3.963899	-4.683645	-0.064799
84	1	0	-2.286067	-4.237551	0.252835
85	1	0	1.978448	-0.206402	2.417733
86	1	0	2.143418	-1.664936	4.395105
87	1	0	0.493315	-4.934142	2.131364
88	1	0	0.322686	-3.483992	0.149650
89	1	0	1.399136	-4.039834	4.273253
90	1	0	3.852211	-1.925096	1.155519
91	1	0	5.176589	-1.980243	-0.021928
92	1	0	3.850628	0.623844	0.844188
93	1	0	5.866877	0.820674	2.208438
94	1	0	5.003513	-0.473288	2.672086
95	1	0	6.007486	2.427921	-1.283938
96	1	0	4.739450	2.473321	-0.102841

HCl

SCF Done: E(RB3LYP) = -460.796000317 A.U.; No imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.000000	0.000000	0.071725
2	1	0	0.000000	0.000000	-1.219330

TSrd

SCF Done: E(RB3LYP) = -2555.60197103 A.U.; An imaginary frequency of -257.5484 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.165236	1.012188	2.190659
2	6	0	-1.931181	1.472556	0.893897
3	6	0	-1.746200	2.834767	0.626464
4	6	0	-1.760201	3.739450	1.690075
5	6	0	-1.976399	3.296224	2.999540

6	6	0	-2.180096	1.937004	3.242317
7	79	0	-0.874759	0.092475	-0.502706
8	16	0	-3.227643	0.515963	-0.795154
9	6	0	-4.071882	-0.812342	0.166509
10	6	0	-5.492757	-1.026375	-0.373685
11	7	0	-6.058574	-2.193780	0.326444
12	15	0	1.494675	-0.311298	-0.213174
13	6	0	1.997318	-1.258751	-1.715345
14	6	0	1.066790	-1.588220	-2.726082
15	6	0	1.492089	-2.311774	-3.849537
16	6	0	2.814497	-2.724276	-3.986364
17	6	0	3.738428	-2.418581	-2.987454
18	6	0	3.328900	-1.695521	-1.870173
19	7	0	-0.335473	-1.205675	-2.633430
20	6	0	-1.229699	-2.383938	-2.602345
21	6	0	2.453761	1.339600	-0.250100
22	6	0	3.994862	1.220003	-0.401711
23	6	0	4.633906	2.629427	-0.447252
24	6	0	4.300973	3.401094	0.843908
25	6	0	2.771890	3.543625	0.971050
26	6	0	2.134711	2.137212	1.042837
27	6	0	2.217640	4.309341	-0.245798
28	6	0	2.562011	3.536894	-1.534042
29	6	0	4.090754	3.400298	-1.665100
30	6	0	1.917108	2.133599	-1.476905
31	6	0	1.818186	-1.441974	1.296155
32	6	0	0.992205	-0.916231	2.503411
33	6	0	1.131938	-1.872208	3.709412
34	6	0	2.613412	-1.977184	4.118427
35	6	0	3.428131	-2.525928	2.931368
36	6	0	3.303331	-1.560216	1.728361
37	6	0	0.598757	-3.264922	3.323711
38	6	0	1.416656	-3.808679	2.136808
39	6	0	1.284200	-2.855894	0.927509
40	6	0	2.900490	-3.919451	2.538155
41	6	0	-0.729637	-0.277947	-3.716919
42	6	0	-6.379477	0.191150	-0.033784
43	7	0	-7.253540	0.547387	-1.004281
44	8	0	-6.311767	0.763139	1.052592
45	1	0	0.776246	-2.559451	-4.626775
46	1	0	3.117424	-3.284869	-4.865685
47	1	0	4.772149	-2.739025	-3.072706
48	1	0	4.062597	-1.472277	-1.106805
49	1	0	0.231219	-2.791452	0.620611
50	1	0	1.844210	-3.266246	0.080196
51	1	0	1.036141	-4.794827	1.841707
52	1	0	-0.926724	-3.049000	-1.790457
53	1	0	-1.214255	-2.941616	-3.548942
54	1	0	-2.251142	-2.038131	-2.419305
55	1	0	-0.464690	-3.202612	3.054529
56	1	0	0.674579	-3.949624	4.178991
57	1	0	0.543166	-1.464725	4.541096
58	1	0	2.995591	-0.991574	4.417120
59	1	0	2.719423	-2.640790	4.986968
60	1	0	4.488180	-2.593901	3.206900
61	1	0	3.921616	-1.934419	0.905916
62	1	0	3.697174	-0.579147	2.016509
63	1	0	3.011613	-4.614739	3.380930

64	1	0	3.489163	-4.327082	1.705019
65	1	0	1.322528	0.086867	2.792764
66	1	0	-0.062922	-0.836343	2.222709
67	1	0	2.138385	1.587267	-2.402817
68	1	0	0.826878	2.240476	-1.415288
69	1	0	2.157869	4.066575	-2.406078
70	1	0	-1.755090	0.055637	-3.533506
71	1	0	-0.687815	-0.756538	-4.705147
72	1	0	-0.066768	0.589936	-3.712724
73	1	0	4.554840	4.394119	-1.720811
74	1	0	4.347231	2.872636	-2.593828
75	1	0	5.720774	2.507766	-0.538464
76	1	0	4.705833	2.872621	1.717893
77	1	0	4.772841	4.392536	0.820623
78	1	0	2.523183	4.082237	1.894283
79	1	0	2.534930	1.613700	1.918568
80	1	0	1.050502	2.224900	1.178556
81	1	0	4.428761	0.652779	0.428187
82	1	0	4.243972	0.692544	-1.328001
83	1	0	2.650401	5.317886	-0.284641
84	1	0	1.129739	4.428622	-0.154358
85	1	0	-2.317816	-0.040937	2.397880
86	1	0	-2.348517	1.579267	4.254498
87	1	0	-1.613095	4.796502	1.485709
88	1	0	-1.608926	3.188779	-0.390060
89	1	0	-1.995462	4.006856	3.820250
90	1	0	-3.500427	-1.739524	0.096495
91	1	0	-4.145032	-0.500003	1.210423
92	1	0	-5.454340	-1.158188	-1.466788
93	1	0	-7.018004	-2.339017	0.011662
94	1	0	-5.548632	-3.026696	0.032604
95	1	0	-7.897770	1.309081	-0.835507
96	1	0	-7.297414	0.076950	-1.896758

CP3

SCF Done: E(RB3LYP) = -2555.66109952 A.U.; No imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.933728	-3.932560	2.407221
2	6	0	3.332205	-2.547627	2.953858
3	6	0	2.392799	-2.157298	4.110000
4	6	0	0.944151	-2.105710	3.588618
5	6	0	0.537004	-3.490059	3.048921
6	6	0	1.480443	-3.880377	1.895536
7	6	0	3.234719	-1.492902	1.824854
8	6	0	1.784246	-1.431051	1.277524
9	6	0	0.837543	-1.058892	2.456958
10	6	0	1.376270	-2.839402	0.758912
11	15	0	1.487568	-0.203155	-0.167267
12	6	0	2.350392	1.493624	-0.003605
13	6	0	3.899167	1.464782	-0.085218
14	6	0	4.463492	2.902362	0.020780
15	6	0	4.032979	3.538056	1.356739
16	6	0	2.494008	3.592143	1.420766
17	6	0	1.928871	2.156478	1.335228

18	6	0	3.932894	3.750808	-1.150286
19	6	0	2.394269	3.799200	-1.083037
20	6	0	1.826447	2.366212	-1.181339
21	6	0	1.953349	4.435544	0.249892
22	79	0	-0.834865	0.159584	-0.325246
23	7	0	-0.033370	-0.876910	-2.901773
24	6	0	-0.351701	0.157187	-3.894197
25	6	0	-3.551661	2.135998	0.436682
26	6	0	-2.795809	2.559124	1.536876
27	6	0	-3.072879	3.795456	2.121733
28	6	0	-4.088887	4.606021	1.606095
29	6	0	-4.834473	4.179985	0.504990
30	6	0	-4.570902	2.940711	-0.084357
31	16	0	-3.254956	0.544976	-0.359135
32	6	0	-3.931854	-0.624056	0.910261
33	6	0	-3.810073	-2.075798	0.444465
34	6	0	-4.799643	-2.355228	-0.708219
35	8	0	-5.870766	-1.761604	-0.810394
36	7	0	-4.199507	-2.932699	1.578824
37	6	0	2.159844	-0.980195	-1.707940
38	6	0	1.370010	-1.211289	-2.861503
39	6	0	1.964387	-1.791321	-3.993673
40	6	0	3.307685	-2.154825	-4.011132
41	6	0	4.089376	-1.942170	-2.875906
42	6	0	3.517768	-1.361696	-1.746517
43	6	0	-0.890856	-2.059692	-3.051871
44	7	0	-4.405645	-3.327744	-1.564267
45	1	0	1.354845	-1.962079	-4.876154
46	1	0	3.738534	-2.602429	-4.902193
47	1	0	5.138347	-2.222308	-2.864482
48	1	0	4.149892	-1.205061	-0.882332
49	1	0	0.347407	-2.812287	0.374048
50	1	0	2.023926	-3.142094	-0.071059
51	1	0	1.192537	-4.860287	1.493738
52	1	0	-0.653254	-2.784753	-2.268549
53	1	0	-0.782680	-2.554411	-4.031683
54	1	0	-1.936069	-1.756169	-2.935503
55	1	0	-0.503865	-3.468948	2.696949
56	1	0	0.590519	-4.239204	3.850229
57	1	0	0.266635	-1.806865	4.398730
58	1	0	2.683145	-1.181033	4.521717
59	1	0	2.475276	-2.888067	4.925686
60	1	0	4.370074	-2.573100	3.309627
61	1	0	3.942038	-1.757740	1.033003
62	1	0	3.534640	-0.516285	2.220997
63	1	0	3.027864	-4.689042	3.197729
64	1	0	3.610760	-4.229541	1.594618
65	1	0	1.085723	-0.068461	2.853389
66	1	0	-0.199362	-1.009333	2.101963
67	1	0	2.120985	1.917354	-2.138543
68	1	0	0.729313	2.404281	-1.165207
69	1	0	2.002012	4.385489	-1.923815
70	1	0	-1.399224	0.451530	-3.771747
71	1	0	-0.208913	-0.179042	-4.934964
72	1	0	0.276323	1.035665	-3.724076
73	1	0	4.345130	4.767382	-1.097602
74	1	0	4.256478	3.319995	-2.107607
75	1	0	5.558346	2.844417	-0.028014

76	1	0	4.426159	2.953798	2.200038
77	1	0	4.450459	4.550043	1.444196
78	1	0	2.176074	4.032377	2.374424
79	1	0	2.307824	1.574331	2.183038
80	1	0	0.834306	2.179325	1.417634
81	1	0	4.323127	0.849895	0.715396
82	1	0	4.218293	1.031040	-1.037974
83	1	0	2.333086	5.463722	0.320010
84	1	0	0.857255	4.493205	0.298689
85	1	0	-2.000450	1.931259	1.926247
86	1	0	-2.490084	4.126567	2.976157
87	1	0	-5.623119	4.808184	0.101840
88	1	0	-5.151164	2.603058	-0.937327
89	1	0	-4.296610	5.569665	2.061805
90	1	0	-3.384720	-0.467232	1.841755
91	1	0	-4.984669	-0.367440	1.038889
92	1	0	-2.781947	-2.265291	0.094368
93	1	0	-4.194256	-3.908081	1.281409
94	1	0	-3.484705	-2.863164	2.302846
95	1	0	-5.029385	-3.617627	-2.306399
96	1	0	-3.522812	-3.809612	-1.471345

Isomeric reductive elimination from 3-coordinate Au(III) intermediate

CP2-iso

SCF Done: E(RB3LYP) = -2555.58050063 A.U.; No imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.080124	2.809115	0.540629
2	6	0	1.933171	1.643783	-0.200722
3	6	0	2.273697	1.539330	-1.541049
4	6	0	2.737664	2.695760	-2.185923
5	6	0	2.868163	3.895113	-1.484910
6	6	0	2.544188	3.950436	-0.127641
7	79	0	1.146785	-0.018772	0.773573
8	16	0	3.337936	-0.433450	1.587945
9	6	0	4.080731	-1.445657	0.230345
10	6	0	5.591239	-1.611144	0.439286
11	6	0	6.312368	-0.272663	0.176521
12	8	0	6.058854	0.422972	-0.805521
13	15	0	-1.275168	-0.080201	0.185098
14	6	0	-2.067886	1.568728	-0.389403
15	6	0	-3.616584	1.494029	-0.384477
16	6	0	-4.213609	2.850047	-0.833267
17	6	0	-3.716039	3.197177	-2.249815
18	6	0	-2.178234	3.302597	-2.238269
19	6	0	-1.576111	1.943513	-1.811551
20	6	0	-3.780966	3.952970	0.150973
21	6	0	-2.243573	4.046499	0.157890
22	6	0	-1.642565	2.691402	0.597611
23	6	0	-1.737530	4.401321	-1.253178
24	6	0	-2.016104	-0.449380	1.864039
25	6	0	-3.135925	-1.252171	2.208319
26	6	0	-3.527116	-1.326457	3.555351
27	6	0	-2.859505	-0.642398	4.566867
28	6	0	-1.762111	0.150122	4.239955

29	6	0	-1.355883	0.237230	2.911269
30	7	0	-3.883279	-2.008216	1.232247
31	6	0	-3.972786	-3.440170	1.563076
32	6	0	-1.327710	-1.497513	-1.106252
33	6	0	-2.688601	-1.670215	-1.828784
34	6	0	-2.607773	-2.845638	-2.831503
35	6	0	-2.256463	-4.146651	-2.084528
36	6	0	-0.888903	-3.985770	-1.391820
37	6	0	-0.951632	-2.817700	-0.379295
38	6	0	-1.528688	-2.547344	-3.889090
39	6	0	-0.165161	-2.393905	-3.189181
40	6	0	-0.225016	-1.227727	-2.174339
41	6	0	0.191840	-3.696923	-2.450616
42	7	0	6.077737	-2.585042	-0.554002
43	6	0	-5.238234	-1.478783	1.007267
44	7	0	7.260757	0.052556	1.086940
45	1	0	-1.219026	0.696008	5.005134
46	1	0	-3.194841	-0.729283	5.596180
47	1	0	-4.384577	-1.940879	3.811585
48	1	0	0.025900	-2.718820	0.113605
49	1	0	-1.684031	-3.039877	0.396736
50	1	0	-0.638866	-4.902073	-0.842231
51	1	0	1.177145	-3.604793	-1.973374
52	1	0	0.254826	-4.530437	-3.162565
53	1	0	0.610460	-2.159190	-3.929091
54	1	0	-1.779274	-1.629990	-4.439131
55	1	0	-1.482602	-3.361174	-4.625012
56	1	0	-3.586628	-2.948887	-3.316887
57	1	0	-3.468627	-1.856167	-1.087988
58	1	0	-2.949222	-0.757181	-2.375511
59	1	0	-2.220044	-4.987377	-2.790332
60	1	0	-3.033422	-4.382049	-1.345671
61	1	0	-0.407323	-0.291795	-2.708974
62	1	0	0.753840	-1.141008	-1.686569
63	1	0	-1.987876	2.457259	1.610358
64	1	0	-0.552322	2.773815	0.630299
65	1	0	-1.919198	4.811882	0.874272
66	1	0	-4.216712	4.916154	-0.146258
67	1	0	-4.152827	3.728672	1.160018
68	1	0	-5.307042	2.757609	-0.834002
69	1	0	-4.037640	2.428492	-2.965803
70	1	0	-4.156399	4.147595	-2.579243
71	1	0	-1.813232	3.536239	-3.246279
72	1	0	-1.884253	1.183029	-2.535819
73	1	0	-0.481988	1.998517	-1.833353
74	1	0	-3.973854	0.699529	-1.047169
75	1	0	-3.969139	1.267364	0.627767
76	1	0	-2.143395	5.372556	-1.566132
77	1	0	-0.643203	4.493875	-1.252079
78	1	0	2.180683	0.611205	-2.092369
79	1	0	2.993378	2.640815	-3.240018
80	1	0	2.659391	4.874874	0.430771
81	1	0	1.846788	2.849639	1.598294
82	1	0	3.232199	4.783189	-1.992449
83	1	0	3.597596	-2.425525	0.209591
84	1	0	3.915893	-0.942355	-0.724829
85	1	0	5.780606	-1.928359	1.477745
86	1	0	7.084180	-2.706107	-0.439774

87	1	0	5.670009	-3.495297	-0.340885
88	1	0	7.795127	0.903018	0.965133
89	1	0	7.453359	-0.518601	1.897031
90	1	0	-4.340782	-3.980086	0.684231
91	1	0	-2.987946	-3.833207	1.825711
92	1	0	-4.660874	-3.650300	2.398203
93	1	0	-5.689764	-2.015842	0.166317
94	1	0	-5.894676	-1.604533	1.884931
95	1	0	-5.197752	-0.419315	0.755863
96	1	0	-0.499726	0.865772	2.689345

TSrd-iso

SCF Done: E(RB3LYP) = -2555.57892494 A.U.; An imaginary frequency of -132.3007 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.411630	-0.766693	2.193748
2	6	0	-2.160383	-0.189025	1.853021
3	6	0	-1.449346	0.479208	2.876741
4	6	0	-1.934382	0.594980	4.176736
5	6	0	-3.165904	0.029517	4.498686
6	6	0	-3.881914	-0.640236	3.511408
7	15	0	-1.302681	-0.072115	0.191379
8	79	0	1.101990	-0.061451	0.751075
9	16	0	3.350310	-0.412865	1.431420
10	6	0	4.020510	-1.466590	0.071741
11	6	0	5.485797	-1.828331	0.355410
12	7	0	5.900971	-2.813258	-0.657966
13	7	0	-4.213877	-1.507242	1.248068
14	6	0	-5.504102	-0.866239	0.948424
15	6	0	-1.444681	-1.606958	-0.947354
16	6	0	-2.788637	-1.748689	-1.705182
17	6	0	-2.781707	-3.042138	-2.553410
18	6	0	-2.575262	-4.266376	-1.640147
19	6	0	-1.222780	-4.140015	-0.910640
20	6	0	-1.213095	-2.854986	-0.052305
21	6	0	-0.084928	-4.076588	-1.946911
22	6	0	-0.297929	-2.849522	-2.853058
23	6	0	-1.644829	-2.974661	-3.590512
24	6	0	-0.289616	-1.563166	-1.994476
25	6	0	-1.908554	1.569476	-0.587920
26	6	0	-3.454091	1.653760	-0.655588
27	6	0	-3.886007	3.008718	-1.266803
28	6	0	-3.298239	3.152090	-2.683786
29	6	0	-1.759454	3.102886	-2.605177
30	6	0	-1.322775	1.742285	-2.013202
31	6	0	-3.377662	4.159066	-0.377468
32	6	0	-1.840067	4.097272	-0.302366
33	6	0	-1.403948	2.741764	0.300780
34	6	0	-1.245523	4.249541	-1.715033
35	6	0	2.288998	1.571042	0.010980
36	6	0	2.616349	1.538722	-1.335896
37	6	0	3.017447	2.744286	-1.930357
38	6	0	3.105878	3.913544	-1.172946
39	6	0	2.795444	3.892427	0.189608
40	6	0	2.392066	2.702953	0.809367

41	6	0	6.378201	-0.579657	0.193037
42	7	0	7.290233	-0.396900	1.176688
43	8	0	6.275655	0.170420	-0.775777
44	6	0	-4.455534	-2.894200	1.679804
45	1	0	-1.347859	1.119002	4.925161
46	1	0	-3.564510	0.102566	5.506386
47	1	0	-4.838820	-1.086885	3.764209
48	1	0	-0.248162	-2.773320	0.468658
49	1	0	-1.986597	-2.917029	0.714303
50	1	0	-1.075695	-5.000519	-0.245656
51	1	0	0.887767	-4.009861	-1.440133
52	1	0	-0.071652	-4.993800	-2.550610
53	1	0	0.520460	-2.776970	-3.580694
54	1	0	-1.792658	-2.116777	-4.260600
55	1	0	-1.646974	-3.877141	-4.216434
56	1	0	-3.748929	-3.121630	-3.066149
57	1	0	-3.609573	-1.768306	-0.985336
58	1	0	-2.940677	-0.889818	-2.368734
59	1	0	-2.592019	-5.188024	-2.237402
60	1	0	-3.394305	-4.341114	-0.913316
61	1	0	-0.381329	-0.691966	-2.647974
62	1	0	0.680308	-1.482399	-1.487734
63	1	0	-1.808986	2.650113	1.315238
64	1	0	-0.312367	2.714860	0.380539
65	1	0	-1.465962	4.897968	0.348373
66	1	0	-3.696185	5.125038	-0.791702
67	1	0	-3.810794	4.080567	0.628954
68	1	0	-4.982247	3.029957	-1.314041
69	1	0	-3.670371	2.347573	-3.332743
70	1	0	-3.622856	4.101521	-3.129936
71	1	0	-1.332215	3.191562	-3.612075
72	1	0	-1.681139	0.946534	-2.673674
73	1	0	-0.228163	1.682770	-1.985886
74	1	0	-3.866713	0.833596	-1.252436
75	1	0	-3.866036	1.568372	0.355374
76	1	0	-1.536141	5.218180	-2.143338
77	1	0	-0.148344	4.233015	-1.669757
78	1	0	2.549860	0.631578	-1.926035
79	1	0	3.258435	2.752264	-2.989312
80	1	0	2.875407	4.795424	0.787793
81	1	0	2.170318	2.678114	1.870044
82	1	0	3.428392	4.838678	-1.640685
83	1	0	3.417541	-2.372984	-0.013203
84	1	0	3.978610	-0.911198	-0.868204
85	1	0	5.573685	-2.209994	1.385542
86	1	0	6.879044	-3.059238	-0.504038
87	1	0	5.378004	-3.675307	-0.504817
88	1	0	7.929701	0.385205	1.120707
89	1	0	7.365306	-1.016086	1.970677
90	1	0	-4.873460	-3.456791	0.838188
91	1	0	-3.520219	-3.368788	1.984521
92	1	0	-5.165340	-2.967594	2.520473
93	1	0	-5.983575	-1.412214	0.128899
94	1	0	-6.194455	-0.869964	1.808840
95	1	0	-5.354638	0.165679	0.631877
96	1	0	-0.487637	0.929394	2.654519

CP3-iso

SCF Done: E(RB3LYP) = -2555.65070232 A.U.; No imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.904285	1.755456	1.253187
2	6	0	3.997070	1.066483	0.441866
3	6	0	3.681806	1.534842	-0.839715
4	6	0	4.292350	2.696732	-1.311576
5	6	0	5.198574	3.393810	-0.505453
6	6	0	5.501257	2.925134	0.773955
7	79	0	0.818104	-0.150576	0.666066
8	16	0	3.217523	-0.408076	1.132564
9	6	0	3.732368	-1.785801	0.005424
10	6	0	5.105279	-2.382524	0.346918
11	6	0	6.237626	-1.442593	-0.115396
12	8	0	6.271473	-0.987059	-1.256240
13	15	0	-1.502710	0.042739	0.202072
14	6	0	-1.711647	1.634891	-0.835696
15	6	0	-3.187012	2.050838	-1.049614
16	6	0	-3.257886	3.359546	-1.873267
17	6	0	-2.572101	3.159062	-3.238917
18	6	0	-1.094481	2.780593	-3.016366
19	6	0	-1.025470	1.460487	-2.215277
20	6	0	-2.548423	4.488498	-1.101599
21	6	0	-1.074006	4.099999	-0.880341
22	6	0	-0.997451	2.787124	-0.069380
23	6	0	-0.378971	3.902790	-2.241096
24	6	0	-2.395414	0.345573	1.821128
25	6	0	-3.775538	0.205969	2.128237
26	6	0	-4.236540	0.614047	3.390515
27	6	0	-3.389250	1.146450	4.357655
28	6	0	-2.032024	1.273412	4.072725
29	6	0	-1.554992	0.874238	2.826778
30	7	0	-4.725760	-0.376346	1.207735
31	6	0	-5.296493	-1.632114	1.723332
32	6	0	-1.939722	-1.591453	-0.695873
33	6	0	-3.278314	-1.579937	-1.475385
34	6	0	-3.534515	-2.970205	-2.103186
35	6	0	-3.580855	-4.045225	-0.998787
36	6	0	-2.231390	-4.077670	-0.253592
37	6	0	-1.960269	-2.700164	0.392211
38	6	0	-2.405343	-3.302264	-3.096848
39	6	0	-1.062549	-3.328016	-2.341958
40	6	0	-0.797008	-1.947659	-1.696368
41	6	0	-1.102618	-4.410576	-1.247700
42	7	0	5.221078	-3.632656	-0.421235
43	6	0	-5.825672	0.527891	0.837312
44	7	0	7.184522	-1.186678	0.816959
45	1	0	-1.342570	1.675394	4.808948
46	1	0	-3.785490	1.448481	5.322897
47	1	0	-5.292567	0.502364	3.617429
48	1	0	-0.995166	-2.721787	0.917431
49	1	0	-2.725837	-2.487350	1.141787
50	1	0	-2.263422	-4.832895	0.542093
51	1	0	-0.137565	-4.458050	-0.724612
52	1	0	-1.274256	-5.397421	-1.698137

53	1	0	-0.244845	-3.537511	-3.043541
54	1	0	-2.374645	-2.553659	-3.900379
55	1	0	-2.588341	-4.276413	-3.570148
56	1	0	-4.497100	-2.938821	-2.629813
57	1	0	-4.092650	-1.300065	-0.803936
58	1	0	-3.236576	-0.830136	-2.274618
59	1	0	-3.785520	-5.029066	-1.442309
60	1	0	-4.398079	-3.834428	-0.297093
61	1	0	-0.714368	-1.193315	-2.482771
62	1	0	0.169118	-1.975639	-1.176454
63	1	0	-1.463348	2.934118	0.912221
64	1	0	0.054579	2.528318	0.107516
65	1	0	-0.562712	4.886693	-0.310878
66	1	0	-2.609638	5.428710	-1.666055
67	1	0	-3.044685	4.659024	-0.136518
68	1	0	-4.314656	3.616169	-2.021224
69	1	0	-3.082600	2.370702	-3.808854
70	1	0	-2.640786	4.080746	-3.831962
71	1	0	-0.601195	2.622076	-3.983769
72	1	0	-1.526737	0.677028	-2.792968
73	1	0	0.020943	1.155291	-2.084424
74	1	0	-3.749346	1.260953	-1.558431
75	1	0	-3.658494	2.217683	-0.076214
76	1	0	-0.406298	4.836544	-2.818413
77	1	0	0.678999	3.646391	-2.092453
78	1	0	2.968623	1.001474	-1.460388
79	1	0	4.053265	3.061108	-2.306297
80	1	0	6.204872	3.463181	1.402101
81	1	0	5.144579	1.382271	2.243604
82	1	0	5.665706	4.301642	-0.875628
83	1	0	2.954991	-2.542791	0.138678
84	1	0	3.712941	-1.433446	-1.027017
85	1	0	5.169236	-2.533390	1.435542
86	1	0	6.161412	-4.012295	-0.313122
87	1	0	4.596263	-4.326078	-0.010862
88	1	0	7.969926	-0.596119	0.575772
89	1	0	7.149126	-1.573831	1.748830
90	1	0	-5.851581	-2.125522	0.918290
91	1	0	-4.504715	-2.303222	2.060755
92	1	0	-5.990200	-1.472508	2.565625
93	1	0	-6.391478	0.069914	0.018920
94	1	0	-6.526207	0.718062	1.667817
95	1	0	-5.435853	1.484961	0.491484
96	1	0	-0.493638	0.980319	2.628798

CP2-cis

SCF Done: E(RB3LYP) = -2555.61288320 A.U.; No imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.122241	-0.940336	3.728543
2	6	0	4.101549	0.524880	3.249782
3	6	0	3.150308	1.348916	4.137773
4	6	0	1.731739	0.754816	4.048581
5	6	0	1.748263	-0.706000	4.536978
6	6	0	2.698906	-1.525434	3.643904

7	6	0	3.618559	0.585627	1.780476
8	6	0	2.191097	-0.010535	1.666164
9	6	0	1.234951	0.800003	2.585525
10	6	0	2.211663	-1.479198	2.177647
11	15	0	1.477855	-0.044891	-0.110557
12	6	0	1.762389	1.521621	-1.168937
13	6	0	3.230704	1.750408	-1.616367
14	6	0	3.324097	3.018895	-2.498197
15	6	0	2.830098	4.246781	-1.709600
16	6	0	1.363696	4.025418	-1.291986
17	6	0	1.271965	2.772443	-0.391488
18	6	0	2.458514	2.830264	-3.758690
19	6	0	0.993388	2.609586	-3.337004
20	6	0	0.890520	1.350246	-2.447223
21	6	0	0.490019	3.833704	-2.547602
22	79	0	-0.873651	-0.840674	-0.225399
23	7	0	0.075870	-2.607918	-1.325624
24	6	0	-0.566925	-2.652891	-2.677892
25	6	0	-2.795271	-1.652453	-0.315161
26	6	0	-3.261531	-2.396335	0.773912
27	6	0	-4.513208	-3.020397	0.712448
28	6	0	-5.310380	-2.887144	-0.427140
29	6	0	-4.854262	-2.126494	-1.505644
30	6	0	-3.600801	-1.503663	-1.448665
31	16	0	-1.883081	1.010699	0.908524
32	6	0	-3.207306	1.639510	-0.210785
33	6	0	-3.911381	2.833001	0.455335
34	6	0	-4.752953	2.344729	1.652500
35	8	0	-5.568910	1.430905	1.545911
36	7	0	-4.828925	3.418749	-0.537366
37	6	0	2.303271	-1.439212	-0.984940
38	6	0	1.549960	-2.520277	-1.476671
39	6	0	2.193522	-3.578858	-2.132879
40	6	0	3.575185	-3.585635	-2.297889
41	6	0	4.337118	-2.528616	-1.802616
42	6	0	3.702308	-1.472900	-1.156427
43	6	0	-0.279251	-3.839055	-0.548991
44	7	0	-4.535827	3.008364	2.813492
45	1	0	1.621438	-4.413908	-2.519627
46	1	0	4.048898	-4.418311	-2.808280
47	1	0	5.416424	-2.522305	-1.916580
48	1	0	4.308947	-0.661481	-0.777264
49	1	0	1.205013	-1.913911	2.111049
50	1	0	2.873380	-2.092780	1.556964
51	1	0	2.707538	-2.573224	3.969813
52	1	0	0.208947	-3.797415	0.425602
53	1	0	0.045591	-4.737196	-1.081716
54	1	0	-1.359794	-3.870664	-0.417215
55	1	0	0.734912	-1.128978	4.501398
56	1	0	2.080082	-0.752506	5.582729
57	1	0	1.041011	1.345770	4.663353
58	1	0	3.143876	2.398854	3.814835
59	1	0	3.499734	1.335081	5.178799
60	1	0	5.113754	0.946072	3.294944
61	1	0	4.324035	0.031132	1.153463
62	1	0	3.626903	1.627689	1.442296
63	1	0	4.489030	-0.991967	4.762267
64	1	0	4.812877	-1.531320	3.111789

65	1	0	1.164014	1.841148	2.255100
66	1	0	0.226415	0.375523	2.537315
67	1	0	1.221847	0.470269	-3.013643
68	1	0	-0.159290	1.187601	-2.172343
69	1	0	0.367960	2.455910	-4.225543
70	1	0	-1.646249	-2.721926	-2.550989
71	1	0	-0.217466	-3.522509	-3.241834
72	1	0	-0.317035	-1.740812	-3.221883
73	1	0	2.534545	3.714566	-4.405410
74	1	0	2.819067	1.972313	-4.342402
75	1	0	4.374080	3.158032	-2.785311
76	1	0	3.457270	4.404952	-0.821630
77	1	0	2.915805	5.149760	-2.328824
78	1	0	1.004910	4.889088	-0.717873
79	1	0	1.893670	2.930521	0.497009
80	1	0	0.241548	2.625057	-0.049737
81	1	0	3.891246	1.862850	-0.749532
82	1	0	3.589174	0.894285	-2.196266
83	1	0	0.534981	4.731784	-3.178020
84	1	0	-0.561304	3.693721	-2.261064
85	1	0	-2.657723	-2.499168	1.671734
86	1	0	-4.863956	-3.603524	1.560147
87	1	0	-5.470892	-2.010012	-2.393140
88	1	0	-3.266722	-0.903762	-2.291354
89	1	0	-6.284098	-3.367122	-0.470847
90	1	0	-3.153636	3.549735	0.810743
91	1	0	-5.320387	4.206299	-0.114131
92	1	0	-4.272181	3.821545	-1.290864
93	1	0	-5.062234	2.750178	3.638103
94	1	0	-3.866476	3.760103	2.892795
95	1	0	-2.757401	1.963041	-1.153913
96	1	0	-3.945288	0.863199	-0.407985

TSrd-cis

SCF Done: E(RB3LYP) = -2555.59679983 A.U.; An imaginary frequency of -226.0526 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.097307	3.127965	-3.622887
2	6	0	-2.972557	3.260242	-2.361742
3	6	0	-2.413650	4.374323	-1.455455
4	6	0	-0.971706	4.019322	-1.045316
5	6	0	-0.090839	3.884342	-2.302310
6	6	0	-0.657377	2.772089	-3.205052
7	6	0	-2.978606	1.913469	-1.599669
8	6	0	-1.538711	1.546200	-1.154816
9	6	0	-0.975080	2.685191	-0.265116
10	6	0	-0.655729	1.434021	-2.431540
11	15	0	-1.360231	-0.112640	-0.228183
12	6	0	-2.220610	-0.218915	1.480089
13	6	0	-3.637429	0.403922	1.570930
14	6	0	-4.213504	0.209773	2.994780
15	6	0	-3.301703	0.911993	4.018959
16	6	0	-1.892540	0.291903	3.953248
17	6	0	-1.309458	0.474057	2.533768
18	6	0	-4.296978	-1.294071	3.322566

19	6	0	-2.884471	-1.908387	3.262468
20	6	0	-2.309872	-1.729594	1.839975
21	6	0	-1.970314	-1.209981	4.286944
22	79	0	0.983000	-0.816130	-0.035862
23	7	0	0.092236	-2.550454	-1.633898
24	6	0	0.427837	-3.855510	-1.016016
25	6	0	2.962955	-1.617907	0.208447
26	6	0	3.800870	-1.572376	-0.915067
27	6	0	4.733263	-2.597504	-1.114886
28	6	0	4.839907	-3.646397	-0.199778
29	6	0	4.005527	-3.677956	0.924834
30	6	0	3.075986	-2.661802	1.143299
31	16	0	2.636413	0.398035	1.340272
32	6	0	3.579316	1.474275	0.182035
33	6	0	4.106901	2.705220	0.941255
34	6	0	2.940684	3.647206	1.301592
35	8	0	2.178804	4.092585	0.444667
36	7	0	5.012325	3.421757	0.029194
37	6	0	-2.125768	-1.397802	-1.304638
38	6	0	-1.346624	-2.429483	-1.873672
39	6	0	-1.958970	-3.385200	-2.698227
40	6	0	-3.326198	-3.349010	-2.956146
41	6	0	-4.109282	-2.345680	-2.386259
42	6	0	-3.509265	-1.386398	-1.575404
43	6	0	0.864229	-2.347287	-2.882827
44	7	0	2.830827	3.948563	2.616756
45	1	0	-1.360214	-4.172770	-3.143783
46	1	0	-3.774034	-4.103325	-3.596168
47	1	0	-5.178429	-2.305714	-2.570442
48	1	0	-4.132815	-0.614588	-1.143212
49	1	0	0.375523	1.176932	-2.155382
50	1	0	-1.031521	0.632725	-3.080778
51	1	0	-0.028016	2.656468	-4.096951
52	1	0	0.623287	-1.369467	-3.304739
53	1	0	0.642257	-3.124085	-3.626485
54	1	0	1.929877	-2.383645	-2.646065
55	1	0	0.940719	3.656817	-2.006439
56	1	0	-0.069013	4.836574	-2.850089
57	1	0	-0.559430	4.795036	-0.389529
58	1	0	-3.045462	4.489502	-0.563717
59	1	0	-2.431064	5.335213	-1.987513
60	1	0	-4.005221	3.496306	-2.649321
61	1	0	-3.379402	1.137815	-2.260397
62	1	0	-3.647803	1.988687	-0.736443
63	1	0	-2.102742	4.070053	-4.187571
64	1	0	-2.503945	2.352163	-4.286117
65	1	0	-1.591732	2.803080	0.633429
66	1	0	0.044583	2.450037	0.062034
67	1	0	-2.949189	-2.254215	1.121467
68	1	0	-1.313635	-2.189926	1.782917
69	1	0	-2.937216	-2.982608	3.481336
70	1	0	1.489042	-3.862216	-0.760700
71	1	0	0.225103	-4.693874	-1.694694
72	1	0	-0.158626	-3.983781	-0.103700
73	1	0	-4.727709	-1.437038	4.322632
74	1	0	-4.961155	-1.801856	2.609922
75	1	0	-5.216867	0.653444	3.023101
76	1	0	-3.252291	1.988819	3.807002

77	1	0	-3.715789	0.801928	5.030241
78	1	0	-1.229498	0.798392	4.666369
79	1	0	-1.210919	1.542800	2.315267
80	1	0	-0.301258	0.045278	2.494592
81	1	0	-3.598120	1.475666	1.346357
82	1	0	-4.315909	-0.059555	0.846877
83	1	0	-2.363838	-1.352578	5.302399
84	1	0	-0.966383	-1.656229	4.265764
85	1	0	3.725219	-0.765434	-1.636965
86	1	0	5.372443	-2.569147	-1.993047
87	1	0	4.087318	-4.488560	1.643696
88	1	0	2.455922	-2.672036	2.034577
89	1	0	5.573081	-4.432163	-0.355027
90	1	0	4.604919	2.371068	1.865646
91	1	0	5.337502	4.276195	0.481728
92	1	0	5.847180	2.853156	-0.110291
93	1	0	2.095571	4.573325	2.921722
94	1	0	3.472403	3.594104	3.311129
95	1	0	4.422893	0.903925	-0.217257
96	1	0	2.942523	1.809389	-0.637757

Prod

SCF Done: E(RB3LYP) = -933.114169000 A.U.; No imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.671547	1.243662	-0.306227
2	6	0	1.696337	0.234064	-0.236514
3	6	0	2.068758	-1.053082	0.173198
4	6	0	3.399160	-1.319088	0.511697
5	6	0	4.367130	-0.317269	0.442049
6	6	0	3.995033	0.965976	0.029331
7	16	0	0.034976	0.701093	-0.706924
8	6	0	-0.957439	-0.803649	-0.356450
9	6	0	-2.446836	-0.497900	-0.554232
10	7	0	-3.181183	-1.772538	-0.466611
11	6	0	-2.954840	0.413892	0.583262
12	7	0	-3.736881	1.444119	0.182996
13	8	0	-2.683426	0.195398	1.762120
14	1	0	1.338959	-1.852574	0.231821
15	1	0	3.673066	-2.321602	0.829589
16	1	0	4.736903	1.757852	-0.029429
17	1	0	2.392546	2.245995	-0.621347
18	1	0	5.398809	-0.531239	0.705659
19	1	0	-0.651775	-1.605709	-1.034762
20	1	0	-0.802014	-1.118962	0.677628
21	1	0	-2.588316	0.012335	-1.520841
22	1	0	-4.178650	-1.590902	-0.580399
23	1	0	-2.920312	-2.350326	-1.265643
24	1	0	-4.135974	2.062387	0.877214
25	1	0	-3.962105	1.611375	-0.787048

LAu(I)-SbF_6

SCF Done: E(RB3LYP) = -2227.29357958 A.U.; No imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.960406	4.138833	-0.499894
2	6	0	-0.079957	4.061412	0.761682
3	6	0	1.187306	4.917649	0.568215
4	6	0	1.978284	4.391923	-0.645467
5	6	0	1.103238	4.476712	-1.909272
6	6	0	-0.159357	3.616788	-1.707682
7	6	0	0.325430	2.593273	1.019936
8	6	0	1.138153	2.040837	-0.187357
9	6	0	2.396662	2.922440	-0.397201
10	6	0	0.246631	2.146497	-1.459211
11	15	0	1.483635	0.195220	0.201354
12	6	0	2.731005	-0.717765	-0.920153
13	6	0	2.246615	-0.639365	-2.392889
14	6	0	3.153112	-1.502519	-3.298952
15	6	0	3.117118	-2.970140	-2.830857
16	6	0	3.629452	-3.054439	-1.379869
17	6	0	2.716975	-2.207080	-0.465674
18	6	0	4.596855	-0.968417	-3.227053
19	6	0	5.099120	-1.057228	-1.773597
20	6	0	4.195298	-0.207694	-0.846878
21	6	0	5.074441	-2.525135	-1.306714
22	6	0	2.140202	0.105626	1.929483
23	6	0	1.484715	-0.584435	2.981128
24	6	0	2.068388	-0.595187	4.257694
25	6	0	3.267618	0.059987	4.522892
26	6	0	3.912556	0.749330	3.496880
27	6	0	3.351615	0.766716	2.222236
28	7	0	0.231787	-1.270075	2.781320
29	6	0	0.342074	-2.725669	2.936221
30	79	0	-0.545376	-0.859940	0.068998
31	9	0	-2.613458	-1.742558	-0.074447
32	6	0	-0.864569	-0.711670	3.582830
33	1	0	1.564736	-1.129093	5.058192
34	1	0	3.692068	0.033663	5.522398
35	1	0	4.846107	1.272267	3.680805
36	1	0	3.873275	1.309743	1.445684
37	1	0	-0.575194	1.983775	1.171833
38	1	0	0.920457	2.534480	1.938334
39	1	0	-0.642993	4.421452	1.632307
40	1	0	-0.932420	0.365723	3.409467
41	1	0	-0.748541	-0.887031	4.665477
42	1	0	-1.803981	-1.172802	3.260313
43	1	0	-1.869246	3.537274	-0.361689
44	1	0	-1.279613	5.174858	-0.675820
45	1	0	-0.782190	3.651730	-2.610776
46	1	0	1.665825	4.125157	-2.784986
47	1	0	0.822861	5.520583	-2.104027
48	1	0	2.889482	4.988138	-0.781856
49	1	0	3.049180	2.888688	0.480747
50	1	0	2.975745	2.562676	-1.255208
51	1	0	0.911647	5.968771	0.409383
52	1	0	1.810590	4.881015	1.472156
53	1	0	0.779724	1.766362	-2.336843
54	1	0	-0.655615	1.535557	-1.340579
55	1	0	3.057669	-2.284905	0.574469

56	1	0	1.694074	-2.603990	-0.503396
57	1	0	3.595023	-4.094780	-1.032191
58	1	0	-0.609776	-3.183429	2.647064
59	1	0	0.573728	-3.037221	3.968740
60	1	0	1.123904	-3.106845	2.273825
61	1	0	5.731735	-3.134154	-1.941571
62	1	0	5.455447	-2.602949	-0.279352
63	1	0	6.120959	-0.662576	-1.707548
64	1	0	4.633693	0.071491	-3.579444
65	1	0	5.250257	-1.554873	-3.886694
66	1	0	2.780194	-1.430646	-4.328506
67	1	0	2.278721	0.397067	-2.747216
68	1	0	1.204881	-0.978448	-2.466112
69	1	0	4.258630	0.845024	-1.142409
70	1	0	4.574281	-0.287559	0.176493
71	1	0	3.741819	-3.589803	-3.487902
72	1	0	2.093227	-3.363479	-2.894273
73	51	0	-3.986796	-0.418854	-0.441406
74	9	0	-3.050816	0.768294	0.664692
75	9	0	-5.288485	0.851643	-0.798666
76	9	0	-4.795829	-1.686930	-1.530668
77	9	0	-4.890201	-1.071889	1.044599
78	9	0	-2.935379	0.148154	-1.877828

LAu(I)-Cl

SCF Done: E(RB3LYP) = -2082.94143912 A.U.; No imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.588510	-1.506714	2.500770
2	6	0	0.114096	-0.243325	2.069226
3	6	0	-0.231878	0.704134	3.055844
4	6	0	-0.116380	0.432262	4.416750
5	6	0	0.358464	-0.811556	4.831999
6	6	0	0.703598	-1.762877	3.876844
7	15	0	-0.074116	0.215276	0.281912
8	79	0	0.370653	-1.565370	-1.155187
9	7	0	0.949577	-2.542595	1.565663
10	6	0	0.086127	-3.724793	1.665207
11	6	0	1.221495	1.584509	-0.048560
12	6	0	1.020421	2.147184	-1.481111
13	6	0	2.146615	3.148041	-1.825809
14	6	0	3.513367	2.440382	-1.752092
15	6	0	3.733401	1.905612	-0.323394
16	6	0	2.616090	0.897176	0.023595
17	6	0	3.706244	3.074944	0.678847
18	6	0	2.335640	3.774025	0.601285
19	6	0	2.112493	4.317664	-0.822893
20	6	0	1.219231	2.762977	0.960059
21	6	0	-1.901892	0.750138	0.019478
22	6	0	-2.276338	2.167122	0.529469
23	6	0	-3.778153	2.446151	0.276439
24	6	0	-4.631161	1.397031	1.016158
25	6	0	-4.285631	-0.008702	0.485544
26	6	0	-2.790306	-0.300413	0.744562
27	6	0	-4.071255	2.382315	-1.233519

28	6	0	-3.721869	0.975349	-1.754656
29	6	0	-2.225473	0.684471	-1.503005
30	6	0	-4.578110	-0.077192	-1.025309
31	6	0	2.371568	-2.898215	1.616560
32	1	0	1.069942	-2.733285	4.198665
33	1	0	0.458040	-1.040161	5.889321
34	1	0	-0.394860	1.190458	5.142463
35	1	0	-0.597845	1.679041	2.763100
36	1	0	-2.541146	-1.309868	0.389016
37	1	0	-2.598551	-0.281456	1.823034
38	1	0	-4.881806	-0.762740	1.015388
39	1	0	-0.960937	-3.422463	1.574034
40	1	0	0.209746	-4.277989	2.611954
41	1	0	0.323242	-4.404296	0.840003
42	1	0	-4.352047	-1.081435	-1.409310
43	1	0	-5.644692	0.107205	-1.211560
44	1	0	-3.905965	0.921370	-2.835384
45	1	0	-3.482994	3.141553	-1.766935
46	1	0	-5.130262	2.604248	-1.422174
47	1	0	-4.008842	3.448722	0.658798
48	1	0	-2.080635	2.265262	1.601457
49	1	0	-1.678383	2.928130	0.015935
50	1	0	-5.698648	1.605398	0.863311
51	1	0	-4.444434	1.450726	2.097514
52	1	0	-1.615310	1.404154	-2.059238
53	1	0	-1.978495	-0.310494	-1.893139
54	1	0	2.781516	0.491584	1.030075
55	1	0	2.656449	0.053326	-0.676930
56	1	0	4.698802	1.386657	-0.264938
57	1	0	2.593266	-3.580838	0.789315
58	1	0	2.666153	-3.393979	2.557455
59	1	0	2.981087	-1.998788	1.494178
60	1	0	4.508226	3.788804	0.447428
61	1	0	3.886720	2.705640	1.697594
62	1	0	2.296666	4.598652	1.324523
63	1	0	1.147605	4.839687	-0.883384
64	1	0	2.890794	5.051494	-1.072090
65	1	0	1.976326	3.524132	-2.842721
66	1	0	0.055525	2.661523	-1.554949
67	1	0	1.009582	1.326633	-2.210814
68	1	0	0.252225	3.277051	0.959667
69	1	0	1.393444	2.391366	1.974770
70	1	0	4.315159	3.141820	-2.019346
71	1	0	3.552619	1.614837	-2.476090
72	17	0	0.824846	-3.336153	-2.745781

Chemoselectivity studies

N-arylation pathway

CP1^{amino}

SCF Done: E(RB3LYP) = -3016.43182834 A.U.; No imaginary frequency

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.728631	-3.836559	1.592673
2	6	0	4.209492	-2.440828	2.031840
3	6	0	3.656852	-2.110845	3.430034

4	6	0	2.118249	-2.132205	3.377847
5	6	0	1.630939	-3.529432	2.952269
6	6	0	2.188626	-3.853694	1.552524
7	6	0	3.720269	-1.377177	1.018018
8	6	0	2.167193	-1.392129	0.950167
9	6	0	1.610622	-1.080763	2.363482
10	6	0	1.683372	-2.807127	0.529490
11	15	0	1.475045	-0.134210	-0.333629
12	6	0	2.292311	1.603480	-0.333084
13	6	0	3.743231	1.595554	-0.897834
14	6	0	4.320448	3.033995	-0.878123
15	6	0	4.328118	3.584721	0.560192
16	6	0	2.885267	3.611729	1.096837
17	6	0	2.323205	2.171484	1.110200
18	6	0	3.462668	3.942354	-1.778139
19	6	0	2.020097	3.963063	-1.240073
20	6	0	1.443547	2.527879	-1.251422
21	6	0	2.012176	4.511338	0.200400
22	79	0	-0.934268	0.033622	-0.377842
23	7	0	-0.717465	-0.804068	-2.523047
24	6	0	-1.230911	0.250251	-3.456642
25	6	0	-1.221946	0.947388	1.465233
26	6	0	-1.577446	0.162562	2.562087
27	6	0	-1.899746	0.788086	3.773388
28	6	0	-1.872784	2.179612	3.881267
29	6	0	-1.540203	2.953227	2.768559
30	6	0	-1.216133	2.339940	1.551101
31	7	0	-3.112150	0.390081	-0.629728
32	6	0	-4.118825	-0.107013	0.347073
33	6	0	-5.119374	-1.077909	-0.302345
34	6	0	1.746367	-0.859250	-2.005974
35	6	0	0.678742	-1.122066	-2.879573
36	6	0	0.928177	-1.687288	-4.136924
37	6	0	2.222873	-2.005413	-4.534738
38	6	0	3.291332	-1.754473	-3.675838
39	6	0	3.051093	-1.186106	-2.429255
40	6	0	-1.563819	-2.035408	-2.616886
41	17	0	-2.155296	-2.935290	0.752067
42	1	0	0.110041	-1.884426	-4.819658
43	1	0	2.390583	-2.445794	-5.512374
44	1	0	4.307753	-1.995951	-3.969076
45	1	0	3.896789	-0.996063	-1.784427
46	1	0	0.587931	-2.835080	0.485330
47	1	0	2.067493	-3.061511	-0.464499
48	1	0	1.834491	-4.840592	1.229167
49	1	0	-1.180918	-2.785121	-1.927098
50	1	0	-1.580809	-2.420943	-3.640072
51	1	0	-2.583761	-1.792467	-2.322315
52	1	0	0.534074	-3.562127	2.938804
53	1	0	1.969617	-4.282975	3.675739
54	1	0	1.706953	-1.876641	4.362417
55	1	0	4.014628	-1.125156	3.757354
56	1	0	4.019966	-2.844563	4.161726
57	1	0	5.306073	-2.409433	2.044694
58	1	0	4.162279	-1.602693	0.044319
59	1	0	4.084259	-0.393810	1.331594
60	1	0	4.097143	-4.596467	2.294329
61	1	0	4.138408	-4.084966	0.604281

62	1	0	1.909328	-0.081491	2.694778
63	1	0	0.521588	-1.103878	2.342915
64	1	0	1.449334	2.140086	-2.278102
65	1	0	0.399251	2.555858	-0.923083
66	1	0	1.388371	4.588728	-1.882457
67	1	0	-2.265500	0.490093	-3.209907
68	1	0	-1.200550	-0.101052	-4.491985
69	1	0	-0.620724	1.148647	-3.358212
70	1	0	3.874704	4.959863	-1.788914
71	1	0	3.477765	3.576431	-2.813443
72	1	0	5.345597	2.985202	-1.265593
73	1	0	4.961017	2.960239	1.204940
74	1	0	4.755925	4.595735	0.570643
75	1	0	2.875556	3.990339	2.126255
76	1	0	2.964165	1.550616	1.745226
77	1	0	1.322954	2.166575	1.552243
78	1	0	4.392376	0.938463	-0.312101
79	1	0	3.746275	1.234506	-1.930093
80	1	0	2.399521	5.538363	0.210674
81	1	0	0.985835	4.553880	0.588100
82	1	0	-1.630501	-0.918186	2.471493
83	1	0	-2.174174	0.176481	4.628581
84	1	0	-1.535048	4.037686	2.833249
85	1	0	-0.982972	2.961235	0.693653
86	1	0	-2.120821	2.659078	4.823770
87	1	0	-3.607612	-0.683066	1.122180
88	6	0	-4.799416	1.133299	0.964552
89	1	0	-3.224205	1.415620	-0.637546
90	1	0	-3.391960	0.086516	-1.564498
91	7	0	-5.585985	0.900863	2.030362
92	8	0	-4.627198	2.249376	0.467848
93	1	0	-5.842582	-1.402623	0.448383
94	16	0	-6.012936	-0.314173	-1.734825
95	1	0	-4.567922	-1.956161	-0.643725
96	1	0	-6.163606	-1.450454	-2.442351
97	1	0	-6.047443	1.680629	2.480699
98	1	0	-5.641388	-0.002283	2.479811

CP2^{amino}

SCF Done: E(RB3LYP) = -2555.59011940 A.U.; No imaginary frequency

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.471323	-4.667382	0.564176
2	6	0	3.574981	-3.628427	0.836225
3	6	0	3.662030	-3.348383	2.348152
4	6	0	2.310887	-2.793039	2.837147
5	6	0	1.196480	-3.822177	2.565969
6	6	0	1.121945	-4.108430	1.053340
7	6	0	3.251779	-2.322296	0.070151
8	6	0	1.900516	-1.734874	0.565242
9	6	0	2.005595	-1.473378	2.091628
10	6	0	0.798276	-2.799534	0.297098
11	15	0	1.362020	-0.132902	-0.338854
12	6	0	2.360683	1.447271	0.102285
13	6	0	3.899724	1.241952	0.117558

14	6	0	4.607757	2.581911	0.434948
15	6	0	4.165888	3.087909	1.820340
16	6	0	2.642026	3.309532	1.811665
17	6	0	1.924547	1.977383	1.495106
18	6	0	4.246158	3.625230	-0.639975
19	6	0	2.721761	3.852466	-0.637321
20	6	0	2.003224	2.522452	-0.963578
21	6	0	2.274808	4.359683	0.746554
22	79	0	-1.073867	0.194063	-0.323696
23	7	0	-0.850568	-0.227791	-2.595850
24	6	0	-1.451367	0.956173	-3.288193
25	6	0	-1.361476	0.602487	1.671505
26	6	0	-1.463627	-0.416810	2.619013
27	6	0	-1.739724	-0.098807	3.955841
28	6	0	-1.915280	1.230106	4.343163
29	6	0	-1.823056	2.245753	3.387861
30	6	0	-1.551879	1.935444	2.050643
31	7	0	-3.129142	0.574848	-0.616693
32	6	0	-4.161776	0.438343	0.404855
33	6	0	-4.552811	-0.990995	0.813564
34	6	0	1.622811	-0.424399	-2.142370
35	6	0	0.543914	-0.417793	-3.042866
36	6	0	0.773729	-0.606814	-4.412566
37	6	0	2.061161	-0.796546	-4.904305
38	6	0	3.141727	-0.805785	-4.023933
39	6	0	2.918603	-0.623607	-2.663046
40	6	0	-1.629580	-1.468603	-2.902210
41	1	0	-0.055758	-0.607305	-5.110159
42	1	0	2.213757	-0.937492	-5.969685
43	1	0	4.153036	-0.953947	-4.388825
44	1	0	3.771217	-0.641594	-1.999532
45	1	0	-0.182983	-2.429049	0.615268
46	1	0	0.730392	-3.005122	-0.778915
47	1	0	0.321401	-4.830249	0.848660
48	1	0	-1.188724	-2.308910	-2.364365
49	1	0	-1.623659	-1.679305	-3.975953
50	1	0	-2.664027	-1.342497	-2.583040
51	1	0	0.231721	-3.444248	2.930350
52	1	0	1.402303	-4.750993	3.114066
53	1	0	2.363093	-2.575129	3.911153
54	1	0	4.465265	-2.628701	2.557059
55	1	0	3.909666	-4.272321	2.887303
56	1	0	4.538722	-4.004279	0.470210
57	1	0	3.196619	-2.551384	-0.998181
58	1	0	4.067621	-1.605999	0.214558
59	1	0	2.701028	-5.606854	1.084096
60	1	0	2.421201	-4.896728	-0.508820
61	1	0	2.813033	-0.762011	2.295230
62	1	0	1.079308	-1.033310	2.474584
63	1	0	2.301560	2.185574	-1.962505
64	1	0	0.917466	2.686791	-0.984960
65	1	0	2.452779	4.584622	-1.409067
66	1	0	-2.437809	1.147896	-2.866925
67	1	0	-1.544726	0.779374	-4.363796
68	1	0	-0.812576	1.823692	-3.114608
69	1	0	4.767393	4.569918	-0.436283
70	1	0	4.576907	3.281726	-1.629505
71	1	0	5.690174	2.402176	0.430128

72	1	0	4.439867	2.359652	2.595795
73	1	0	4.683660	4.025785	2.061425
74	1	0	2.308147	3.649116	2.800336
75	1	0	2.156706	1.249277	2.278139
76	1	0	0.844910	2.134205	1.514173
77	1	0	4.181397	0.498997	0.871915
78	1	0	4.256503	0.882271	-0.851042
79	1	0	2.765389	5.315584	0.973692
80	1	0	1.191869	4.543967	0.752023
81	1	0	-1.347666	-1.457745	2.336766
82	1	0	-1.819189	-0.898456	4.687323
83	1	0	-1.966003	3.283756	3.675950
84	1	0	-1.498771	2.733991	1.316615
85	1	0	-2.129169	1.473362	5.379943
86	1	0	-3.817496	0.935038	1.319048
87	6	0	-5.437183	1.229166	-0.003124
88	1	0	-3.386754	-0.094468	-1.345905
89	7	0	-5.208575	2.263868	-0.838147
90	8	0	-6.544427	0.949356	0.460279
91	1	0	-5.339697	-0.949456	1.567317
92	16	0	-5.225394	-2.008887	-0.581823
93	1	0	-3.692136	-1.513833	1.231233
94	1	0	-4.143004	-2.786452	-0.782405
95	1	0	-5.980391	2.823904	-1.172901
96	1	0	-4.286089	2.359469	-1.243675

TS$^{rd\text{-}amino}$

SCF Done: E(RB3LYP) = -2555.56744685 A.U.; An imaginary frequency of -334.7644 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.193150	-2.178034	1.375260
2	6	0	-1.854839	-1.746812	1.268319
3	6	0	-0.885139	-2.382623	2.072455
4	6	0	-1.272718	-3.410762	2.943975
5	6	0	-2.599875	-3.820038	3.034058
6	6	0	-3.567088	-3.199467	2.244091
7	15	0	-1.401992	-0.368108	0.126376
8	79	0	0.961179	-0.056959	0.418834
9	7	0	3.023248	0.235688	0.520750
10	6	0	4.036910	-0.219780	-0.411987
11	6	0	5.211298	0.756006	-0.685238
12	8	0	6.204100	0.359498	-1.293610
13	7	0	0.518131	-1.993508	2.028818
14	6	0	1.382890	-3.119896	1.616172
15	6	0	-1.729102	-0.993278	-1.650697
16	6	0	-3.127884	-1.628113	-1.875223
17	6	0	-3.258737	-2.121164	-3.336957
18	6	0	-2.193721	-3.199592	-3.610255
19	6	0	-0.794349	-2.591368	-3.399299
20	6	0	-0.658825	-2.084533	-1.945712
21	6	0	-0.589214	-1.411896	-4.370495
22	6	0	-1.662202	-0.338991	-4.103360
23	6	0	-3.064442	-0.943066	-4.311094
24	6	0	-1.544214	0.178343	-2.651693
25	6	0	-2.413673	1.165388	0.670069

26	6	0	-3.923215	1.113481	0.316509
27	6	0	-4.635386	2.381808	0.846023
28	6	0	-4.021424	3.632813	0.190336
29	6	0	-2.524678	3.704906	0.546573
30	6	0	-1.803597	2.440840	0.024875
31	6	0	-4.474002	2.464063	2.376819
32	6	0	-2.975949	2.547969	2.728542
33	6	0	-2.255824	1.281286	2.213524
34	6	0	-2.359047	3.799182	2.075051
35	6	0	1.843426	1.702342	-0.479938
36	6	0	1.966058	1.739235	-1.869858
37	6	0	2.056153	2.982016	-2.508111
38	6	0	2.041347	4.167551	-1.770222
39	6	0	1.932497	4.110409	-0.377521
40	6	0	1.837544	2.878526	0.280107
41	6	0	0.966889	-1.434479	3.325407
42	6	0	4.612244	-1.604881	-0.045959
43	16	0	5.493387	-1.677436	1.567567
44	7	0	5.098303	2.022764	-0.214539
45	1	0	-0.526130	-3.897368	3.563216
46	1	0	-2.874045	-4.617985	3.717591
47	1	0	-4.607324	-3.504707	2.300190
48	1	0	-3.961516	-1.714234	0.771791
49	1	0	0.351091	-1.680442	-1.798708
50	1	0	-0.777028	-2.923131	-1.247399
51	1	0	-0.025071	-3.354798	-3.571409
52	1	0	1.067181	-3.482571	0.635547
53	1	0	1.353293	-3.950946	2.333510
54	1	0	2.411683	-2.761751	1.550698
55	1	0	0.415210	-0.985565	-4.242541
56	1	0	-0.659208	-1.762737	-5.408672
57	1	0	-1.517553	0.509467	-4.783997
58	1	0	-3.834592	-0.178121	-4.142155
59	1	0	-3.176992	-1.290203	-5.346856
60	1	0	-4.261792	-2.547832	-3.463671
61	1	0	-3.268017	-2.482154	-1.205239
62	1	0	-3.924700	-0.907476	-1.663019
63	1	0	-2.290282	-3.574501	-4.637900
64	1	0	-2.340406	-4.056632	-2.939056
65	1	0	-2.315579	0.938948	-2.487429
66	1	0	-0.571972	0.662231	-2.500939
67	1	0	-2.674343	0.397565	2.707803
68	1	0	-1.191169	1.329858	2.480064
69	1	0	-2.851479	2.595631	3.817822
70	1	0	1.977488	-1.034218	3.204203
71	1	0	0.981911	-2.193567	4.119278
72	1	0	0.299287	-0.622331	3.620947
73	1	0	-5.001233	3.346542	2.762967
74	1	0	-4.926893	1.584208	2.853845
75	1	0	-5.699313	2.308787	0.587456
76	1	0	-4.151032	3.592245	-0.899813
77	1	0	-4.538130	4.535456	0.542863
78	1	0	-2.068222	4.580600	0.067741
79	1	0	-1.889602	2.403957	-1.065381
80	1	0	-0.738310	2.506482	0.260767
81	1	0	-4.057643	1.051077	-0.768940
82	1	0	-4.401228	0.234373	0.758620
83	1	0	-2.852888	4.704079	2.453748

84	1	0	-1.295211	3.878578	2.337211
85	1	0	1.977924	0.828426	-2.459160
86	1	0	2.136194	3.011978	-3.591335
87	1	0	1.927528	5.023554	0.211199
88	1	0	1.759377	2.844517	1.362663
89	1	0	2.121179	5.126202	-2.273286
90	1	0	3.556900	-0.366870	-1.388454
91	1	0	3.356404	0.826414	1.274055
92	1	0	5.363888	-1.878936	-0.788091
93	1	0	3.814998	-2.349586	-0.062498
94	1	0	4.436552	-1.369633	2.348673
95	1	0	5.818478	2.679201	-0.489639
96	1	0	4.204561	2.413346	0.052910

CP3^{amino}

SCF Done: E(RB3LYP) = -2555.66126622 A.U.; No imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.076742	1.570680	-1.240110
2	6	0	-3.564086	1.061561	-0.041666
3	6	0	-3.485759	1.878442	1.091702
4	6	0	-3.929425	3.199541	1.019761
5	6	0	-4.442446	3.715123	-0.173940
6	6	0	-4.511975	2.897069	-1.302417
7	79	0	-0.843195	-0.163339	-0.183639
8	7	0	-0.025650	-0.239965	-2.991568
9	6	0	-0.824050	0.823514	-3.613776
10	15	0	1.476761	0.102199	-0.180922
11	6	0	1.859916	1.767923	0.699096
12	6	0	3.315428	1.936172	1.209786
13	6	0	3.496217	3.329589	1.858314
14	6	0	2.545355	3.466510	3.061762
15	6	0	1.092532	3.316371	2.573404
16	6	0	0.902157	1.930757	1.916438
17	6	0	3.185711	4.428968	0.823808
18	6	0	1.727660	4.283484	0.344919
19	6	0	1.541885	2.900273	-0.318005
20	6	0	0.772209	4.418873	1.546102
21	6	0	2.173175	0.204613	-1.893536
22	6	0	3.547795	0.479105	-2.052850
23	6	0	4.143195	0.561582	-3.308954
24	6	0	3.368680	0.365834	-4.452126
25	6	0	2.009253	0.099694	-4.318641
26	6	0	1.391501	0.018917	-3.060310
27	6	0	2.257948	-1.451322	0.614486
28	6	0	3.809215	-1.507856	0.594194
29	6	0	4.300021	-2.827938	1.237761
30	6	0	3.765099	-4.024710	0.429203
31	6	0	2.225104	-3.991980	0.440220
32	6	0	1.730032	-2.672870	-0.193509
33	6	0	3.800153	-2.920947	2.692615
34	6	0	2.259613	-2.896419	2.703944
35	6	0	1.768077	-1.569759	2.082928
36	6	0	1.714713	-4.087213	1.891410
37	7	0	-3.079373	-0.313730	-0.005872

38	6	0	-3.542186	-1.164880	1.131091
39	6	0	-2.917435	-2.570071	1.060532
40	16	0	-3.283130	-3.513343	-0.483048
41	6	0	-5.070706	-1.312681	1.344038
42	7	0	-5.923337	-0.841385	0.407248
43	8	0	-5.445581	-1.909458	2.351076
44	6	0	-0.393455	-1.566410	-3.499745
45	1	0	1.404907	-0.046976	-5.208984
46	1	0	3.817597	0.422737	-5.439620
47	1	0	5.204576	0.776235	-3.388177
48	1	0	4.173279	0.634201	-1.183843
49	1	0	0.633007	-2.667432	-0.218058
50	1	0	2.077003	-2.610633	-1.232812
51	1	0	1.829416	-4.828700	-0.149534
52	1	0	0.187880	-2.333650	-2.981673
53	1	0	-0.231832	-1.678780	-4.585232
54	1	0	-1.455564	-1.737822	-3.295164
55	1	0	0.616137	-4.087093	1.908313
56	1	0	2.042753	-5.032535	2.343967
57	1	0	1.893531	-2.951980	3.737010
58	1	0	4.196515	-2.085013	3.285081
59	1	0	4.166633	-3.846428	3.156611
60	1	0	5.397353	-2.828153	1.220977
61	1	0	4.174211	-1.459654	-0.436590
62	1	0	4.241083	-0.661566	1.137061
63	1	0	4.125210	-4.966476	0.864508
64	1	0	4.137906	-3.982335	-0.603260
65	1	0	2.151575	-0.733928	2.679812
66	1	0	0.671814	-1.520572	2.121292
67	1	0	2.200313	2.824042	-1.190003
68	1	0	0.510012	2.797012	-0.681472
69	1	0	1.502033	5.056672	-0.400562
70	1	0	-1.882583	0.631789	-3.413240
71	1	0	-0.689057	0.888863	-4.706463
72	1	0	-0.557717	1.787265	-3.171420
73	1	0	3.337401	5.419604	1.272821
74	1	0	3.874256	4.352922	-0.028762
75	1	0	4.537505	3.417948	2.193368
76	1	0	2.774220	2.701324	3.816153
77	1	0	2.683127	4.444090	3.542966
78	1	0	0.403741	3.389659	3.424807
79	1	0	1.083538	1.145617	2.658578
80	1	0	-0.138721	1.827012	1.587348
81	1	0	3.548818	1.164334	1.951223
82	1	0	4.035190	1.833361	0.391951
83	1	0	0.884416	5.409233	2.007299
84	1	0	-0.271294	4.333997	1.212836
85	1	0	-3.073928	1.498068	2.020480
86	1	0	-3.868902	3.827333	1.903729
87	1	0	-4.908988	3.282700	-2.236591
88	1	0	-4.132372	0.940198	-2.124329
89	1	0	-4.784671	4.744222	-0.222267
90	1	0	-3.167155	-0.711458	2.051415
91	1	0	-3.340221	-0.782622	-0.876993
92	1	0	-3.333269	-3.152883	1.882985
93	1	0	-1.835487	-2.513481	1.191015
94	1	0	-2.195796	-3.130995	-1.184151
95	1	0	-6.914009	-0.906154	0.607246

96	1	0	-5.647379	-0.204801	-0.326389

$TS^{neutralNH2}$

SCF Done: E(RB3LYP) = -3016.38979831 A.U.; An imaginary frequency of -275.4366 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.254759	1.240065	2.248812
2	6	0	2.045982	0.544901	2.029753
3	6	0	1.402988	-0.020807	3.147788
4	6	0	1.941092	0.167022	4.430232
5	6	0	3.122701	0.873741	4.624090
6	6	0	3.792664	1.402061	3.521617
7	15	0	1.366626	0.393565	0.312316
8	79	0	-0.610543	-1.012489	0.609537
9	7	0	-3.464691	-0.887908	-0.651823
10	6	0	-3.937070	0.207581	0.200775
11	6	0	-4.198505	1.427962	-0.701256
12	8	0	-4.286672	1.306676	-1.922740
13	7	0	0.208854	-0.842311	3.012377
14	6	0	-0.949051	-0.243737	3.719267
15	6	0	1.026287	2.195656	-0.299946
16	6	0	2.065256	3.237893	0.199769
17	6	0	1.681273	4.656364	-0.286600
18	6	0	0.302037	5.036540	0.281944
19	6	0	-0.743484	4.023546	-0.219313
20	6	0	-0.364773	2.603638	0.259458
21	6	0	-0.791879	4.046177	-1.760038
22	6	0	0.594977	3.675580	-2.321375
23	6	0	1.640219	4.691354	-1.825298
24	6	0	0.997804	2.258090	-1.850834
25	6	0	2.686515	-0.586635	-0.686147
26	6	0	3.976137	0.219585	-1.002625
27	6	0	4.977928	-0.672185	-1.777192
28	6	0	4.345412	-1.151658	-3.096866
29	6	0	3.081078	-1.971845	-2.781093
30	6	0	2.067968	-1.087428	-2.019085
31	6	0	5.354372	-1.888009	-0.909214
32	6	0	4.085679	-2.707476	-0.601511
33	6	0	3.074338	-1.826737	0.168482
34	6	0	3.452153	-3.192949	-1.918917
35	6	0	-1.526310	-1.278121	-1.499427
36	6	0	-1.436605	-0.287608	-2.478095
37	6	0	-1.145386	-0.663978	-3.790774
38	6	0	-0.999428	-2.012742	-4.132522
39	6	0	-1.170271	-2.988612	-3.149516
40	6	0	-1.467865	-2.636794	-1.825579
41	6	0	0.475236	-2.219354	3.500035
42	6	0	-5.177792	-0.175277	1.045998
43	16	0	-6.737429	-0.479647	0.118077
44	7	0	-4.346019	2.604198	-0.055735
45	1	0	1.434335	-0.258442	5.289649
46	1	0	3.519773	0.999944	5.626784
47	1	0	4.725251	1.943634	3.645086
48	1	0	3.789478	1.674418	1.417552
49	1	0	-1.130467	1.896050	-0.075639

50	1	0	-0.354184	2.569259	1.356637
51	1	0	-1.731496	4.270287	0.188071
52	1	0	-1.135896	0.756213	3.320661
53	1	0	-0.774028	-0.171405	4.801075
54	1	0	-1.824660	-0.871019	3.543143
55	1	0	-1.555164	3.346098	-2.126424
56	1	0	-1.082501	5.044859	-2.111967
57	1	0	0.564771	3.674706	-3.418123
58	1	0	2.629371	4.450024	-2.237682
59	1	0	1.383879	5.700693	-2.173566
60	1	0	2.442598	5.354843	0.082994
61	1	0	2.106009	3.244634	1.292237
62	1	0	3.067435	2.994036	-0.170980
63	1	0	0.027875	6.050961	-0.036506
64	1	0	0.331708	5.040212	1.379964
65	1	0	1.986824	2.022777	-2.256976
66	1	0	0.302659	1.523283	-2.259950
67	1	0	3.516293	-1.510537	1.119714
68	1	0	2.180091	-2.419207	0.404194
69	1	0	4.341584	-3.567584	0.030099
70	1	0	-0.405205	-2.832227	3.309226
71	1	0	0.697079	-2.232250	4.575054
72	1	0	1.327331	-2.633394	2.956340
73	1	0	6.086737	-2.513816	-1.436336
74	1	0	5.827979	-1.555857	0.024585
75	1	0	5.873073	-0.073231	-1.987090
76	1	0	4.092654	-0.292060	-3.732434
77	1	0	5.064657	-1.764597	-3.656427
78	1	0	2.607836	-2.303976	-3.713636
79	1	0	1.777126	-0.244819	-2.652617
80	1	0	1.163049	-1.668261	-1.819560
81	1	0	3.744314	1.109072	-1.597886
82	1	0	4.460304	0.556545	-0.081878
83	1	0	4.156613	-3.838331	-2.460304
84	1	0	2.557366	-3.795502	-1.711207
85	1	0	-1.060907	0.108783	-4.550108
86	1	0	-1.077219	-4.042661	-3.397292
87	1	0	-1.608756	-3.403522	-1.074344
88	1	0	-0.785515	-2.297979	-5.157861
89	1	0	-3.148122	0.453858	0.921987
90	1	0	-3.938118	-0.849214	-1.555197
91	1	0	-3.574451	-1.795589	-0.200850
92	1	0	-5.414864	0.641735	1.732708
93	1	0	-4.937923	-1.051637	1.653115
94	1	0	-6.405112	-1.675586	-0.409729
95	1	0	-4.543420	3.438038	-0.593682
96	1	0	-4.210239	2.706582	0.940282
97	1	0	-1.634230	0.748464	-2.240898
98	17	0	-2.213733	-2.755641	1.478708

Cysteine
SCF Done: E(RB3LYP) = -721.921135171 A.U.; No imaginary frequency

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.982560	0.796248	0.437882

2	16	0	-2.293296	-0.272678	-0.285576
3	6	0	0.382134	0.702233	-0.252879
4	7	0	1.250985	1.776258	0.260658
5	6	0	1.068685	-0.630760	0.041084
6	8	0	2.285422	-0.682821	-0.535098
7	8	0	0.611632	-1.542039	0.701125
8	1	0	-1.365294	1.814900	0.327011
9	1	0	-0.883866	0.586691	1.504890
10	1	0	0.233075	0.745775	-1.344879
11	1	0	2.168224	1.696062	-0.175900
12	1	0	0.873422	2.671424	-0.048357
13	1	0	-1.763714	-1.450258	0.101407
14	1	0	2.688013	-1.542999	-0.304306

Zwitterionic cysteine (**2**)
SCF Done: E(RB3LYP) = -721.923194649 A.U.; No imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.768907	-0.648010	0.370975
2	16	0	-2.527897	-0.158567	0.114661
3	6	0	0.255634	0.116654	-0.465741
4	7	0	0.170442	1.600555	-0.229268
5	6	0	1.714900	-0.295878	-0.032236
6	8	0	2.355952	0.625466	0.552722
7	8	0	2.041226	-1.467103	-0.285385
8	1	0	-0.590834	-0.485572	1.438983
9	1	0	-0.637762	-1.711677	0.169727
10	1	0	0.106759	-0.074905	-1.529182
11	1	0	1.042033	1.761032	0.351110
12	1	0	0.248722	2.142212	-1.092956
13	1	0	-2.612395	-0.493813	-1.190102
14	1	0	-0.690456	1.892405	0.246027

CP2$^{\textbf{carboxylate}}$
SCF Done: E(RB3LYP) = -2575.48037866 A.U.; No imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.229163	-1.050211	2.301026
2	6	0	-1.895513	-0.776143	1.934670
3	6	0	-0.885912	-0.998236	2.887015
4	6	0	-1.218758	-1.453237	4.168435
5	6	0	-2.542776	-1.707864	4.513701
6	6	0	-3.552637	-1.512967	3.573007
7	15	0	-1.495757	-0.138406	0.249041
8	79	0	0.883662	0.005180	0.459323
9	8	0	2.960023	0.211679	0.900957
10	6	0	3.741558	-0.742157	0.469551
11	8	0	3.372158	-1.780525	-0.077793
12	7	0	0.533955	-0.788913	2.565091
13	6	0	1.279838	-2.082223	2.678143
14	6	0	-2.031521	-1.476180	-1.015480
15	6	0	-3.573912	-1.634911	-1.114738

16	6	0	-3.918314	-2.770869	-2.109910
17	6	0	-3.303198	-4.094974	-1.617518
18	6	0	-1.771626	-3.947423	-1.539372
19	6	0	-1.413557	-2.822590	-0.540552
20	6	0	-1.209850	-3.602864	-2.932046
21	6	0	-1.834141	-2.280934	-3.415845
22	6	0	-3.364464	-2.427155	-3.504831
23	6	0	-1.479347	-1.145582	-2.427929
24	6	0	-2.308141	1.594676	0.097176
25	6	0	-3.802556	1.605040	0.525947
26	6	0	-4.373909	3.039810	0.406670
27	6	0	-4.251810	3.542723	-1.043450
28	6	0	-2.765873	3.551113	-1.450021
29	6	0	-2.209572	2.110602	-1.362183
30	6	0	-3.596878	3.978335	1.348288
31	6	0	-2.111970	3.983776	0.939784
32	6	0	-1.536911	2.552312	1.049931
33	6	0	-1.974138	4.482562	-0.512060
34	6	0	1.404696	0.800948	-1.369893
35	6	0	1.871769	-0.042997	-2.378907
36	6	0	2.369956	0.511893	-3.563848
37	6	0	2.410260	1.897285	-3.734035
38	6	0	1.961156	2.732643	-2.710435
39	6	0	1.458659	2.186950	-1.521736
40	6	0	1.146728	0.231449	3.473531
41	6	0	5.248043	-0.446065	0.694096
42	7	0	6.086464	-1.637865	0.648532
43	6	0	5.692497	0.566432	-0.372757
44	16	0	7.492781	0.943103	-0.168692
45	1	0	-0.441893	-1.619231	4.905997
46	1	0	-2.778815	-2.061638	5.512267
47	1	0	-4.589257	-1.713897	3.823173
48	1	0	-4.032169	-0.898411	1.594242
49	1	0	-0.321637	-2.737044	-0.466083
50	1	0	-1.790439	-3.086242	0.453973
51	1	0	-1.324427	-4.880520	-1.174980
52	1	0	0.826102	-2.817729	2.013183
53	1	0	1.251227	-2.453503	3.707196
54	1	0	2.315011	-1.916241	2.386178
55	1	0	-0.115924	-3.513419	-2.888746
56	1	0	-1.439521	-4.410077	-3.639878
57	1	0	-1.426063	-2.013267	-4.398386
58	1	0	-3.814318	-1.495760	-3.874274
59	1	0	-3.628012	-3.218092	-4.219208
60	1	0	-5.010869	-2.859869	-2.151863
61	1	0	-4.005569	-1.884152	-0.141866
62	1	0	-4.036259	-0.702950	-1.457726
63	1	0	-3.567545	-4.908770	-2.305308
64	1	0	-3.710208	-4.360513	-0.632564
65	1	0	-1.897679	-0.205924	-2.799528
66	1	0	-0.396253	-1.022360	-2.390953
67	1	0	-1.621271	2.199464	2.085374
68	1	0	-0.469664	2.575872	0.803938
69	1	0	-1.540070	4.632952	1.614132
70	1	0	2.172020	0.405282	3.145459
71	1	0	1.150018	-0.121989	4.509232
72	1	0	0.575169	1.158231	3.405944
73	1	0	-4.007105	4.994963	1.289757

74	1	0	-3.704166	3.646895	2.389828
75	1	0	-5.429598	3.003780	0.702727
76	1	0	-4.826491	2.897022	-1.721044
77	1	0	-4.672853	4.553181	-1.126494
78	1	0	-2.663511	3.891823	-2.487626
79	1	0	-2.799277	1.469272	-2.025398
80	1	0	-1.174226	2.085794	-1.715981
81	1	0	-4.394827	0.925235	-0.095253
82	1	0	-3.902040	1.282334	1.565663
83	1	0	-2.356378	5.508437	-0.593311
84	1	0	-0.916849	4.511217	-0.807256
85	1	0	1.877767	-1.118569	-2.245699
86	1	0	2.731206	-0.147732	-4.348223
87	1	0	1.999463	3.812475	-2.824742
88	1	0	1.133456	2.853640	-0.730290
89	1	0	2.797642	2.322889	-4.655279
90	1	0	5.358545	0.019173	1.678161
91	1	0	5.911567	-2.204819	1.476985
92	1	0	5.785329	-2.211239	-0.140473
93	1	0	7.444880	2.181751	-0.703365
94	1	0	5.523506	0.158851	-1.374490
95	1	0	5.122174	1.491066	-0.271381

TS$^{rd\text{-}carboxylate}$

SCF Done: E(RB3LYP) = -2575.43500864 A.U.; An imaginary frequency of -388.9289 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.602622	-3.474010	2.477241
2	6	0	3.923950	-2.007749	2.825313
3	6	0	3.089020	-1.566295	4.041914
4	6	0	1.591845	-1.699837	3.703325
5	6	0	1.264709	-3.166633	3.364765
6	6	0	2.102254	-3.603328	2.147937
7	6	0	3.594899	-1.101411	1.614393
8	6	0	2.090278	-1.223965	1.255766
9	6	0	1.249376	-0.801647	2.492855
10	6	0	1.763088	-2.709673	0.933360
11	15	0	1.544744	-0.187430	-0.259193
12	6	0	2.242103	1.589168	-0.361027
13	6	0	3.765744	1.663699	-0.648526
14	6	0	4.214900	3.142625	-0.734974
15	6	0	3.901681	3.866140	0.588675
16	6	0	2.383919	3.814483	0.850424
17	6	0	1.936570	2.338674	0.963393
18	6	0	3.472757	3.835037	-1.893181
19	6	0	1.956897	3.776888	-1.627473
20	6	0	1.500131	2.303656	-1.527357
21	6	0	1.632719	4.501753	-0.306339
22	79	0	-0.810136	-0.118526	-0.413444
23	7	0	-0.253787	-1.328928	-2.609602
24	6	0	-0.837632	-0.474749	-3.666681
25	6	0	-2.096564	0.984842	1.137401
26	6	0	-2.302565	0.325356	2.341521
27	6	0	-2.407205	1.123602	3.488949
28	6	0	-2.351383	2.516281	3.402712

29	6	0	-2.201299	3.132250	2.155648
30	6	0	-2.101201	2.366959	0.989580
31	8	0	-2.979181	0.277545	-0.384860
32	6	0	-3.748198	-0.803379	-0.187601
33	6	0	-5.190631	-0.591489	-0.706095
34	6	0	-5.921593	0.318692	0.296392
35	7	0	-5.917827	-1.834487	-0.900918
36	6	0	2.096899	-1.072800	-1.780057
37	6	0	1.181900	-1.503073	-2.767342
38	6	0	1.662044	-2.139152	-3.921174
39	6	0	3.021723	-2.372404	-4.107482
40	6	0	3.930295	-1.974197	-3.127301
41	6	0	3.467905	-1.331644	-1.982108
42	6	0	-0.950836	-2.632916	-2.531078
43	16	0	-7.661267	0.588627	-0.268824
44	1	0	0.959652	-2.463811	-4.682152
45	1	0	3.366196	-2.868445	-5.009927
46	1	0	4.993114	-2.157944	-3.249632
47	1	0	4.191248	-1.028694	-1.236675
48	1	0	0.697974	-2.813428	0.684635
49	1	0	2.334218	-3.047072	0.061706
50	1	0	1.867177	-4.642564	1.885635
51	1	0	-0.527708	-3.220647	-1.713517
52	1	0	-0.865416	-3.205560	-3.465147
53	1	0	-2.009826	-2.455780	-2.328267
54	1	0	0.193487	-3.276069	3.147080
55	1	0	1.485949	-3.811559	4.225604
56	1	0	0.985680	-1.369883	4.556494
57	1	0	3.327257	-0.527633	4.308659
58	1	0	3.335628	-2.187225	4.913357
59	1	0	4.993109	-1.903217	3.048685
60	1	0	4.225779	-1.397960	0.770190
61	1	0	3.844587	-0.064882	1.865306
62	1	0	3.859447	-4.125723	3.322842
63	1	0	4.208551	-3.802662	1.621963
64	1	0	1.435504	0.245542	2.751992
65	1	0	0.182386	-0.889355	2.264801
66	1	0	1.700488	1.786288	-2.474282
67	1	0	0.415985	2.274375	-1.363720
68	1	0	1.413863	4.249573	-2.455592
69	1	0	-1.893166	-0.304018	-3.435877
70	1	0	-0.769407	-0.936465	-4.661648
71	1	0	-0.319961	0.486743	-3.683709
72	1	0	3.799818	4.879662	-1.980414
73	1	0	3.711009	3.342130	-2.845486
74	1	0	5.296007	3.159364	-0.921936
75	1	0	4.445772	3.394212	1.418136
76	1	0	4.239873	4.909511	0.534972
77	1	0	2.151061	4.318031	1.797086
78	1	0	2.472519	1.870409	1.796507
79	1	0	0.865051	2.288349	1.191700
80	1	0	4.338439	1.156135	0.134215
81	1	0	3.995504	1.170802	-1.598284
82	1	0	1.930364	5.556585	-0.373434
83	1	0	0.550562	4.483998	-0.119302
84	1	0	-2.363114	-0.753610	2.398642
85	1	0	-2.537992	0.636184	4.450951
86	1	0	-2.176954	4.215174	2.075188

87	1	0	-2.018592	2.833178	0.014579
88	1	0	-2.443531	3.120685	4.299552
89	1	0	-5.127097	-0.069229	-1.665379
90	1	0	-5.530484	-2.342344	-1.694268
91	1	0	-5.783754	-2.435524	-0.087860
92	1	0	-7.820630	1.786656	0.332078
93	8	0	-3.377212	-1.827561	0.356102
94	1	0	-5.933165	-0.143491	1.288217
95	1	0	-5.416869	1.283685	0.365991

CP3[carboxylate]

SCF Done: E(RB3LYP) = -2575.49704007 A.U.; No imaginary frequency

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.323307	-0.119145	2.289412
2	6	0	-1.955868	0.035719	1.976242
3	6	0	-1.045595	0.241757	3.043950
4	6	0	-1.533347	0.272095	4.359579
5	6	0	-2.885755	0.110414	4.646316
6	6	0	-3.788051	-0.084630	3.601834
7	15	0	-1.448116	-0.024769	0.198790
8	79	0	0.845883	0.172575	0.007135
9	8	0	3.122957	0.412909	-0.419852
10	6	0	3.978094	-0.484926	-1.067439
11	8	0	4.992900	-0.112795	-1.590380
12	7	0	0.367784	0.432700	2.820052
13	6	0	1.191261	-0.613709	3.440797
14	6	0	-1.917068	-1.756855	-0.480233
15	6	0	-3.429632	-2.108594	-0.474018
16	6	0	-3.641184	-3.546123	-1.011596
17	6	0	-2.901541	-4.546961	-0.103650
18	6	0	-1.396058	-4.219674	-0.111290
19	6	0	-1.174006	-2.785684	0.420782
20	6	0	-0.848366	-4.326053	-1.547602
21	6	0	-1.598055	-3.331006	-2.453096
22	6	0	-3.103652	-3.656633	-2.450488
23	6	0	-1.388588	-1.890683	-1.934903
24	6	0	-2.221541	1.510701	-0.648023
25	6	0	-3.771095	1.513228	-0.717503
26	6	0	-4.268053	2.827104	-1.369202
27	6	0	-3.702255	2.946850	-2.796628
28	6	0	-2.162691	2.967613	-2.731440
29	6	0	-1.659956	1.654541	-2.089631
30	6	0	-3.806210	4.031125	-0.526171
31	6	0	-2.266396	4.048922	-0.467421
32	6	0	-1.761633	2.742363	0.185282
33	6	0	-1.693036	4.170696	-1.891913
34	6	0	3.559801	1.769652	-0.340502
35	6	0	3.219824	2.646764	-1.363751
36	6	0	3.611129	3.983127	-1.247379
37	6	0	4.328603	4.411743	-0.126859
38	6	0	4.659887	3.505556	0.884320
39	6	0	4.275813	2.165705	0.782847
40	6	0	0.823492	1.778207	3.197894
41	6	0	3.494874	-1.936694	-0.979999

42	7	0	4.056575	-2.775903	-2.024283
43	6	0	3.869315	-2.479076	0.412890
44	16	0	3.349647	-4.247532	0.538896
45	1	0	-0.832807	0.431028	5.173801
46	1	0	-3.230394	0.140823	5.675916
47	1	0	-4.848266	-0.208554	3.799876
48	1	0	-4.048216	-0.268990	1.500857
49	1	0	-0.098889	-2.564899	0.438564
50	1	0	-1.537488	-2.713549	1.453187
51	1	0	-0.859027	-4.916423	0.544783
52	1	0	0.850607	-1.596711	3.104975
53	1	0	1.167383	-0.591181	4.543035
54	1	0	2.229884	-0.476792	3.122513
55	1	0	0.228930	-4.112177	-1.558460
56	1	0	-0.976868	-5.349335	-1.924810
57	1	0	-1.205465	-3.388377	-3.476239
58	1	0	-3.642460	-2.964607	-3.111877
59	1	0	-3.272649	-4.670379	-2.837330
60	1	0	-4.718006	-3.757037	-0.998510
61	1	0	-3.831837	-2.059050	0.541775
62	1	0	-3.995733	-1.404163	-1.092391
63	1	0	-3.066125	-5.572325	-0.460900
64	1	0	-3.296547	-4.495323	0.920056
65	1	0	-1.918849	-1.197581	-2.596290
66	1	0	-0.323615	-1.630513	-1.977672
67	1	0	-2.148352	2.672372	1.208760
68	1	0	-0.665685	2.763390	0.250798
69	1	0	-1.926291	4.893221	0.145576
70	1	0	1.863395	1.900660	2.879024
71	1	0	0.770708	1.963556	4.283660
72	1	0	0.215240	2.529096	2.687112
73	1	0	-4.176849	4.964896	-0.969554
74	1	0	-4.223592	3.967320	0.487927
75	1	0	-5.364394	2.795939	-1.404288
76	1	0	-4.044157	2.104185	-3.412862
77	1	0	-4.072682	3.864986	-3.271675
78	1	0	-1.747529	3.035118	-3.745027
79	1	0	-1.979188	0.812053	-2.711344
80	1	0	-0.562597	1.645523	-2.068975
81	1	0	-4.131711	0.662839	-1.305787
82	1	0	-4.201200	1.430709	0.285154
83	1	0	-2.029442	5.108026	-2.354732
84	1	0	-0.595470	4.204024	-1.857330
85	1	0	2.662312	2.292645	-2.224820
86	1	0	3.355165	4.685172	-2.035014
87	1	0	5.218050	3.836796	1.754621
88	1	0	4.524506	1.444754	1.554788
89	1	0	4.629885	5.451450	-0.042259
90	1	0	2.404819	-1.949839	-1.075858
91	1	0	3.687103	-2.501293	-2.932644
92	1	0	5.066199	-2.641023	-2.070822
93	1	0	3.171909	-4.242862	1.876742
94	1	0	4.950302	-2.407040	0.566181
95	1	0	3.366276	-1.905027	1.192916

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3. Solution-Phase Electronic Energies and Thermal Corrections

Table S1. Single Point Electronic Energies, Zero-Point Vibrational Energies, Thermal Corrections to Enthalpies and Gibbs Free Energies [a]

Stationary point	SP (a.u., in water)	ZPE (a.u.)	ΔH (a.u.)	ΔG (a.u.)
Favorable pathway for S-arylation				
CP0	-2314.37728692	0.731169	0.766326	0.666974
1	-702.05615433	0.120034	0.129854	0.085997
CP1	-3016.42775083	0.850817	0.89649	0.771399
HCl	-460.79600032	0.00664	0.009945	-0.011255
CP2	-2555.62089144	0.842659	0.885671	0.767788
TS^{rd}	-2555.60197103	0.839445	0.882797	0.76085
CP3	-2555.66109952	0.840762	0.884578	0.761307
Prod	-933.11416900	0.203046	0.217461	0.160419
SbF_6^-	-604.73322838	0.013364	0.022634	-0.020148
LAu(I)-SbF_6	-2227.29357958	0.650631	0.68956	0.578252
Cl^-	-460.36592171	0	0.00236	-0.015023
LAu(I)-Cl	-2082.94143912	0.636932	0.667568	0.576341
Isomeric pathways for reductive elimination				
CP2-iso	-2555.58050063	0.839771	0.883901	0.761798
TS^{rd}-iso	-2555.57892494	0.838752	0.882396	0.759854
CP3-iso	-2555.65070232	0.840672	0.884524	0.760729
CP2-cis	-2555.61288320	0.842642	0.885728	0.766713
TS^{rd}-cis	-2555.59679983	0.840057	0.883142	0.763763
Chemoselectivity of possible N-arylation and O-arylation				
$CP1^{amino}$	-3016.43182834	0.854611	0.899988	0.77694
$CP2^{amino}$	-2555.59011940	0.839433	0.882378	0.764458
$TS^{rd\text{-}amino}$	-2555.56744685	0.837209	0.879809	0.762812
$CP3^{amino}$	-2555.66126622	0.840075	0.883275	0.761672
$TS^{neutralNH2}$	-3016.38979831	0.852017	0.896983	0.775451
Cysteine	-721.92113517	0.108047	0.117242	0.07458
2	-721.92319465	0.109627	0.11847	0.076625
$CP2^{carboxylate}$	-2575.48037866	0.828021	0.870784	0.752915
$TS^{rd\text{-}carboxylate}$	-2575.43500864	0.823701	0.866862	0.745135
$CP3^{carboxylate}$	-2575.49704007	0.825291	0.869138	0.744576

a. SP: Solution-phase single point electronic energy;
ZPE: Zero-point vibrational energy;
ΔH: Thermal correction to enthalpy;
ΔG: Thermal correction to Gibbs free energy.

4. Full citation of Gaussian09 program

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