

Supporting Information:

Formation and Intramolecular Capture of α -Imino Gold Carbenoids in the Au(I)-Catalyzed [3 + 2] Reaction of Anthranils, 1,2,4-Oxadiazoles and 4,5-Dihydro-1,2,4-Oxadiazoles with Ynamides

Contents

Solvation Effects S-2

Cartesian coordinates of A-Series S-6

Cartesian coordinates of B-Series S-42

Cartesian coordinates of C-Series S-72

Tables of partial charges of crucial structures of B/C-Series S-103

Energy diagrams of B/C-Series including alternative attack of N-4 of oxadiazole S-106

List of Figures

S1 A-series reaction mechanism..... S-5

S2 B-series reaction mechanism..... S-41

S3 C-series reaction mechanism..... S-71

S4 B-series reaction mechanism S-106

S5 C-series reaction mechanism S-107

Solvation Effects

Structure	Gas phase SCF energy	Solv. Effect		Solution phase SCF energy
A-series	A.U.	kcal/mol		A.U.
1a	-1660.631455	-20.9		-1660.664707
2	-399.0803095	-2.0		-399.083469
3a1	-2059.743484	-22.1		-2059.778775
3a2	-2059.752059	-21.3		-2059.785955
4a1	-2059.811325	-22.2		-2059.846655
4a2	-2059.785408	-23.0		-2059.822135
5a1 _{anti}	-2059.789509	-24.6		-2059.828742
5a1 _{syn}	-2059.780881	-24.0		-2059.819176

5a2 _{anti}	-2059.80376	-21.7	-21.7	-2059.838396
5a2 _{syn}	-2059.799664	-21.5		-2059.833853
6a1 _{anti}	-2059.779871	-24.7		-2059.819204
6a1	-2059.869334	-22.7		-2059.905476
6a1 _{syn}	-2059.776651	-25.1		-2059.816668
6a2 _{anti}	-2059.786424	-25.3		-2059.826684
6a2	-2059.862758	-22.6		-2059.898715
6a2 _{syn}	-2059.78844	-23.0		-2059.825098
TS _{3a1}	-2059.704011	-20.7		-2059.736946
TS _{3a2}	-2059.727328	-19.8		-2059.758827
TS _{4a1}	-2059.736971	-21.7		-2059.771558
TS _{4a2}	-2059.739043	-20.4		-2059.771592
TS _{5a1_anti}	-2059.776951	-21.9		-2059.811906
TS _{5a1_syn}	-2059.763183	-21.9		-2059.79813
TS _{5a2_anti}	-2059.767457	-21.7	-22.1	-2059.802044
TS _{5a2_syn}	-2059.766955	-20.9		-2059.800304
TS _{6a1_anti'}	-2059.754691	-23.9		-2059.792787
TS _{6a1_anti}	-2059.769403	-23.1		-2059.806289
TS _{6a1_syn}	-2059.758855	-24.1		-2059.7972
TS _{6a2_anti'}	-2059.758562	-24.0		-2059.796773
TS _{6a2_anti}	-2059.769206	-23.2		-2059.806154
TS _{6a2_syn'}	-2059.757416	-21.9		-2059.792272
TS _{6a2_syn}	-2059.767057	-22.4		-2059.802723

average values in boldface

Structure	Gas phase SCF energy	Solv. Effect		Solution phase SCF energy
B-series	A.U.	kcal/mol		A.U.
1b	-1429.919991	-24.1		-1429.95846
2b	-762.3983785	-2.0		-762.4015868
3b1	-2192.357401	-20.5		-2192.390039
3b2	-2192.361702	-20.9		-2192.395084
4b1	-2192.37417	-24.6		-2192.413441
4b2	-2192.386678	-24.3		-2192.425423
5b1	-2192.357917	-20.2		-2192.390075
5b2	-2192.3574	-23.8		-2192.395386
6b1B	-2192.356339	-20.0	-20.4	-2192.388167
6b1	-2192.439821	-23.0		-2192.476486

6b2B	-2192.357399	-20.1		-2192.38943
6b2	-2192.452758	-21.1		-2192.486364
TS _{3b1}	-2192.332326	-21.3		-2192.366303
TS _{3b2}	-2192.326364	-20.2		-2192.358629
TS _{4b1}	-2192.350205	-19.4		-2192.381146
TS _{4b2}	-2192.346655	-20.3		-2192.37904
TS _{5b1}	-2192.33341	-20.8	-21.0	-2192.36649
TS _{5b2}	-2192.337623	-24.3		-2192.376423
TS _{6b1A}	-2192.33584	-22.2		-2192.37118
TS _{6b1B'}	-2192.343166	-20.6		-2192.375942
TS _{6b1B}	-2192.344463	-20.2		-2192.376607
TS _{6b2A}	-2192.334355	-22.0		-2192.369348
TS _{6b2B'}	-2192.339445	-20.3		-2192.371753
TS _{6b2B}	-2192.351036	-20.5		-2192.383777

average values in boldface

Structure	Gas phase SCF energy	Solv. Effect		Solution phase SCF energy
C-series	A.U.	kcal/mol		A.U.
1b	-1586.315612	-41.3		-1586.381375
2c	-724.3060386	-6.8		-724.3168507
3c1	-2310.682937	-36.5		-2310.741157
3c2	-2310.680006	-36.7		-2310.738434
4c1'	-1965.619604	-39.3	-33.4	-1965.682154
4c1	-2310.680308	-34.9		-2310.735894
4c2'	-1965.631635	-38.8		-1965.693535
5c1	-1965.600329	-34.9		-1965.655971
5c2	-1965.604836	-39.6		-1965.667921
6c1A	-1965.595689	-36.5		-1965.653913

6c1B	-1965.606333	-35.4		-1965.662751
6c1	-1965.706768	-35.9		-1965.764042
6c2A	-1965.590613	-38.7		-1965.65235
6c2B	-1965.603713	-36.1		-1965.661316
6c2	-1965.702307	-39.7		-1965.765556
benzaldehyde	-345.0592262	-3.3		-345.0644655
TS _{3c1}	-2310.646406	-37.6		-2310.706364
TS _{3c2}	-2310.633541	-36.2		-2310.69122
TS _{4c1'}	-2310.677423	-34.7		-2310.732662
TS _{4c1}	-2310.664582	-34.2		-2310.719099
TS _{4c2}	-2310.663918	-37.3		-2310.723312
TS _{5c1}	-1965.577278	-36.2	-36.8	-1965.635043
TS _{5c2}	-1965.576943	-38.2		-1965.637822
TS _{6c1A'}	-1965.595822	-36.4		-1965.653908
TS _{6c1A}	-1965.587062	-36.1		-1965.644633
TS _{6c1B}	-1965.597359	-35.8		-1965.654478
TS _{6c2A}	-1965.582648	-40.2		-1965.646778
TS _{6c2B}	-1965.591864	-38.5		-1965.653285
TS _{6c1B'}	-1965.589463	-36.6		-1965.647745
TS _{6c2A'}	-1965.588634	-37.6		-1965.648502
TS _{6c2B'}	-1965.585258	-36.4		-1965.643268

average values in boldface

Cartesian coordinates of A-Series

S - 5

51

scf done: -1660.664707

C	5.139051	-0.573601	-1.654363
C	5.592180	0.423811	-0.851957
N	3.797469	-0.732642	-1.372568
C	3.407965	0.141625	-0.418196
N	4.514937	0.848953	-0.100532
Au	1.499307	0.348154	0.343815
C	2.938388	-1.691860	-2.043771
C	4.585049	1.919528	0.875561
H	5.650812	-1.189387	-2.394006
H	6.583361	0.863730	-0.741488
H	3.455293	-2.662795	-2.113982
H	2.009488	-1.822666	-1.465101
H	2.690348	-1.340062	-3.060168
H	5.447459	1.758400	1.543151
H	4.692818	2.895287	0.371660
H	3.660297	1.919936	1.473569
C	-0.753442	-0.586475	1.503668
C	-0.522057	0.580960	1.027055
N	-1.009754	-1.834807	1.635666
C	-1.361502	1.758507	0.841531
C	-0.846820	-2.648712	2.843192
S	-1.421020	-2.734908	0.102558
O	-2.060390	-3.940937	0.589651
C	-2.562677	-1.616835	-0.622823
O	-0.186020	-2.763710	-0.661165
H	-1.788241	-3.174725	3.066981
H	-0.042332	-3.389047	2.692437
H	-0.581850	-1.976872	3.673837
C	-2.680318	1.768813	1.330777
C	-3.515669	2.850469	1.084054
C	-3.049609	3.936887	0.339290
C	-1.743099	3.940462	-0.147396
C	-0.901307	2.861179	0.107287
H	-3.045927	0.913245	1.913096
H	-4.539895	2.849120	1.474180
H	-3.709050	4.790134	0.143907
H	-1.375015	4.794245	-0.726650
H	0.126968	2.858976	-0.275471
C	-2.109127	-0.691711	-1.565459
C	-3.003637	0.253709	-2.048117
C	-4.334495	0.285230	-1.606513
C	-4.760746	-0.673967	-0.675623
C	-3.883714	-1.626253	-0.171877
H	-1.068208	-0.714509	-1.907295
H	-2.664290	0.991802	-2.785349
C	-5.268636	1.339381	-2.106780
H	-5.805219	-0.673287	-0.341982
H	-4.217417	-2.373111	0.557189
H	-6.325251	1.056541	-1.961268
H	-5.099488	2.290568	-1.563689
H	-5.105525	1.548617	-3.178940

14

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scf done: -399.083469
C      -0.725546      -1.583504      0.000000
C       0.508775      -2.170618      0.000000
C       1.713680      -1.389747      0.000000
C       1.697989      -0.023338      0.000000
C       0.424861       0.620318      0.000000
C      -0.782150      -0.160104      0.000000
C      -1.759208       0.807414      0.000000
O      -1.194425       2.008322      0.000000
N       0.171274       1.920772      0.000000
H      -1.642188      -2.182634      0.000000
H       0.592893      -3.263124      0.000000
H       2.674670      -1.917282      0.000000
H       2.615649       0.573064      0.000000
H      -2.849919       0.790009      0.000000

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TS_{3a1}

65

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scf done: -2059.736946
C       6.120458       1.287426      -0.552737
C       6.360899       0.498129      -1.644030
C       5.587814      -0.679909      -1.894576
C       4.570899      -1.086633      -1.070477
C       4.297834      -0.279663       0.067011
C       5.069922       0.898830       0.321309
C       4.507277       1.394482       1.476702
O       3.524696       0.606294       1.873132
N       3.378776      -0.453339       1.019063
H       6.710793       2.187434      -0.354843
H       7.160315       0.761690      -2.344487
H       5.826328      -1.279393      -2.780520
H       3.995137      -1.996028      -1.269907
H       4.703084       2.266831       2.102236
C       1.291525      -0.948042       0.672563
C       0.549181       0.029003       1.044142
Au      -1.432907      -0.709346       0.626082
C      -3.397119      -1.206715       0.229812
N      -4.454775      -0.369281       0.309834
C      -5.621091      -1.031326      -0.018855
C      -5.273994      -2.310749      -0.314107
N      -3.904299      -2.397177      -0.156187
C      -3.140487      -3.611568      -0.371491
C      -4.373643       1.019527       0.727144
H      -6.590834      -0.533648      -0.015751
H      -5.875365      -3.164793      -0.625399
H      -3.418657      -4.375936       0.373736
H      -3.333620      -4.003622      -1.384084
H      -2.067277      -3.381733      -0.269992
H      -5.338049       1.511180       0.522983
H      -4.156771       1.086451       1.807531
H      -3.578107       1.539175       0.164138
C       1.502139      -2.201709       0.006802
N       0.738164       1.337836       1.460048
S       1.229971       2.444404       0.246543
C      -0.151100       1.868165       2.484200
H      -0.138278       1.180650       3.346221
H      -1.198712       1.976666       2.126106
H       0.232329       2.846028       2.817193
O       1.676716       3.629292       0.960809

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O	2.108183	1.709204	-0.649311
C	-0.278553	2.808477	-0.609030
C	-1.061597	3.888786	-0.204013
C	-2.288139	4.101425	-0.826909
C	-2.743331	3.250635	-1.842892
C	-1.931414	2.175569	-2.231647
C	-0.699971	1.949393	-1.626774
H	-0.705407	4.560720	0.584820
H	-2.908754	4.952075	-0.519472
C	-4.058982	3.492206	-2.514593
H	-2.270674	1.507413	-3.033301
H	-0.057459	1.122696	-1.950413
H	-4.748671	4.063538	-1.868436
H	-3.925594	4.078339	-3.444687
H	-4.548687	2.543926	-2.801718
C	2.061828	-3.292878	0.691922
C	2.270291	-4.494607	0.026609
C	1.930841	-4.615098	-1.323324
C	1.383047	-3.532482	-2.013869
C	1.172381	-2.326131	-1.354831
H	2.339801	-3.175101	1.744800
H	2.704471	-5.346420	0.560878
H	2.100766	-5.563904	-1.844534
H	1.127225	-3.628752	-3.074565
H	0.757463	-1.459452	-1.884388

3a1

65

scf done: -2059.778775

C	4.753876	1.841919	1.649569
C	4.461387	1.394648	2.911451
C	3.183309	0.841730	3.226406
C	2.178876	0.707155	2.295682
C	2.475090	1.159273	0.995423
C	3.735015	1.734666	0.666839
C	3.603071	2.097334	-0.661496
O	2.414376	1.776450	-1.121877
N	1.699787	1.175110	-0.104454
H	5.728588	2.272913	1.400911
H	5.213678	1.464300	3.703421
H	2.998296	0.513444	4.255123
H	1.198768	0.282674	2.534029
H	4.264488	2.598084	-1.371519
C	0.316784	0.918388	-0.295254
C	-0.195510	-0.320739	-0.037925
Au	-2.267655	-0.516024	0.166451
C	-4.339472	-0.586667	0.382506
N	-5.140746	0.482712	0.596937
C	-6.462027	0.092904	0.690542
C	-6.482936	-1.254780	0.524861
N	-5.172593	-1.650432	0.338531
C	-4.768263	-3.023918	0.113061
C	-4.664949	1.845778	0.751545
H	-7.267413	0.806853	0.863435
H	-7.309358	-1.965434	0.516582
H	-5.227099	-3.411145	-0.812610
H	-3.671673	-3.056896	0.013118
H	-5.075652	-3.656368	0.963233
H	-4.214856	1.990007	1.749245
H	-3.908448	2.071181	-0.019862

H	-5.514478	2.537156	0.635268
C	-0.475933	2.098928	-0.694502
N	0.672542	-1.423423	0.121743
S	1.634224	-1.895477	-1.221846
C	0.186494	-2.525277	0.950380
H	-0.087825	-2.119267	1.939313
H	0.974425	-3.281923	1.085155
H	-0.701758	-3.018427	0.506352
O	1.558192	-3.349088	-1.269776
O	1.246526	-1.085204	-2.368118
C	3.308711	-1.466131	-0.798849
C	4.103482	-0.864960	-1.770800
C	5.447448	-0.617734	-1.490305
C	6.003831	-0.961157	-0.254004
C	5.177160	-1.568195	0.704489
C	3.840297	-1.834883	0.438075
H	3.667236	-0.592137	-2.738170
H	6.080608	-0.151688	-2.255856
C	7.447664	-0.707767	0.048540
H	5.599846	-1.843154	1.679476
H	3.213778	-2.321858	1.195062
H	8.026864	-1.650941	0.026683
H	7.908230	-0.022762	-0.684215
H	7.579269	-0.279121	1.059600
C	-0.343360	3.321156	-0.019439
C	-1.118333	4.418494	-0.384456
C	-2.026808	4.314145	-1.439461
C	-2.149910	3.110080	-2.131900
C	-1.375264	2.010272	-1.766616
H	0.364468	3.408401	0.816952
H	-1.015113	5.364059	0.160071
H	-2.630854	5.181035	-1.730644
H	-2.843051	3.030217	-2.977223
H	-1.437867	1.071295	-2.330295

TS_{3a2}

65

scf done: -2059.758827

C	-5.577215	1.336032	0.048563
C	-5.419191	2.072242	-1.092852
C	-4.118596	2.430904	-1.578075
C	-2.963348	2.064491	-0.940345
C	-3.102389	1.294067	0.246302
C	-4.399959	0.932044	0.738384
C	-4.114247	0.193677	1.863907
O	-2.802300	0.118497	2.031609
N	-2.156727	0.805183	1.044045
H	-6.568963	1.066626	0.425897
H	-6.298600	2.407143	-1.652992
H	-4.053176	3.027871	-2.494631
H	-1.973155	2.350486	-1.311752
H	-4.721320	-0.315349	2.614032
C	-0.235730	0.155543	0.851419
N	-0.353900	-1.117656	1.174315
C	0.542583	1.134117	0.484072
Au	2.469065	0.301404	0.123518
C	4.279347	-0.611194	-0.269471
N	5.503382	-0.069554	-0.450896
C	6.437523	-1.054847	-0.705520
C	5.771865	-2.238490	-0.679728

N	4.450014	-1.945314	-0.412477
C	3.389432	-2.929029	-0.272197
C	5.813293	1.345337	-0.394261
H	7.487420	-0.825063	-0.886726
H	6.119828	-3.260160	-0.831695
H	3.078146	-3.016818	0.783715
H	2.515506	-2.638737	-0.879291
H	3.761750	-3.906201	-0.617272
H	4.885542	1.900118	-0.183808
H	6.544939	1.544210	0.407022
H	6.228665	1.683829	-1.358601
S	-0.555727	-2.294937	-0.103918
C	-0.213373	-1.613038	2.545228
C	-2.293038	-2.308045	-0.404372
O	0.118272	-1.748419	-1.270706
O	-0.144491	-3.547227	0.509098
H	-1.044360	-2.293893	2.800449
H	0.747340	-2.142746	2.671533
H	-0.248715	-0.742837	3.219264
C	-2.809232	-1.516080	-1.430493
C	-4.180679	-1.528873	-1.656651
C	-5.037892	-2.316727	-0.876370
C	-4.485407	-3.101653	0.146329
C	-3.115997	-3.111092	0.387056
H	-2.139411	-0.905426	-2.046595
H	-4.599219	-0.913801	-2.463057
C	-6.508792	-2.341084	-1.149003
H	-5.144484	-3.731068	0.756827
H	-2.686349	-3.748943	1.167652
H	-6.759816	-3.143569	-1.869855
H	-7.091665	-2.539762	-0.232110
H	-6.856083	-1.389708	-1.589897
C	0.241994	2.548588	0.264798
C	0.647745	3.169743	-0.926895
C	0.328034	4.502169	-1.173920
C	-0.367310	5.243951	-0.218812
C	-0.739916	4.645654	0.984937
C	-0.444393	3.306599	1.225723
H	1.208796	2.587619	-1.669119
H	0.636094	4.969470	-2.116154
H	-0.607458	6.296377	-0.407219
H	-1.268928	5.229594	1.746772
H	-0.738725	2.837384	2.170976

3a2

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scf done: -2059.785955

C	-5.107898	1.725300	-0.313728
C	-4.838640	2.001578	-1.627141
C	-3.533425	1.809998	-2.178576
C	-2.472962	1.341888	-1.440708
C	-2.738843	1.064968	-0.084711
C	-4.032914	1.249858	0.485610
C	-3.881913	0.850469	1.798935
O	-2.640155	0.477487	2.037610
N	-1.922032	0.599581	0.871289
H	-6.104336	1.867807	0.114674
H	-5.633157	2.378433	-2.278884
H	-3.377784	2.043126	-3.237569

H	-1.476982	1.180418	-1.864831
H	-4.565257	0.781832	2.647576
C	-0.542365	0.205604	0.878288
N	-0.375807	-1.153079	1.212749
C	0.432496	1.084115	0.540812
Au	2.332630	0.306358	0.148649
C	4.154736	-0.593194	-0.301436
N	5.368515	-0.035004	-0.509338
C	6.309824	-1.004152	-0.796679
C	5.660867	-2.196943	-0.764538
N	4.342492	-1.923746	-0.461908
C	3.305573	-2.927332	-0.290178
C	5.659911	1.382987	-0.447774
H	7.351334	-0.757965	-1.003806
H	6.018643	-3.212469	-0.934292
H	3.096735	-3.091920	0.781773
H	2.376961	-2.607075	-0.791711
H	3.647116	-3.874531	-0.736477
H	4.730528	1.921807	-0.204994
H	6.411471	1.585455	0.334143
H	6.042949	1.737560	-1.419925
S	-0.553799	-2.291735	-0.024978
C	0.310597	-1.518427	2.446154
C	-2.317103	-2.331021	-0.243592
O	0.020627	-1.772164	-1.264967
O	-0.095705	-3.560698	0.526181
H	0.134689	-2.582723	2.668923
H	1.403005	-1.337754	2.384482
H	-0.106384	-0.907626	3.266567
C	-2.870784	-1.970258	-1.469242
C	-4.256321	-1.962707	-1.606128
C	-5.092466	-2.315339	-0.539814
C	-4.503487	-2.693309	0.676747
C	-3.122006	-2.709262	0.831382
H	-2.214735	-1.692302	-2.301143
H	-4.702452	-1.669989	-2.565389
C	-6.579743	-2.305564	-0.708355
H	-5.145684	-2.986321	1.516687
H	-2.668264	-3.003411	1.786115
H	-7.104009	-2.291121	0.263052
H	-6.912496	-1.432861	-1.299895
H	-6.921390	-3.208467	-1.250514
C	0.114882	2.509429	0.361312
C	0.534738	3.177528	-0.800672
C	0.179312	4.503916	-1.029774
C	-0.567929	5.203740	-0.082673
C	-0.954199	4.567328	1.097062
C	-0.622251	3.233133	1.315621
H	1.135066	2.630939	-1.540204
H	0.500907	5.001128	-1.952124
H	-0.834230	6.252542	-0.255456
H	-1.516735	5.119263	1.859104
H	-0.918947	2.744472	2.253161

TS_{4a1}

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scf done: -2059.771558

C	-4.451336	-2.093906	-1.696791
C	-4.018461	-1.794983	-2.966669
C	-2.721051	-1.255523	-3.177206

C	-1.849803	-0.985039	-2.143135
C	-2.293451	-1.272103	-0.834755
C	-3.574344	-1.841066	-0.618028
C	-3.652152	-2.076625	0.760609
O	-2.631707	-1.702009	1.418980
N	-1.613168	-1.066602	0.301616
H	-5.443506	-2.521350	-1.515035
H	-4.666630	-1.981889	-3.828564
H	-2.400021	-1.046441	-4.204023
H	-0.850947	-0.564379	-2.306217
H	-4.468248	-2.560881	1.317767
C	-0.323374	-0.826222	0.627798
C	0.189640	0.471491	0.468186
Au	2.219466	0.573111	-0.066834
C	4.225109	0.575120	-0.625546
N	5.006623	-0.512752	-0.818196
C	6.288924	-0.136868	-1.165579
C	6.304207	1.220354	-1.191026
N	5.030707	1.636919	-0.857369
C	4.636454	3.029474	-0.775968
C	4.588885	-1.893097	-0.658881
H	7.072655	-0.868191	-1.363383
H	7.102962	1.926523	-1.417990
H	3.577792	3.081179	-0.475582
H	5.250720	3.556158	-0.026040
H	4.761074	3.520036	-1.756437
H	4.842098	-2.469003	-1.565001
H	5.089901	-2.347519	0.213523
H	3.498550	-1.926200	-0.498150
C	0.528130	-1.997554	0.930464
N	-0.587773	1.591714	0.475632
C	-0.051597	2.841172	-0.075396
S	-1.910531	1.804546	1.605643
H	-0.847275	3.597353	-0.141011
H	0.757512	3.244782	0.562338
H	0.339610	2.640797	-1.086298
O	-1.742023	0.833013	2.671108
O	-1.906964	3.228766	1.901648
C	-3.389301	1.432312	0.695802
C	0.326349	-3.222627	0.277300
C	1.138560	-4.318067	0.556026
C	2.157482	-4.213752	1.504485
C	2.351106	-3.008923	2.178905
C	1.539611	-1.911212	1.899125
H	-0.471858	-3.319813	-0.470884
H	0.974273	-5.264720	0.028687
H	2.789325	-5.080312	1.730240
H	3.129370	-2.926947	2.946514
H	1.665317	-0.977482	2.461235
C	-4.468531	0.918082	1.412865
C	-5.679266	0.713761	0.755687
C	-5.825069	1.009166	-0.605067
C	-4.720354	1.524278	-1.297353
C	-3.507384	1.749869	-0.656434
H	-4.356631	0.674015	2.475434
H	-6.533826	0.311955	1.314503
C	-7.128426	0.793688	-1.308245
H	-4.814892	1.750583	-2.366878
H	-2.655526	2.151807	-1.218152
H	-7.752022	0.041084	-0.794380
H	-7.716145	1.731442	-1.345781

H	-6.975477	0.468647	-2.353522
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scf done: -2059.846655

C	4.174577	-1.062910	-1.873313
C	3.371955	-2.044756	-2.435784
C	2.012730	-1.779404	-2.622640
C	1.466445	-0.557140	-2.246441
C	2.264505	0.432461	-1.648729
C	3.646296	0.171693	-1.469281
C	4.572651	1.173310	-0.917894
O	4.273140	2.230318	-0.412510
N	1.748981	1.686032	-1.366449
H	5.250619	-1.236588	-1.740271
H	3.800680	-3.003081	-2.749128
H	1.365982	-2.536283	-3.083382
H	0.406765	-0.339511	-2.431999
H	5.652717	0.871194	-1.002575
C	0.959858	1.984891	-0.411835
C	0.455241	0.935064	0.523151
Au	-1.403166	0.153384	-0.030474
C	-3.280146	-0.525094	-0.594182
N	-4.213208	-1.098970	0.197552
C	-5.340190	-1.414253	-0.534057
C	-5.096786	-1.026774	-1.813363
N	-3.829494	-0.481975	-1.828221
C	-3.161753	0.028149	-3.012269
C	-4.077573	-1.357120	1.620390
H	-6.216243	-1.875389	-0.078196
H	-5.714118	-1.083982	-2.709802
H	-2.630218	0.961717	-2.766532
H	-2.439603	-0.711094	-3.400690
H	-3.914560	0.238147	-3.787858
H	-3.128508	-0.928027	1.980824
H	-4.914658	-0.892204	2.167395
H	-4.081423	-2.444064	1.811485
C	0.513591	3.369922	-0.186397
N	1.183335	0.641323	1.552498
C	2.414363	1.316708	1.980473
S	0.676430	-0.749188	2.652893
H	2.685534	2.092134	1.245800
H	3.240309	0.588398	2.044753
H	2.258172	1.760498	2.976958
O	-0.755611	-0.611392	2.845904
C	1.037583	-2.131474	1.630318
O	1.620255	-0.647324	3.746701
C	-0.448284	3.678597	0.786579
C	-0.823229	5.001499	1.004439
C	-0.235843	6.022107	0.258212
C	0.731577	5.721197	-0.703605
C	1.107787	4.402781	-0.925554
H	-0.920569	2.881847	1.377575
H	-1.577932	5.237195	1.762379
H	-0.528943	7.063630	0.431648
H	1.201030	6.526425	-1.279172
H	1.879228	4.145728	-1.659609
C	2.377394	-2.464836	1.412780
C	2.667017	-3.523824	0.565000
C	1.644891	-4.260644	-0.053100

C	0.313086	-3.913282	0.205906
C	-0.004196	-2.850645	1.045068
H	3.182965	-1.906573	1.903517
H	3.713401	-3.793087	0.377172
C	1.978362	-5.408028	-0.951542
H	-0.494443	-4.491375	-0.259060
H	-1.047360	-2.592375	1.255606
H	1.155221	-5.633836	-1.651667
H	2.895340	-5.210986	-1.535651
H	2.166826	-6.325632	-0.360786

TS_{4a2}

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scf done: -2059.771592

C	-3.985591	4.113527	-0.872044
C	-3.165115	4.968165	-1.566107
C	-1.887548	4.534851	-2.007552
C	-1.401252	3.266877	-1.763238
C	-2.224797	2.387296	-1.034596
C	-3.507939	2.811592	-0.598255
C	-4.077979	1.716333	0.059224
O	-3.322469	0.696977	0.144830
N	-1.970346	1.100795	-0.718398
H	-4.977314	4.421479	-0.526312
H	-3.490690	5.988951	-1.787610
H	-1.260050	5.237225	-2.567459
H	-0.414710	2.944467	-2.111214
H	-5.095833	1.634623	0.469371
C	-0.821306	0.406501	-0.464159
C	0.258269	0.995101	0.176170
Au	2.140975	0.123983	0.005485
C	3.982482	-0.845028	-0.091227
N	4.228238	-2.088121	0.380657
C	5.544732	-2.439798	0.165088
C	6.133518	-1.388002	-0.460789
N	5.158245	-0.420526	-0.606860
C	5.383363	0.860985	-1.243020
C	3.243463	-2.920892	1.052809
H	5.944921	-3.405229	0.474720
H	7.153547	-1.241084	-0.815709
H	5.636623	0.722860	-2.308211
H	4.462110	1.459360	-1.164534
H	6.207439	1.395397	-0.740525
H	2.328020	-3.003866	0.442516
H	3.672466	-3.924058	1.201882
H	2.981523	-2.488442	2.033705
N	-0.770500	-0.890232	-1.000593
C	0.043436	2.184342	0.990858
C	-1.297903	-1.151980	-2.327664
S	-0.663708	-2.209814	0.066041
C	-2.307557	-2.862909	0.164730
O	0.176083	-3.200939	-0.598264
O	-0.301489	-1.663974	1.368435
H	-0.932650	-0.366514	-3.012310
H	-0.912729	-2.119500	-2.691105
H	-2.407426	-1.166117	-2.353559
C	-1.016293	2.253122	1.915390
C	-1.239114	3.412625	2.650413
C	-0.422187	4.528594	2.462430
C	0.648905	4.465318	1.569315

C	0.897556	3.294702	0.862422
H	-1.643632	1.366311	2.074342
H	-2.054196	3.447680	3.382369
H	-0.606375	5.445455	3.033546
H	1.304993	5.332944	1.437503
H	1.748016	3.231364	0.171213
C	-2.686673	-3.910249	-0.675274
C	-3.983875	-4.403142	-0.591963
C	-4.905591	-3.870018	0.319141
C	-4.489738	-2.827869	1.158853
C	-3.197935	-2.318366	1.090510
H	-1.961612	-4.346197	-1.371151
H	-4.288369	-5.233706	-1.240604
C	-6.305314	-4.396341	0.382920
H	-5.193413	-2.418658	1.894418
H	-2.873738	-1.515571	1.761837
H	-6.341790	-5.478626	0.166265
H	-6.761839	-4.223936	1.373244
H	-6.949574	-3.896141	-0.366519

4a2

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scf done: -2059.822135

C	5.071771	-1.653280	-1.890333
C	4.410833	-2.822081	-2.237629
C	3.016631	-2.804018	-2.328765
C	2.301329	-1.641240	-2.065862
C	2.958722	-0.459589	-1.688455
C	4.373082	-0.469291	-1.609060
C	5.165656	0.725256	-1.275137
O	4.747845	1.798130	-0.903778
N	2.257153	0.721196	-1.521595
H	6.168030	-1.636248	-1.830450
H	4.971071	-3.738371	-2.449488
H	2.475715	-3.712580	-2.617685
H	1.208311	-1.625974	-2.165772
H	6.272422	0.562191	-1.393615
C	1.495808	1.074295	-0.561536
C	1.157477	0.111869	0.507606
Au	-0.651778	-0.854435	0.247269
C	-2.532150	-1.720734	-0.005421
N	-3.238720	-1.827155	-1.152466
C	-4.501525	-2.323735	-0.901700
C	-4.578311	-2.537054	0.438195
N	-3.358429	-2.165659	0.967350
C	-3.041259	-2.208282	2.381718
C	-2.764661	-1.429516	-2.464474
H	-5.224068	-2.495382	-1.699949
H	-5.381804	-2.937042	1.056864
H	-3.569753	-1.403579	2.922964
H	-3.337301	-3.182827	2.803889
H	-1.954997	-2.074384	2.508128
H	-1.667050	-1.522763	-2.497255
H	-3.206180	-2.089968	-3.228184
H	-3.043732	-0.381077	-2.676500
N	0.928474	2.338322	-0.600247
C	2.144509	-0.193652	1.475360
C	1.319648	3.228462	-1.689174
S	-0.116016	2.882063	0.630462
C	-1.732479	2.338996	0.135869

O	-0.068313	4.329996	0.589255
O	0.265814	2.140720	1.830217
H	0.929029	2.857671	-2.653863
H	0.931412	4.235672	-1.477861
H	2.420856	3.261013	-1.744652
C	3.283963	0.639025	1.644778
C	4.228286	0.343432	2.610266
C	4.060290	-0.786160	3.419704
C	2.945988	-1.622035	3.275673
C	1.992786	-1.325719	2.319016
H	3.414451	1.518306	1.002502
H	5.102028	0.989612	2.741837
H	4.812870	-1.019881	4.181436
H	2.832506	-2.500408	3.918775
H	1.109690	-1.963791	2.188774
C	-2.562780	1.743944	1.084014
C	-3.843938	1.351618	0.704825
C	-4.302892	1.540100	-0.604105
C	-3.446164	2.153528	-1.531180
C	-2.169300	2.564997	-1.169818
H	-2.202471	1.583321	2.106530
H	-4.507113	0.884340	1.444391
C	-5.684213	1.129914	-1.009517
H	-3.795631	2.320208	-2.558054
H	-1.520501	3.054231	-1.905849
H	-5.701376	0.726727	-2.039291
H	-6.102894	0.368158	-0.328430
H	-6.371554	1.998169	-0.996837

TS_{5a1syn}

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scf done: -2059.798130

C	2.250910	4.193290	1.376240
C	1.150422	4.586806	0.583486
C	0.131957	3.694440	0.353985
C	0.216456	2.356064	0.864505
C	1.410982	1.956781	1.562099
C	2.411941	2.899874	1.861895
C	3.693884	2.546727	2.512607
O	4.128912	1.432298	2.639904
N	1.502897	0.614978	1.763495
H	3.040871	4.926048	1.589478
H	1.091256	5.614534	0.212373
H	-0.791539	4.016715	-0.144525
H	-0.717006	2.046317	1.363612
H	4.272085	3.442131	2.871330
C	0.839511	-0.018131	0.841570
C	0.110247	0.804336	-0.207239
Au	-1.983137	0.286634	-0.132136
C	-3.965184	-0.293282	0.079081
N	-4.395420	-1.397249	0.731913
C	-5.771508	-1.492584	0.670334
C	-6.206106	-0.417258	-0.035409
N	-5.082971	0.304531	-0.389411
C	-5.126316	1.541463	-1.144141
C	-3.538150	-2.388599	1.356419
H	-6.316997	-2.313748	1.135565
H	-7.210486	-0.097074	-0.312546
H	-5.649820	2.324149	-0.569102
H	-4.094239	1.868844	-1.346229

H	-5.651031	1.382611	-2.101123
H	-3.303874	-3.203739	0.649276
H	-2.596854	-1.911981	1.676377
H	-4.048924	-2.808166	2.238011
C	0.696736	-1.475893	0.895377
N	0.659493	0.956933	-1.470105
C	-0.167891	1.532104	-2.523035
S	2.394613	1.109367	-1.729654
H	-1.067462	0.902991	-2.652401
H	-0.483871	2.563127	-2.261658
H	0.391587	1.564734	-3.468737
O	2.540763	1.329994	-3.159904
O	2.918554	2.077431	-0.773052
C	2.998720	-0.496306	-1.323002
C	0.170164	-2.210767	-0.180624
C	0.052278	-3.593937	-0.096775
C	0.451463	-4.259012	1.063395
C	0.987704	-3.540044	2.134429
C	1.118558	-2.159697	2.048673
H	-0.138674	-1.694666	-1.098037
H	-0.352577	-4.158818	-0.943955
H	0.350986	-5.348312	1.131571
H	1.309584	-4.063357	3.041415
H	1.553392	-1.581678	2.870992
C	2.720349	-1.546780	-2.201637
C	3.167533	-2.818665	-1.880414
C	3.895825	-3.054763	-0.702276
C	4.188056	-1.972770	0.135519
C	3.748717	-0.687013	-0.164595
H	2.151283	-1.364791	-3.120919
H	2.945651	-3.657676	-2.551697
C	4.359621	-4.436301	-0.366537
H	4.763387	-2.140035	1.054036
H	3.962445	0.146608	0.513526
H	4.578335	-4.541930	0.710425
H	3.604414	-5.193231	-0.646327
H	5.287007	-4.686252	-0.917916

5a1_{syn}

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scf done: -2059.819176

C	2.297998	3.603454	1.369778
C	2.993340	2.928442	0.301505
C	2.448889	1.852326	-0.312500
C	1.068557	1.444088	0.066986
C	0.644037	1.877421	1.431131
C	1.138431	3.137815	1.932086
C	0.526251	3.865747	3.063065
O	-0.499627	3.565602	3.613451
N	-0.106147	1.013960	2.043689
H	2.739860	4.521850	1.780904
H	3.970185	3.308916	-0.015601
H	2.957538	1.364571	-1.153726
H	0.442821	2.092787	-0.610567
H	1.111142	4.777963	3.366220
C	-0.162484	-0.138308	1.264018
C	0.509417	0.031063	0.020161
Au	-1.713911	0.261672	-0.618515
C	-3.636666	0.409858	-1.324355
N	-4.700573	-0.182258	-0.740795

C	-5.850975	0.099433	-1.447417
C	-5.486208	0.884998	-2.494377
N	-4.120141	1.063738	-2.400408
C	-3.343009	1.851747	-3.337485
C	-4.633566	-1.000501	0.460080
H	-6.825527	-0.281888	-1.142341
H	-6.074203	1.333919	-3.294759
H	-3.692019	2.897941	-3.334743
H	-2.284714	1.821491	-3.034538
H	-3.441324	1.437399	-4.354778
H	-4.184687	-0.425903	1.288120
H	-5.654239	-1.301562	0.740728
H	-4.025317	-1.903797	0.278416
C	-0.856375	-1.305313	1.828518
N	1.087026	-1.005060	-0.740259
S	2.318567	-1.963813	-0.020125
C	1.062857	-0.953126	-2.192555
H	1.407994	-1.918621	-2.597866
H	0.021270	-0.805768	-2.533304
H	1.690064	-0.138978	-2.613793
C	3.870022	-1.239429	-0.478791
O	2.147014	-1.789581	1.414866
O	2.211822	-3.262239	-0.667995
C	-0.943200	-2.542298	1.161814
C	-1.653817	-3.592336	1.726255
C	-2.285466	-3.432963	2.963466
C	-2.200197	-2.215044	3.633597
C	-1.490932	-1.156596	3.072055
H	-0.442933	-2.688308	0.198714
H	-1.705515	-4.552986	1.202396
H	-2.838487	-4.268186	3.407826
H	-2.685216	-2.086720	4.607462
H	-1.416792	-0.196043	3.590394
C	4.401678	-1.477471	-1.747600
C	5.598782	-0.864711	-2.098967
C	6.286727	-0.040983	-1.195574
C	5.739265	0.157244	0.078709
C	4.535357	-0.435055	0.445827
H	3.893094	-2.148516	-2.448327
H	6.023510	-1.040968	-3.094850
C	7.598550	0.571983	-1.572541
H	6.273564	0.785811	0.802053
H	4.110759	-0.282599	1.444297
H	7.804947	1.487668	-0.991520
H	8.429179	-0.133013	-1.373831
H	7.638556	0.820630	-2.647816

TS_{5alanti}
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scf done: -2059.811906

C	-1.243711	-2.196743	3.161912
C	-0.162080	-2.873041	2.555837
C	0.801222	-2.150566	1.892973
C	0.691507	-0.731637	1.803736
C	-0.443088	-0.062837	2.368987
C	-1.419807	-0.823103	3.066107
C	-2.687713	-0.256915	3.583338
O	-3.199693	0.772596	3.229035
N	-0.596559	1.231793	2.017629
H	-2.004447	-2.780924	3.697357

H	-0.082096	-3.960686	2.648620
H	1.684205	-2.650475	1.474234
H	1.629913	-0.158902	1.839087
H	-3.186088	-0.918882	4.344895
C	-0.023792	1.454099	0.860280
C	0.407519	0.256660	0.092488
Au	-1.450511	-0.567251	-0.621623
C	-3.391422	-1.037806	-1.129191
N	-4.436496	-0.242919	-0.807191
C	-5.618517	-0.803525	-1.244239
C	-5.296333	-1.975254	-1.852695
N	-3.923109	-2.099377	-1.770802
C	-3.176204	-3.215274	-2.315533
C	-4.318152	1.032405	-0.112662
H	-6.582901	-0.321879	-1.082935
H	-5.917402	-2.730971	-2.333480
H	-3.293754	-3.255690	-3.411666
H	-2.111385	-3.080023	-2.069671
H	-3.533920	-4.162019	-1.877140
H	-3.707377	1.733050	-0.708009
H	-5.325004	1.457943	0.017520
H	-3.851701	0.899937	0.880330
C	-0.003971	2.806934	0.290889
N	1.496815	0.249728	-0.707934
C	1.590887	-0.633932	-1.862927
S	2.949843	1.162895	-0.320553
C	4.220391	-0.067573	-0.290537
O	2.710336	1.640259	1.036752
O	3.195629	2.060188	-1.434281
H	1.553238	-1.694100	-1.543870
H	0.759169	-0.428683	-2.560090
H	2.536367	-0.458674	-2.401543
C	0.099761	3.039870	-1.089096
C	0.071422	4.339711	-1.582513
C	-0.051327	5.418128	-0.706558
C	-0.158939	5.194705	0.666888
C	-0.143984	3.897522	1.162764
H	0.195638	2.202115	-1.790112
H	0.148850	4.512987	-2.661220
H	-0.064450	6.441535	-1.098066
H	-0.256342	6.040892	1.355728
H	-0.238003	3.705033	2.236426
C	4.355174	-0.894609	0.827094
C	5.371053	-1.841117	0.842013
C	6.262723	-1.967284	-0.234358
C	6.115852	-1.106244	-1.329176
C	5.102232	-0.155071	-1.367361
H	3.694804	-0.782498	1.694732
H	5.494472	-2.487410	1.719483
C	7.338781	-3.005506	-0.209924
H	6.819770	-1.176043	-2.166937
H	5.000790	0.528177	-2.217605
H	7.748484	-3.139621	0.806797
H	6.941610	-3.988526	-0.530180
H	8.168788	-2.750041	-0.890818

5a1_{anti}

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scf done: -2059.828742

C	-5.234106	-0.862945	1.392972
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C	-4.698455	-2.127725	0.953308
C	-3.439723	-2.216349	0.463754
C	-2.591611	-0.994058	0.471605
C	-3.343747	0.292098	0.497268
C	-4.593480	0.336675	1.216788
C	-5.243931	1.589572	1.650344
O	-4.769836	2.690835	1.555950
N	-2.795566	1.231538	-0.214211
H	-6.225468	-0.854186	1.867111
H	-5.319283	-3.024433	1.047316
H	-2.990235	-3.179619	0.195428
H	-2.116585	-1.056207	1.490061
H	-6.254231	1.422389	2.116759
C	-1.721362	0.671394	-0.902273
C	-1.493471	-0.682435	-0.527242
Au	0.170746	0.434150	0.616471
C	1.833312	1.146748	1.596132
N	2.778984	1.929041	1.033192
C	3.825436	2.121030	1.911692
C	3.512748	1.444155	3.048101
N	2.283428	0.853468	2.832845
C	1.608410	0.014586	3.804430
C	2.735077	2.433168	-0.329060
H	4.691982	2.731099	1.656176
H	4.045240	1.342470	3.993744
H	1.399636	0.586834	4.723978
H	0.658698	-0.337336	3.370749
H	2.238514	-0.857258	4.052616
H	3.451579	3.264039	-0.426418
H	2.999786	1.631448	-1.043215
H	1.721691	2.802641	-0.561586
C	-1.084165	1.485993	-1.948528
N	-0.936386	-1.671664	-1.378493
S	0.013941	-2.894505	-0.668794
C	-1.715516	-2.003953	-2.573307
H	-1.213249	-2.813620	-3.124448
H	-2.741870	-2.335077	-2.318283
H	-1.775615	-1.114305	-3.226161
O	0.003269	-4.002736	-1.610033
C	1.645984	-2.197466	-0.614818
O	-0.430897	-3.078034	0.712522
C	2.315859	-2.115903	0.602628
C	3.593173	-1.560470	0.634750
C	4.207446	-1.092837	-0.532193
C	3.518499	-1.220316	-1.750713
C	2.249800	-1.781523	-1.802782
H	1.828690	-2.475789	1.515760
H	4.126725	-1.486616	1.591650
C	5.580552	-0.497454	-0.502428
H	3.999403	-0.880417	-2.676743
H	1.729467	-1.899658	-2.761573
H	5.638768	0.417353	-1.121672
H	5.896198	-0.245554	0.525063
H	6.325838	-1.205087	-0.914040
C	-0.050850	0.993222	-2.766217
C	0.538768	1.808930	-3.723079
C	0.108544	3.128595	-3.881226
C	-0.916696	3.625724	-3.078014
C	-1.512242	2.812871	-2.117994
H	0.297339	-0.036304	-2.639061
H	1.340578	1.411477	-4.355836

H	0.572999	3.769964	-4.638599
H	-1.259947	4.658574	-3.201628
H	-2.317624	3.192233	-1.481869

TS_{5a2syn}
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scf done: -2059.819176

C	2.297998	3.603454	1.369778
C	2.993340	2.928442	0.301505
C	2.448889	1.852326	-0.312500
C	1.068557	1.444088	0.066986
C	0.644037	1.877421	1.431131
C	1.138431	3.137815	1.932086
C	0.526251	3.865747	3.063065
O	-0.499627	3.565602	3.613451
N	-0.106147	1.013960	2.043689
H	2.739860	4.521850	1.780904
H	3.970185	3.308916	-0.015601
H	2.957538	1.364571	-1.153726
H	0.442821	2.092787	-0.610567
H	1.111142	4.777963	3.366220
C	-0.162484	-0.138308	1.264018
C	0.509417	0.031063	0.020161
Au	-1.713911	0.261672	-0.618515
C	-3.636666	0.409858	-1.324355
N	-4.700573	-0.182258	-0.740795
C	-5.850975	0.099433	-1.447417
C	-5.486208	0.884998	-2.494377
N	-4.120141	1.063738	-2.400408
C	-3.343009	1.851747	-3.337485
C	-4.633566	-1.000501	0.460080
H	-6.825527	-0.281888	-1.142341
H	-6.074203	1.333919	-3.294759
H	-3.692019	2.897941	-3.334743
H	-2.284714	1.821491	-3.034538
H	-3.441324	1.437399	-4.354778
H	-4.184687	-0.425903	1.288120
H	-5.654239	-1.301562	0.740728
H	-4.025317	-1.903797	0.278416
C	-0.856375	-1.305313	1.828518
N	1.087026	-1.005060	-0.740259
S	2.318567	-1.963813	-0.020125
C	1.062857	-0.953126	-2.192555
H	1.407994	-1.918621	-2.597866
H	0.021270	-0.805768	-2.533304
H	1.690064	-0.138978	-2.613793
C	3.870022	-1.239429	-0.478791
O	2.147014	-1.789581	1.414866
O	2.211822	-3.262239	-0.667995
C	-0.943200	-2.542298	1.161814
C	-1.653817	-3.592336	1.726255
C	-2.285466	-3.432963	2.963466
C	-2.200197	-2.215044	3.633597
C	-1.490932	-1.156596	3.072055
H	-0.442933	-2.688308	0.198714
H	-1.705515	-4.552986	1.202396
H	-2.838487	-4.268186	3.407826
H	-2.685216	-2.086720	4.607462
H	-1.416792	-0.196043	3.590394
C	4.401678	-1.477471	-1.747600

C	5.598782	-0.864711	-2.098967
C	6.286727	-0.040983	-1.195574
C	5.739265	0.157244	0.078709
C	4.535357	-0.435055	0.445827
H	3.893094	-2.148516	-2.448327
H	6.023510	-1.040968	-3.094850
C	7.598550	0.571983	-1.572541
H	6.273564	0.785811	0.802053
H	4.110759	-0.282599	1.444297
H	7.804947	1.487668	-0.991520
H	8.429179	-0.133013	-1.373831
H	7.638556	0.820630	-2.647816

5a2_{syn}

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scf done: -2059.833853

C	0.074092	3.213438	2.013152
C	-0.743986	3.503457	3.052553
C	-1.651109	2.510422	3.565880
C	-1.864651	1.291326	2.970452
C	-1.147065	1.047182	1.743229
C	0.095139	1.825713	1.483573
H	0.853649	1.333774	2.157468
N	-1.486967	0.267500	0.759422
H	0.798027	3.942116	1.626770
H	-0.718353	4.490416	3.524983
H	-2.241276	2.756042	4.459816
C	-2.884345	0.383868	3.528836
C	-0.646231	0.550351	-0.294870
C	0.430011	1.457997	0.035096
Au	1.910048	-0.215384	0.150589
C	3.261425	-1.768778	0.313670
N	4.566516	-1.784441	-0.034329
C	5.121402	-3.020670	0.231013
C	4.130379	-3.787018	0.756351
N	2.996956	-3.001475	0.797164
C	1.708194	-3.431653	1.317581
C	5.304566	-0.672399	-0.599901
H	6.166140	-3.244255	0.015133
H	4.129231	-4.822279	1.097291
H	1.717160	-4.527705	1.419648
H	1.526530	-2.980568	2.308258
H	0.896896	-3.138876	0.629623
H	4.597004	0.135545	-0.845051
H	6.050666	-0.297799	0.121586
H	5.818948	-0.992345	-1.521164
N	-0.902247	-0.041463	-1.481452
C	0.871846	2.595019	-0.833611
O	-3.180566	-0.699665	3.094797
H	-3.377880	0.794422	4.452004
C	-0.075377	0.234565	-2.644260
S	-1.688940	-1.649578	-1.445619
O	-1.551471	-2.104045	-2.819177
C	-3.387515	-1.344811	-1.109075
O	-1.060651	-2.384015	-0.358723
H	0.988201	-0.015830	-2.436626
H	-0.428308	-0.377511	-3.485913
H	-0.145947	1.300137	-2.914585
C	2.215207	2.965985	-0.959055
C	2.578118	4.096248	-1.690891

C	1.601558	4.874125	-2.309869
C	0.257867	4.523137	-2.183026
C	-0.102847	3.399685	-1.442906
H	2.991187	2.358266	-0.473271
H	3.635684	4.368648	-1.780661
H	1.887375	5.758214	-2.890398
H	-0.517904	5.131513	-2.661385
H	-1.164726	3.135663	-1.336454
C	-4.219673	-0.993601	-2.174311
C	-5.572503	-0.806307	-1.922801
C	-6.100468	-0.971794	-0.633349
C	-5.234559	-1.334979	0.406467
C	-3.876291	-1.525002	0.182474
H	-3.816167	-0.885999	-3.186782
H	-6.242423	-0.537899	-2.748778
C	-7.556587	-0.745313	-0.374510
H	-5.628078	-1.472412	1.421134
H	-3.206069	-1.783836	1.006008
H	-7.908026	-1.316414	0.502402
H	-7.757007	0.324649	-0.169603
H	-8.173149	-1.027318	-1.246263

TS5a2anti

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scf done: -2059.802044

C	2.350004	-1.257501	3.335123
C	3.450043	-0.491792	2.885584
C	3.231402	0.734382	2.304606
C	1.903659	1.237327	2.188292
C	0.797329	0.450605	2.633656
C	1.036843	-0.833675	3.189772
C	-0.040928	-1.828639	3.394873
O	-1.104940	-1.826539	2.828141
N	-0.434968	0.893925	2.299369
H	2.531491	-2.254442	3.759219
H	4.466265	-0.878899	3.009808
H	4.070193	1.354866	1.968193
H	1.789969	2.327174	2.227051
H	0.239811	-2.662030	4.094830
C	-0.358045	1.502537	1.143934
C	0.896209	1.391492	0.360468
Au	1.150009	-0.583205	-0.410393
C	1.313987	-2.503331	-1.153210
N	2.390473	-3.079930	-1.730373
C	2.101223	-4.375012	-2.112849
C	0.808797	-4.604721	-1.761533
N	0.345927	-3.444618	-1.173797
C	-0.998650	-3.240770	-0.663383
C	3.667911	-2.416657	-1.916303
H	2.836178	-5.015086	-2.600621
H	0.180047	-5.487016	-1.880133
H	-1.576951	-4.168184	-0.797948
H	-0.967265	-2.985422	0.410812
H	-1.495073	-2.423027	-1.214859
H	4.353298	-3.097710	-2.443861
H	3.536658	-1.500838	-2.517167
H	4.105567	-2.148842	-0.939402
N	-1.463818	2.191027	0.682544
C	1.446224	2.549194	-0.344840
S	-2.072769	1.893357	-0.901688

C	-2.457823	2.630228	1.659803
H	-3.187740	3.277769	1.147667
H	-2.974153	1.778162	2.138899
H	-1.947380	3.222190	2.437559
O	-2.684565	3.124246	-1.363818
O	-0.981004	1.273022	-1.639680
C	-3.337687	0.697721	-0.569038
C	-4.604566	0.891044	-1.113750
C	-5.588819	-0.064316	-0.875062
C	-5.330594	-1.191042	-0.085517
C	-4.046323	-1.348556	0.458612
C	-3.043149	-0.418446	0.219141
H	-4.813653	1.781174	-1.716451
H	-6.587423	0.072582	-1.307326
C	-6.408314	-2.186735	0.208093
H	-3.829091	-2.215349	1.096246
H	-2.058159	-0.555567	0.687373
H	-6.900421	-1.957261	1.173344
H	-7.193506	-2.179422	-0.567675
H	-6.004922	-3.211690	0.289159
C	2.418481	2.355787	-1.344195
C	2.983068	3.433386	-2.016175
C	2.587749	4.732425	-1.699106
C	1.632734	4.950054	-0.702222
C	1.073025	3.873281	-0.030017
H	2.724538	1.330865	-1.593444
H	3.732574	3.260864	-2.795911
H	3.027624	5.584144	-2.229788
H	1.325018	5.970478	-0.450077
H	0.328161	4.061728	0.752638

5a2_{anti}

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scf done: -2059.838396

C	-1.124081	1.486788	2.919639
C	-0.982429	0.809905	4.081103
C	0.153787	-0.052597	4.283042
C	1.090646	-0.335197	3.320555
C	0.891626	0.257168	2.019805
C	-0.066478	1.392326	1.887639
H	0.573590	2.295760	2.090289
N	1.399025	-0.120768	0.880608
H	-1.961065	2.177176	2.750999
H	-1.714407	0.916324	4.887707
H	0.261240	-0.544043	5.260095
C	2.171802	-1.286384	3.646277
C	0.751773	0.594775	-0.106500
C	-0.334160	1.422711	0.379813
Au	-1.851468	-0.157890	-0.039596
C	-3.273377	-1.605746	-0.406803
N	-4.613404	-1.432834	-0.429266
C	-5.247677	-2.618708	-0.740314
C	-4.272388	-3.548887	-0.908680
N	-3.067851	-2.906825	-0.701976
C	-1.778974	-3.576332	-0.754515
C	-5.287150	-0.164256	-0.224869
H	-6.332526	-2.692521	-0.814714
H	-4.325166	-4.609263	-1.155096
H	-1.757232	-4.254693	-1.622693
H	-0.971400	-2.833873	-0.861090

H	-1.613344	-4.161662	0.166138
H	-4.804083	0.382797	0.601108
H	-5.247742	0.451177	-1.140721
H	-6.339701	-0.353817	0.037762
N	1.143345	0.430156	-1.383004
C	-0.660978	2.777897	-0.175135
O	3.042084	-1.655533	2.901907
H	2.125697	-1.650538	4.709601
C	0.465479	1.115838	-2.473217
S	2.052789	-1.057213	-1.813747
H	-0.630085	0.957746	-2.403023
H	0.675687	2.197271	-2.442005
H	0.826528	0.704928	-3.426560
O	2.099179	-0.990332	-3.264980
C	3.670553	-0.795148	-1.178927
O	1.382317	-2.161869	-1.150319
C	-1.972982	3.187173	-0.436141
C	-2.242337	4.480401	-0.884928
C	-1.202028	5.386529	-1.076046
C	0.110756	4.997119	-0.807877
C	0.374417	3.707908	-0.354551
H	-2.799238	2.476677	-0.291120
H	-3.276335	4.780369	-1.088661
H	-1.413277	6.400961	-1.431993
H	0.935400	5.704285	-0.951236
H	1.411068	3.407498	-0.140536
C	4.052106	-1.403202	0.013622
C	5.349500	-1.203857	0.470019
C	6.259652	-0.415638	-0.245530
C	5.838363	0.182184	-1.443582
C	4.549314	-0.004256	-1.923562
H	3.340436	-1.997106	0.591052
H	5.654939	-1.666831	1.416085
C	7.662645	-0.235777	0.241638
H	6.542180	0.801816	-2.012566
H	4.229791	0.450177	-2.867477
H	8.082454	0.736337	-0.071658
H	7.724023	-0.308363	1.341666
H	8.323166	-1.022514	-0.172602

TS_{6a1syn}

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scf done: -2059.797200

C	-0.741812	4.838169	0.800105
C	-0.747008	4.618630	-0.609032
C	-0.529543	3.374155	-1.138924
C	-0.304223	2.290055	-0.243866
C	-0.289161	2.495817	1.195093
C	-0.516668	3.832941	1.708593
C	-0.530033	4.143007	3.158564
O	-0.480751	3.329800	4.040298
N	0.181255	1.382549	1.844222
H	-0.917064	5.853015	1.178723
H	-0.912356	5.471385	-1.275291
H	-0.470889	3.205551	-2.220196
H	-1.406706	2.254239	0.628282
H	-0.611518	5.243744	3.370051
C	0.468831	0.477075	0.927831
C	0.110381	0.897921	-0.445556
Au	-1.786120	-0.287942	-0.412157

C	-3.459127	-1.473197	-0.245368
N	-4.604275	-1.469333	-0.958720
C	-5.458609	-2.452594	-0.500272
C	-4.821286	-3.078350	0.523474
N	-3.594569	-2.463027	0.664099
C	-2.590364	-2.813424	1.656553
C	-4.916849	-0.575113	-2.056969
H	-6.440777	-2.616947	-0.942963
H	-5.132514	-3.904260	1.163037
H	-1.641434	-3.085990	1.163110
H	-2.412378	-1.963695	2.337627
H	-2.952539	-3.673099	2.240473
H	-5.838539	-0.011476	-1.835228
H	-4.081641	0.130877	-2.186857
H	-5.056597	-1.149138	-2.988524
C	1.032256	-0.822156	1.329938
N	0.903779	0.618634	-1.597057
C	0.380678	-0.005826	-2.798531
S	2.436874	1.364936	-1.643278
C	3.562996	0.131747	-1.059328
O	2.371629	2.433557	-0.647421
O	2.728244	1.643264	-3.042356
H	1.135632	0.051021	-3.599329
H	-0.524972	0.520179	-3.161562
H	0.127883	-1.071370	-2.626234
C	1.309377	-1.839269	0.404212
C	1.862383	-3.044021	0.825076
C	2.140154	-3.252544	2.176969
C	1.864085	-2.248584	3.105669
C	1.315716	-1.040813	2.686016
H	1.107969	-1.685245	-0.661119
H	2.083841	-3.826039	0.089422
H	2.574440	-4.203107	2.507937
H	2.079684	-2.408160	4.168021
H	1.097814	-0.241689	3.402206
C	3.970095	-0.878185	-1.931222
C	4.775485	-1.900494	-1.441909
C	5.182078	-1.923949	-0.100570
C	4.782726	-0.876717	0.739594
C	3.972379	0.151570	0.273046
H	3.669955	-0.857138	-2.985363
H	5.106140	-2.698442	-2.118172
C	6.002771	-3.054221	0.435801
H	5.111393	-0.871583	1.786464
H	3.656979	0.966559	0.934064
H	5.356607	-3.791667	0.952967
H	6.538722	-3.590571	-0.366526
H	6.743855	-2.703023	1.175887

6a1_{syn}

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scf done: -2059.816668

C	-2.706369	-2.012252	2.134061
C	-2.554931	-2.514626	0.784872
C	-1.639920	-1.983180	-0.064747
C	-0.842403	-0.870513	0.398528
C	-0.675972	-0.609797	1.875286
C	-1.860070	-1.100359	2.668959
C	-1.939210	-0.794131	4.107082
O	-1.056046	-0.280743	4.744411

N	-0.221782	0.749158	2.013276
H	-3.509291	-2.422190	2.762119
H	-3.220379	-3.313676	0.439189
H	-1.581076	-2.324625	-1.103474
H	0.163059	-1.220503	2.301563
H	-2.903962	-1.118890	4.585103
C	-0.029549	1.246749	0.837760
C	-0.462116	0.307244	-0.257810
Au	1.531578	-0.930732	-0.242564
C	3.554929	-1.245897	-0.302838
N	4.275732	-2.189658	-0.939717
C	5.623414	-1.976743	-0.733308
C	5.730074	-0.871640	0.051662
N	4.447136	-0.437537	0.307755
C	4.102385	0.737617	1.096248
C	3.735841	-3.281035	-1.728371
H	6.383532	-2.632848	-1.157695
H	6.604881	-0.359859	0.452649
H	3.732902	1.550632	0.445377
H	3.321169	0.482818	1.832003
H	5.000632	1.079900	1.632132
H	4.091548	-4.245814	-1.330496
H	2.636804	-3.248482	-1.670027
H	4.049686	-3.182387	-2.781033
C	0.700360	2.512805	0.650361
N	-0.787447	0.710510	-1.566650
C	-0.615638	-0.182639	-2.703410
S	-2.153164	1.774475	-1.664589
C	-3.504117	0.740834	-1.179977
O	-1.954344	2.779300	-0.635896
O	-2.265099	2.109091	-3.072368
H	-0.724568	0.401815	-3.629925
H	0.410471	-0.595018	-2.679403
H	-1.341277	-1.021837	-2.729811
C	1.232302	2.895172	-0.589240
C	2.014780	4.042383	-0.694404
C	2.266888	4.824797	0.431666
C	1.734019	4.454268	1.667648
C	0.960497	3.304589	1.777632
H	1.028110	2.296049	-1.482668
H	2.423760	4.332806	-1.668644
H	2.876551	5.731417	0.345512
H	1.924616	5.068927	2.554522
H	0.549179	2.993872	2.743844
C	-3.926077	0.766643	0.150622
C	-4.924695	-0.111314	0.550301
C	-5.507209	-1.011320	-0.353652
C	-5.086239	-0.988289	-1.690229
C	-4.091095	-0.114220	-2.114823
H	-3.476664	1.473721	0.857462
H	-5.268348	-0.099095	1.592803
C	-6.561986	-1.963308	0.115803
H	-5.556271	-1.665116	-2.413828
H	-3.778885	-0.084035	-3.164994
H	-6.867856	-2.665937	-0.677973
H	-6.205726	-2.553628	0.982381
H	-7.465570	-1.421288	0.453396

TS_{6a1anti}

scf done: -2059.806289

C	-1.647089	4.530475	0.013973
C	-1.356213	4.096544	-1.311066
C	-0.777717	2.876584	-1.545436
C	-0.433821	2.059759	-0.424867
C	-0.663506	2.526245	0.933638
C	-1.343301	3.785153	1.129507
C	-1.720806	4.302595	2.466722
O	-1.512931	3.752604	3.513145
N	-0.303735	1.576454	1.859389
H	-2.140040	5.500631	0.155986
H	-1.612557	4.748682	-2.151951
H	-0.577839	2.521894	-2.562750
H	0.444388	2.816878	0.288350
H	-2.243374	5.297021	2.415252
C	0.203053	0.562844	1.187203
C	0.102240	0.705067	-0.281274
Au	-1.770256	-0.477565	-0.460934
C	-3.473713	-1.633910	-0.478586
N	-4.397051	-1.811662	-1.446303
C	-5.383032	-2.678436	-1.017510
C	-5.055484	-3.047151	0.248451
N	-3.880427	-2.395566	0.560731
C	-3.160728	-2.524234	1.817686
C	-4.391000	-1.175178	-2.749115
H	-6.226321	-2.953432	-1.650965
H	-5.553212	-3.714035	0.952294
H	-3.761149	-3.131755	2.511886
H	-2.186921	-3.017503	1.654797
H	-2.991556	-1.529283	2.262716
H	-5.214946	-0.445250	-2.824420
H	-3.430154	-0.654758	-2.884863
H	-4.506448	-1.936136	-3.538695
C	0.853807	-0.551263	1.883192
N	1.175812	0.254272	-1.114737
C	0.947507	-0.453908	-2.362346
S	2.528565	1.291692	-1.114240
C	3.910868	0.213205	-0.907713
O	2.624790	1.946671	-2.414050
O	2.360941	2.101603	0.101098
H	1.915424	-0.767687	-2.792985
H	0.415950	0.157499	-3.119423
H	0.362688	-1.369802	-2.162346
C	4.737209	-0.048605	-1.999068
C	5.819296	-0.905924	-1.827134
C	6.087799	-1.493678	-0.584595
C	5.238279	-1.203919	0.494009
C	4.152289	-0.351438	0.346299
H	4.534750	0.422938	-2.966785
H	6.476723	-1.122068	-2.678029
C	7.274798	-2.385948	-0.401233
H	5.437170	-1.656185	1.473683
H	3.499595	-0.122336	1.197713
H	8.159800	-1.798680	-0.087273
H	7.097232	-3.145072	0.380745
H	7.545134	-2.903323	-1.338374
C	1.098358	-1.784357	1.258643
C	1.757907	-2.800145	1.942268
C	2.190357	-2.593333	3.253242
C	1.950335	-1.371406	3.882919

C	1.282690	-0.356497	3.204578
H	0.767423	-1.953890	0.227543
H	1.940793	-3.760583	1.447837
H	2.715713	-3.392174	3.788992
H	2.287381	-1.208118	4.912445
H	1.090660	0.610752	3.680821

6a1_{anti}

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scf done: -2059.819204

N	0.249296	0.648553	2.130586
C	0.098305	1.289682	1.016185
C	-0.651011	0.484199	-0.014505
C	-0.948524	-0.730049	0.619943
C	-1.628945	-1.932218	0.237943
C	-1.434844	-3.037123	1.016299
C	-0.530191	-3.022256	2.140014
C	0.027648	-1.873812	2.613718
C	-0.461957	-0.590531	2.024559
C	1.000801	-1.949345	3.719205
O	1.568766	-1.015019	4.221902
H	1.194689	-3.005064	4.056541
H	-0.270414	-3.976607	2.616332
H	-1.916477	-3.982572	0.744048
H	-2.227912	-1.982550	-0.679116
C	0.724193	2.600762	0.792433
H	-1.424237	-0.403856	2.582395
Au	1.321456	-0.630799	-0.545663
C	3.272780	-1.133946	-0.898878
N	4.292619	-0.610384	-0.184957
C	5.494252	-1.104164	-0.644783
C	5.206204	-1.953257	-1.667048
N	3.833493	-1.955629	-1.807951
C	3.119401	-2.738729	-2.798074
C	4.138817	0.365428	0.886113
H	6.447277	-0.809794	-0.205490
H	5.852975	-2.555165	-2.305105
H	3.459789	-2.466526	-3.810974
H	2.043193	-2.524695	-2.706500
H	3.294114	-3.814754	-2.631394
H	3.784244	1.329562	0.479879
H	3.413522	0.002020	1.634398
H	5.114349	0.513765	1.373526
N	-1.295320	1.027617	-1.148380
S	-2.726325	1.894926	-0.797444
O	-2.461585	2.556599	0.470871
O	-3.053992	2.623246	-2.010162
C	-3.945623	0.639016	-0.523404
C	-1.151330	0.443560	-2.471201
H	-1.725486	1.052872	-3.188109
H	-1.499323	-0.608494	-2.530472
C	0.881204	3.148210	-0.488953
C	1.557347	4.353885	-0.658329
C	2.073477	5.028840	0.446525
C	1.914967	4.493005	1.726034
C	1.247805	3.286293	1.898439
H	0.466143	2.634414	-1.362152
H	1.674346	4.773667	-1.663512
H	2.598284	5.981364	0.311379
H	2.314745	5.023957	2.597130

H	1.122724	2.848875	2.894498
C	-4.219779	0.230037	0.781650
C	-5.130009	-0.801801	0.986954
C	-5.771303	-1.427114	-0.090497
C	-5.481790	-0.986262	-1.390542
C	-4.579960	0.046911	-1.617388
H	-3.736024	0.736032	1.625151
H	-5.359867	-1.124671	2.009872
C	-6.778653	-2.509351	0.139581
H	-5.990012	-1.456203	-2.241504
H	-4.382341	0.405384	-2.634014
H	-6.788998	-3.240446	-0.688095
H	-6.590906	-3.049095	1.084216
H	-7.798952	-2.083981	0.206207
H	-0.089125	0.487900	-2.780614

TS_{6a2syn}

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scf done: -2059.802723

C	0.893032	2.461508	3.813207
C	-0.255763	3.158949	3.338281
C	-0.800706	2.888113	2.109320
C	-0.203143	1.874927	1.305630
C	0.979882	1.152689	1.775061
C	1.527692	1.489034	3.078724
C	2.722907	0.822103	3.645368
O	3.294559	-0.117093	3.160113
N	1.531783	0.421195	0.765553
H	1.295179	2.713990	4.802444
H	-0.702657	3.932428	3.971182
H	-1.658557	3.448240	1.720541
H	-0.148129	0.699442	2.114770
H	3.058367	1.276145	4.616414
C	0.776148	0.602914	-0.303753
C	-0.424543	1.443285	-0.070757
Au	-1.867056	-0.258421	0.128497
C	-3.174762	-1.839288	0.278201
N	-4.496807	-1.815957	0.001172
C	-5.049300	-3.066367	0.190196
C	-4.040362	-3.880026	0.597631
N	-2.897278	-3.108197	0.642245
C	-1.597828	-3.595879	1.077129
C	-5.221567	-0.644955	-0.458228
H	-6.105669	-3.266329	0.012324
H	-4.032098	-4.938862	0.855532
H	-1.462621	-3.413541	2.157350
H	-1.544219	-4.679202	0.886716
H	-0.791853	-3.093536	0.516421
H	-6.291785	-0.892833	-0.529553
H	-5.093147	0.185384	0.256437
H	-4.856706	-0.331403	-1.451390
N	1.062919	-0.050619	-1.473252
C	-0.907994	2.523897	-0.997871
C	0.281086	0.193324	-2.674319
S	1.846123	-1.615284	-1.339979
H	0.661328	-0.450235	-3.480209
H	-0.793373	-0.039325	-2.512081
H	0.377436	1.246948	-2.982921
O	1.226545	-2.313953	-0.221367
O	1.748013	-2.163316	-2.684488

C	3.538565	-1.268377	-0.990598
C	0.038805	3.423371	-1.510223
C	-0.349605	4.480423	-2.328918
C	-1.697778	4.668971	-2.632446
C	-2.650266	3.795077	-2.112823
C	-2.257713	2.729395	-1.303212
H	1.101251	3.281204	-1.267046
H	0.406334	5.165390	-2.728875
H	-2.006340	5.500965	-3.275004
H	-3.711599	3.938371	-2.344482
H	-3.015839	2.040121	-0.905858
C	4.385712	-0.982068	-2.062459
C	5.727085	-0.731382	-1.801364
C	6.230292	-0.771148	-0.493046
C	5.349612	-1.063278	0.556730
C	4.003479	-1.316050	0.321500
H	4.000098	-0.965469	-3.087459
H	6.405295	-0.503786	-2.632893
C	7.683830	-0.534594	-0.227026
H	5.720474	-1.084413	1.589000
H	3.320186	-1.517276	1.149794
H	8.140337	0.113575	-0.995656
H	7.846215	-0.073216	0.763113
H	8.243510	-1.490399	-0.233873

6a2_{syn}

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scf done: -2059.825098

C	0.702530	1.884087	3.914766
C	-0.555629	2.502983	3.547799
C	-1.144459	2.260147	2.348935
C	-0.468874	1.381641	1.426362
C	0.623792	0.455889	1.894900
C	1.306059	0.950730	3.140997
C	2.506996	0.259076	3.639018
O	2.948896	-0.765918	3.183613
N	1.394986	0.114220	0.739776
H	1.169109	2.167383	4.867108
H	-1.005613	3.224613	4.238104
H	-2.040236	2.806601	2.031564
H	0.164830	-0.507652	2.248554
H	2.982196	0.763399	4.523665
C	0.804920	0.607439	-0.295664
C	-0.380145	1.476972	0.034548
Au	-1.928991	-0.217323	0.267277
C	-3.108326	-1.874906	0.007457
N	-2.690789	-3.142664	0.205368
C	-3.710362	-4.026109	-0.073029
C	-4.783213	-3.283421	-0.455541
N	-4.391727	-1.962141	-0.399548
C	-5.259069	-0.848772	-0.733604
C	-1.359957	-3.517108	0.664907
H	-3.583661	-5.104411	0.020867
H	-5.786100	-3.576090	-0.765976
H	-4.684601	0.087257	-0.653779
H	-5.632173	-0.957810	-1.765442
H	-6.114256	-0.810421	-0.038280
H	-1.280238	-4.614739	0.651791
H	-0.584203	-3.090161	0.005089
H	-1.204420	-3.160232	1.697865

N	1.167190	0.257369	-1.576848
C	-0.864453	2.654996	-0.734034
C	0.508451	0.810217	-2.751279
S	1.985744	-1.276870	-1.755853
H	-0.588776	0.662400	-2.709918
H	0.895517	0.291086	-3.639939
H	0.725482	1.886550	-2.852557
C	3.618706	-1.014920	-1.139090
O	1.281998	-2.252769	-0.933999
O	2.057604	-1.465750	-3.197488
C	0.079616	3.651186	-1.022657
C	-0.297566	4.811276	-1.692255
C	-1.626087	4.997311	-2.074980
C	-2.573233	4.019568	-1.780439
C	-2.194716	2.855310	-1.112973
H	1.125667	3.506872	-0.720525
H	0.452428	5.578500	-1.913831
H	-1.923635	5.909257	-2.604024
H	-3.618845	4.159673	-2.075630
H	-2.948768	2.087610	-0.892596
C	3.946591	-1.385868	0.163312
C	5.250623	-1.186559	0.601010
C	6.224136	-0.629304	-0.238422
C	5.858801	-0.266827	-1.542682
C	4.562439	-0.458893	-2.004349
H	3.187338	-1.794421	0.834658
H	5.513275	-1.462173	1.629752
C	7.631822	-0.450353	0.237087
H	6.610708	0.170183	-2.211259
H	4.286102	-0.190001	-3.029486
H	8.130255	0.394759	-0.269757
H	7.674733	-0.280618	1.327433
H	8.234302	-1.355652	0.026480

TS6a2anti

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scf done: -2059.806154

C	4.330764	0.071639	2.598406
C	4.724160	0.080801	1.225734
C	3.872594	-0.342324	0.243465
C	2.573699	-0.833359	0.616710
C	2.195412	-0.911900	2.030164
C	3.111012	-0.392951	3.025755
C	2.785804	-0.344453	4.469849
O	1.773321	-0.749305	4.972738
N	0.901837	-1.308789	2.170073
H	5.033680	0.449874	3.351765
H	5.722218	0.444975	0.962106
H	4.150160	-0.304109	-0.815649
H	2.874463	-1.864589	1.421603
H	3.604814	0.121112	5.084125
C	0.433045	-1.502403	0.943515
C	1.374138	-1.182289	-0.136099
Au	0.715099	0.943303	-0.493745
C	0.142587	2.884399	-0.859156
N	0.681546	4.017984	-0.357165
C	0.017595	5.125046	-0.847993
C	-0.955361	4.662574	-1.674277
N	-0.864448	3.285014	-1.666461
C	-1.723505	2.415945	-2.453043

C	1.783070	4.091467	0.583170
H	0.297158	6.139756	-0.564402
H	-1.703079	5.187889	-2.268459
H	-2.779601	2.678212	-2.272700
H	-1.500304	2.531105	-3.527421
H	-1.555455	1.366664	-2.158962
H	2.578985	4.740400	0.181220
H	1.436040	4.496837	1.548895
H	2.184697	3.077052	0.739657
N	-0.818647	-2.064805	0.821617
C	1.487742	-1.949540	-1.415505
C	-1.435320	-2.664773	2.005284
S	-1.878012	-1.866330	-0.520284
C	-3.270643	-1.068342	0.222723
O	-1.237384	-0.929520	-1.436125
O	-2.268234	-3.193607	-0.956572
H	-2.225198	-3.361497	1.680335
H	-0.668296	-3.230252	2.555771
H	-1.859985	-1.899344	2.680123
C	1.144929	-3.306400	-1.457086
C	1.311042	-4.046267	-2.625545
C	1.837407	-3.447300	-3.768294
C	2.191024	-2.099507	-3.736458
C	2.012049	-1.357120	-2.571549
H	0.730444	-3.796641	-0.567775
H	1.027989	-5.104669	-2.639311
H	1.968192	-4.030633	-4.686451
H	2.599369	-1.615988	-4.631098
H	2.269200	-0.288398	-2.564696
C	-3.134471	0.241200	0.688945
C	-4.236977	0.866504	1.255062
C	-5.473928	0.209497	1.352346
C	-5.575373	-1.102182	0.873988
C	-4.481028	-1.750824	0.309485
H	-2.171400	0.765241	0.620010
H	-4.142208	1.890581	1.636500
C	-6.661475	0.907341	1.936080
H	-6.534036	-1.629246	0.948990
H	-4.559090	-2.777995	-0.062929
H	-6.370031	1.594391	2.750142
H	-7.175440	1.516023	1.166659
H	-7.401535	0.190375	2.331535

6a2_{anti}

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scf done: -2059.826684

C	0.148806	-4.365717	-0.555341
C	-0.543413	-3.923516	-1.741905
C	-1.255279	-2.759453	-1.758829
C	-1.338018	-2.019433	-0.530261
C	-1.092484	-2.732053	0.755998
C	-0.022124	-3.771048	0.658693
C	0.747077	-4.264394	1.812883
O	0.685269	-3.833197	2.935753
N	-1.187604	-1.767036	1.806275
H	0.843880	-5.211555	-0.638033
H	-0.433456	-4.507539	-2.661895
H	-1.687404	-2.355629	-2.682527
H	-2.028740	-3.351698	0.853517
H	1.446984	-5.104012	1.544412

C	-1.652243	-0.672866	1.287025
C	-1.767991	-0.722708	-0.218302
Au	0.524376	-0.448755	-0.580901
C	2.549290	-0.106914	-0.651543
N	3.398035	-0.391656	0.359204
C	4.687396	-0.044930	0.012022
C	4.631743	0.460656	-1.248434
N	3.307777	0.414573	-1.637456
C	2.833190	0.845268	-2.938579
C	3.001160	-0.958928	1.638070
H	5.529342	-0.194480	0.688137
H	5.413986	0.844104	-1.903959
H	1.733314	0.786548	-2.957313
H	3.144161	1.887084	-3.126838
H	3.244957	0.195818	-3.729567
H	3.905392	-1.203546	2.215982
H	2.387842	-0.237035	2.205075
H	2.414280	-1.879018	1.482137
N	-1.990701	0.375959	2.128509
C	-2.653457	0.049773	-1.125413
C	-1.931175	0.069943	3.561462
S	-1.949286	2.050325	1.692806
O	-2.122304	2.750002	2.953283
C	-0.295486	2.356037	1.122801
O	-2.857332	2.274610	0.585240
H	-2.510497	-0.848549	3.742488
H	-0.891625	-0.115288	3.891658
H	-2.370123	0.902985	4.124615
C	-4.022200	0.081439	-0.832713
C	-4.907814	0.732419	-1.682612
C	-4.437857	1.359305	-2.837074
C	-3.080285	1.318181	-3.144684
C	-2.192011	0.659284	-2.295428
H	-4.389153	-0.389910	0.087581
H	-5.975411	0.758363	-1.438409
H	-5.135587	1.880834	-3.501512
H	-2.707176	1.802812	-4.053728
H	-1.120053	0.633182	-2.542641
C	-0.106586	2.828471	-0.174968
C	1.170999	3.220580	-0.568259
C	2.255730	3.144714	0.313347
C	2.033488	2.655276	1.610653
C	0.764119	2.275666	2.029215
H	-0.962613	2.907463	-0.855168
H	1.322983	3.618729	-1.579632
C	3.615552	3.623669	-0.089763
H	2.874741	2.601253	2.314145
H	0.592219	1.943620	3.060735
H	4.414618	2.993357	0.341581
H	3.739344	3.646891	-1.187584
H	3.788270	4.655167	0.274760

TS_{6a1syn'}

TS_{6a1anti'}

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scf done: -2059.792787

C	-1.659352	-2.880798	2.478303
C	-2.223024	-2.855034	1.177493

C	-1.952426	-1.827055	0.297499
C	-1.107455	-0.785823	0.729196
C	-0.645756	-0.741015	2.083891
C	-0.856046	-1.866822	2.956757
C	-0.324769	-1.931608	4.332030
O	0.267448	-1.041039	4.883441
N	0.239558	0.386945	2.266898
H	-1.872200	-3.732548	3.136710
H	-2.871915	-3.679895	0.864589
H	-2.365536	-1.831241	-0.718673
H	-1.111798	0.270125	2.604930
H	-0.534141	-2.909134	4.845888
C	0.246829	1.049307	1.095593
C	-0.527899	0.353780	0.075318
Au	1.520730	-0.573994	-0.439988
C	3.365282	-1.266696	-0.997911
N	4.489396	-0.518664	-0.973793
C	5.566861	-1.264362	-1.404002
C	5.094172	-2.503747	-1.698928
N	3.737972	-2.484183	-1.442300
C	2.863092	-3.625392	-1.632406
C	4.545466	0.877416	-0.567786
H	6.573824	-0.851107	-1.458262
H	5.600550	-3.397767	-2.062292
H	1.857348	-3.366560	-1.266368
H	2.805569	-3.888623	-2.702041
H	3.244529	-4.489785	-1.064013
H	4.055764	1.007883	0.412431
H	5.599923	1.182367	-0.486140
H	4.039713	1.516636	-1.311664
C	1.005147	2.304109	0.983299
N	-1.109062	0.986039	-1.049445
C	-0.837453	0.591874	-2.419313
S	-2.465021	1.956800	-0.708404
O	-2.293860	2.351902	0.685010
O	-2.543080	2.923776	-1.791244
C	-3.866340	0.876102	-0.803160
H	-1.395641	1.256269	-3.099139
H	0.238445	0.728279	-2.646912
H	-1.118999	-0.460629	-2.628174
C	1.031052	3.070080	-0.193716
C	1.807867	4.222144	-0.263283
C	2.566769	4.628080	0.834508
C	2.540192	3.877702	2.010062
C	1.765737	2.725225	2.085814
H	0.424885	2.780582	-1.057769
H	1.810580	4.816245	-1.183721
H	3.174060	5.538369	0.776261
H	3.125954	4.196003	2.879519
H	1.739779	2.132399	3.005926
C	-4.403777	0.354852	0.373213
C	-5.461899	-0.543925	0.290071
C	-5.989397	-0.930645	-0.948622
C	-5.433548	-0.381540	-2.113645
C	-4.383135	0.526637	-2.052346
H	-3.996424	0.660051	1.343453
H	-5.895580	-0.953809	1.210673
C	-7.149288	-1.872710	-1.028205
H	-5.847223	-0.663211	-3.089785
H	-3.980416	0.974357	-2.967781
H	-7.179292	-2.558503	-0.163361

H	-8.105722	-1.314395	-1.032497
H	-7.123859	-2.474517	-1.953752

6a1

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scf done: -2059.905476

C	-1.996630	4.440383	-0.342417
C	-1.595316	3.939845	-1.587302
C	-0.904963	2.733203	-1.688535
C	-0.603325	2.028002	-0.518626
C	-0.969800	2.570085	0.721090
C	-1.693795	3.763691	0.841448
C	-2.083900	4.268373	2.161587
O	-1.825934	3.697399	3.200000
N	-0.489983	1.743701	1.720229
H	-2.547759	5.387164	-0.282909
H	-1.824448	4.507297	-2.495130
H	-0.583656	2.357512	-2.666557
H	-2.651240	5.234879	2.158053
C	0.167307	0.692027	1.198768
C	0.077945	0.747589	-0.237574
Au	-1.712901	-0.609115	-0.302578
C	-3.372187	-1.814030	-0.444872
N	-3.562239	-2.992102	0.187600
C	-4.787954	-3.527654	-0.152095
C	-5.370815	-2.654940	-1.014592
N	-4.484769	-1.609170	-1.181278
C	-4.740412	-0.462070	-2.032547
C	-2.595936	-3.623921	1.068284
H	-5.138072	-4.476112	0.254983
H	-6.337793	-2.679120	-1.516969
H	-5.682702	0.026020	-1.733179
H	-3.911079	0.255019	-1.923044
H	-4.812233	-0.778070	-3.086926
H	-2.150834	-2.867595	1.735559
H	-3.108711	-4.384195	1.677645
H	-1.795012	-4.108843	0.483255
C	0.935348	-0.237922	2.018791
N	1.165457	0.246477	-1.011757
H	-0.686722	1.928247	2.706670
C	0.933541	-0.472689	-2.252853
S	2.492863	1.335705	-1.056214
H	1.903233	-0.754919	-2.700429
H	0.386480	-1.408945	-2.037327
H	0.366876	0.114535	-3.003429
O	2.495300	2.028899	-2.340709
O	2.401299	2.082393	0.195090
C	3.889704	0.252596	-0.989235
C	1.108629	-1.578155	1.637995
C	1.885266	-2.431566	2.412733
C	2.504079	-1.958077	3.571405
C	2.344140	-0.626355	3.952662
C	1.564391	0.231195	3.182117
H	0.615757	-1.954506	0.732425
H	2.009241	-3.477674	2.112195
H	3.115616	-2.632661	4.180806
H	2.837839	-0.247741	4.853900
H	1.477862	1.287178	3.463386
C	4.662822	0.048939	-2.129493
C	5.762352	-0.801080	-2.049877

C	6.099094	-1.439332	-0.850084
C	5.301649	-1.207180	0.281510
C	4.202440	-0.361380	0.224458
H	4.404563	0.559239	-3.063889
H	6.378667	-0.970789	-2.941191
C	7.302695	-2.324483	-0.763223
H	5.556033	-1.698207	1.229413
H	3.590374	-0.171506	1.114778
H	7.150586	-3.149210	-0.044415
H	7.562696	-2.758391	-1.744493
H	8.185022	-1.752215	-0.415853

TS_{6a2syn'}

65

scf done: -2059.792272

C	0.515987	1.346833	4.273481
C	-0.642881	2.087540	3.928916
C	-1.081006	2.175433	2.623634
C	-0.362656	1.494872	1.619134
C	0.782981	0.694647	1.966772
C	1.257721	0.670775	3.329660
C	2.403203	-0.158851	3.740307
O	2.916641	-1.002516	3.047441
N	1.504399	0.362171	0.770503
H	0.831441	1.299036	5.323162
H	-1.186175	2.618073	4.717891
H	-1.944250	2.796793	2.358570
H	0.765555	-0.481747	1.607418
H	2.756028	0.035818	4.787699
C	0.756068	0.808376	-0.246749
C	-0.418833	1.564719	0.182218
Au	-1.801758	-0.275568	0.076346
C	-2.921728	-1.979939	-0.091228
N	-2.526926	-3.192752	0.348509
C	-3.488728	-4.139055	0.063143
C	-4.501807	-3.491483	-0.569605
N	-4.133322	-2.163280	-0.654923
C	-4.947666	-1.139862	-1.281654
C	-1.263905	-3.454209	1.022083
H	-3.366103	-5.187939	0.332432
H	-5.448527	-3.854699	-0.969338
H	-5.922800	-1.065415	-0.771672
H	-4.425448	-0.173074	-1.210032
H	-5.109929	-1.384038	-2.344898
H	-0.420702	-3.129345	0.388359
H	-1.231555	-2.917521	1.986391
H	-1.182206	-4.535243	1.212256
N	1.107962	0.454598	-1.529618
C	-1.040884	2.737393	-0.503055
C	0.307590	0.902796	-2.656356
S	1.893429	-1.106820	-1.708741
C	3.560396	-0.833753	-1.207593
O	1.235079	-2.039986	-0.799706
O	1.862444	-1.345863	-3.142794
H	0.721799	0.471439	-3.578613
H	-0.752202	0.580144	-2.555498
H	0.340856	2.001464	-2.732246
C	4.416778	-0.190063	-2.102735
C	5.738849	0.011125	-1.729463
C	6.216032	-0.428699	-0.485258

C	5.327865	-1.073446	0.384752
C	3.998966	-1.283307	0.034706
H	4.051441	0.143619	-3.080204
H	6.424004	0.518270	-2.419849
C	7.651443	-0.233113	-0.110691
H	5.678558	-1.412191	1.367423
H	3.308660	-1.764188	0.732308
H	8.054356	0.709978	-0.520850
H	7.790255	-0.226921	0.984485
H	8.276695	-1.053368	-0.514406
C	-0.198742	3.757501	-0.968518
C	-0.726946	4.906253	-1.551382
C	-2.108111	5.062805	-1.663042
C	-2.955742	4.065538	-1.185768
C	-2.425669	2.911680	-0.610436
H	0.889042	3.644950	-0.868508
H	-0.052606	5.689794	-1.914400
H	-2.524548	5.967410	-2.119582
H	-4.042225	4.183044	-1.263851
H	-3.104971	2.131569	-0.238416

TS_{6a2anti'}

65

scf done: -2059.796773

C	0.856671	0.118633	4.322498
C	2.186161	0.379463	3.911284
C	2.615333	0.072216	2.635395
C	1.706401	-0.545195	1.752915
C	0.421256	-0.967648	2.226760
C	-0.058470	-0.517148	3.505391
C	-1.433738	-0.741740	3.983210
O	-2.299003	-1.320882	3.375505
N	-0.330952	-1.545896	1.138845
H	0.534792	0.427376	5.325028
H	2.875166	0.858806	4.614357
H	3.626998	0.327248	2.298310
H	0.338752	-2.195326	2.167378
H	-1.626562	-0.306747	5.001147
C	0.503184	-1.538821	0.084203
C	1.764953	-0.864671	0.348772
Au	0.770216	1.145978	-0.167070
C	-0.206715	2.906774	-0.533724
N	-1.499314	3.127082	-0.212905
C	-1.870077	4.404717	-0.579723
C	-0.775520	4.985923	-1.137014
N	0.236617	4.047112	-1.099589
C	1.577766	4.280122	-1.600574
C	-2.381719	2.130104	0.372325
H	-2.875929	4.788445	-0.409931
H	-0.623010	5.982110	-1.552056
H	1.547654	4.497091	-2.681528
H	2.037769	5.130723	-1.070300
H	2.181700	3.374819	-1.430659
H	-2.667772	1.376244	-0.383468
H	-1.875696	1.621531	1.211763
H	-3.289356	2.628647	0.748892
N	0.117459	-2.112279	-1.101518
C	3.057348	-1.075171	-0.358775
C	0.689587	-1.664316	-2.360578

S	-1.326122	-3.097462	-1.141276
H	0.085374	-2.069435	-3.185670
H	1.725024	-2.023179	-2.489679
H	0.685765	-0.553809	-2.408125
C	-2.668123	-1.967524	-0.899351
O	-1.372285	-3.573511	-2.513756
O	-1.229884	-4.018825	-0.027719
C	-3.254486	-1.841261	0.358695
C	-4.340414	-0.984043	0.503421
C	-4.847897	-0.260850	-0.583840
C	-4.230431	-0.406121	-1.835079
C	-3.146100	-1.259883	-2.004881
H	-2.858611	-2.389249	1.217774
H	-4.805914	-0.877363	1.491258
C	-6.035917	0.634372	-0.417806
H	-4.620458	0.149774	-2.696895
H	-2.690468	-1.395141	-2.992330
H	-6.976304	0.073909	-0.585641
H	-6.090878	1.053181	0.603044
H	-6.025839	1.468131	-1.142522
C	3.921023	-0.013311	-0.653958
C	5.158590	-0.250382	-1.250081
C	5.548612	-1.552434	-1.556403
C	4.699545	-2.618080	-1.258102
C	3.465346	-2.381941	-0.658829
H	3.622477	1.018248	-0.417152
H	5.821914	0.590921	-1.479236
H	6.519677	-1.738804	-2.028060
H	5.002550	-3.645044	-1.489988
H	2.801745	-3.223066	-0.419755

6a2

65

scf done: -2059.898715

C	0.256702	-3.595801	2.910415
C	1.039189	-2.622748	3.547552
C	1.077554	-1.313088	3.079530
C	0.306781	-0.958791	1.960309
C	-0.475081	-1.953269	1.337653
C	-0.505553	-3.284675	1.784504
C	-1.317306	-4.282216	1.083547
O	-1.980198	-4.035707	0.097404
N	-1.118747	-1.393360	0.264596
H	0.238485	-4.623806	3.293411
H	1.633923	-2.898522	4.424377
H	1.713860	-0.571223	3.575105
H	-1.712436	-1.941502	-0.361731
H	-1.289424	-5.315078	1.517785
C	-0.772651	-0.076960	0.147775
C	0.151705	0.269718	1.174995
Au	1.907657	-0.120371	-0.253238
C	3.613534	-0.298740	-1.368536
N	4.197943	-1.413307	-1.856215
C	5.338364	-1.085634	-2.562810
C	5.458736	0.266155	-2.508054
N	4.391186	0.731088	-1.767373
C	4.117544	2.132669	-1.499220
C	3.729544	-2.774088	-1.673270
H	5.963277	-1.844808	-3.032827
H	6.210307	0.936775	-2.924623

H	5.054163	2.704493	-1.588176
H	3.379458	2.528755	-2.218475
H	3.723526	2.245213	-0.475986
H	3.497300	-3.229834	-2.650401
H	4.503246	-3.374365	-1.166253
H	2.819551	-2.758946	-1.053264
N	-1.354485	0.743979	-0.800266
C	0.437201	1.652457	1.643726
C	-1.390722	0.313062	-2.190568
S	-2.630502	1.794589	-0.284664
H	-1.652369	1.177028	-2.824715
H	-0.381003	-0.029589	-2.482020
H	-2.121426	-0.501407	-2.378940
O	-2.499990	1.872216	1.159948
O	-2.541699	2.960990	-1.144596
C	-4.093778	0.887384	-0.688559
C	0.676123	2.704401	0.743946
C	0.897708	3.997272	1.206176
C	0.891428	4.266733	2.574974
C	0.648116	3.233125	3.475339
C	0.419131	1.938315	3.013984
H	0.660715	2.517129	-0.337932
H	1.070983	4.806194	0.487556
H	1.065457	5.285817	2.937595
H	0.620811	3.435359	4.551915
H	0.183708	1.145812	3.732996
C	-4.786686	1.176056	-1.863019
C	-5.915102	0.425286	-2.176323
C	-6.357655	-0.605079	-1.337009
C	-5.638714	-0.868935	-0.161452
C	-4.513574	-0.127359	0.175174
H	-4.448494	1.988430	-2.515476
H	-6.471288	0.646019	-3.095478
C	-7.589700	-1.387054	-1.666633
H	-5.978907	-1.668749	0.507597
H	-3.971530	-0.321203	1.108010
H	-7.513657	-2.432113	-1.317867
H	-8.476517	-0.944944	-1.171973
H	-7.791781	-1.392996	-2.751870

Cartesian coordinates of B-Series

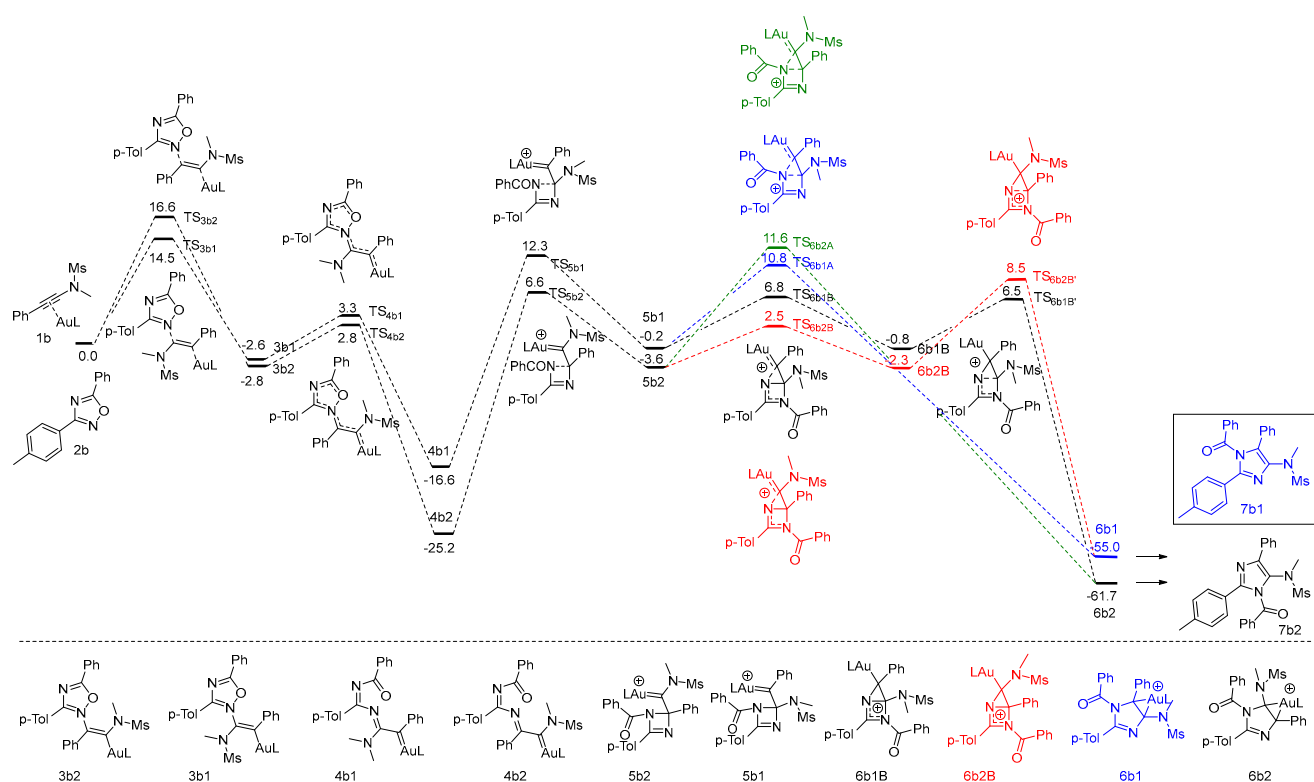


Figure S2. B-series reaction mechanism

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scf done: -1429.958460
C      -1.695926      2.089645      -0.034247
N      -2.571859      2.227485      -1.054851
C      -3.215743      3.445743      -0.978289
C      -2.729658      4.075845      0.122128
N      -1.798637      3.227403      0.686854
C      -2.776430      1.259880      -2.117049
C      -1.070505      3.529812      1.904710
Au     -0.482158      0.456421      0.324310
C      0.661462      -1.320253      0.714498
C      1.690644      -1.128030      -0.014310
C      0.196963      -2.413218      1.560578
N      2.626030      -0.902472      -0.866610
S      2.385913      -1.544326      -2.530487
C      3.901925      -0.231976      -0.584999
O      3.725603      -1.713102      -3.051913
O      1.443734      -2.632251      -2.383502
C      1.593906      -0.164449      -3.313478
C      -0.848992      -2.230134      2.476485
C      -1.273350      -3.285313      3.278378
C      -0.668500      -4.536163      3.162795
C      0.364474      -4.733008      2.243689
C      0.798175      -3.679267      1.449760
H      -3.963846      3.752060      -1.709481
H      -2.967018      5.046052      0.558617
H      -2.637871      0.241773      -1.719832
H      -3.804130      1.356445      -2.501257
H      -2.065507      1.431090      -2.944681
H      -1.766934      3.606367      2.756698
H      -0.349878      2.720420      2.098835
H      -0.526651      4.482484      1.792671
H      4.022303      0.644103      -1.245629
H      3.889381      0.098642      0.464549
H      4.736247      -0.931415      -0.751619
H      1.385428      -0.483838      -4.349344
H      0.655098      0.056643      -2.776731
H      2.287221      0.692353      -3.310013
H      -1.326068      -1.245615      2.560599
H      -2.086396      -3.131917      3.996202
H      -1.007262      -5.367890      3.790501
H      0.834296      -5.717712      2.146122
H      1.599691      -3.830390      0.715941

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2b

30

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scf done: -762.401587
C      -1.741037      -0.992482      -0.345467
C      -2.581278      -0.523615      0.669265
C      -3.931252      -0.858725      0.670783
C      -4.478269      -1.663643      -0.334904
C      -3.625138      -2.131473      -1.344348
C      -2.276138      -1.802925      -1.355174
C      -5.938732      -1.996757      -0.349223
C      -0.321485      -0.639306      -0.340956
N      0.254723      0.144886      0.622389
N      0.517127      -1.047393      -1.265931
O      1.718104      -0.494282      -0.881536
C      1.495347      0.197400      0.240041
C      2.608341      0.893156      0.870596

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C	2.374461	1.618986	2.045915
C	3.421687	2.291209	2.665369
C	4.704185	2.242849	2.116885
C	4.939462	1.520724	0.946566
C	3.896244	0.845585	0.321225
H	-2.159682	0.105651	1.460616
H	-4.580688	-0.488974	1.474667
H	-4.033780	-2.770927	-2.137372
H	-1.618951	-2.176111	-2.148666
H	-6.123340	-2.999940	-0.774159
H	-6.374147	-1.965133	0.665517
H	-6.506504	-1.274887	-0.969035
H	1.360962	1.644757	2.460740
H	3.238003	2.858613	3.584415
H	5.528757	2.773381	2.606590
H	5.946584	1.483432	0.516863
H	4.074042	0.276834	-0.597727

TS_{3b1}

71

scf done: -2192.366303

N	-4.135733	-0.246246	-0.206984
C	-3.211993	0.514571	0.429736
C	-3.545145	-1.405401	-0.307495
O	-2.321361	-1.410525	0.227902
N	-2.103247	-0.146788	0.711324
C	-3.379353	1.923156	0.760800
C	-2.784236	2.466346	1.906426
C	-2.939118	3.815973	2.196970
C	-3.676789	4.655940	1.350974
C	-4.260467	4.099879	0.204086
C	-4.129037	2.748052	-0.086076
C	-3.867059	6.103863	1.679462
C	-4.054885	-2.635600	-0.883342
C	-3.301171	-3.817218	-0.836501
C	-3.815593	-4.981632	-1.394524
C	-5.074641	-4.971275	-1.997112
C	-5.826015	-3.795836	-2.041897
C	-5.320577	-2.627267	-1.485252
C	-0.190270	0.459267	0.284082
C	0.623590	-0.443908	0.754562
C	0.348378	-1.572625	1.645529
C	-0.371277	-1.396249	2.836887
C	-0.639360	-2.482840	3.664043
C	-0.207463	-3.760468	3.308630
C	0.515762	-3.944740	2.129921
C	0.808644	-2.856299	1.313447
Au	2.627426	-0.135967	0.131830
N	-0.345072	1.625462	-0.310603
C	0.052883	2.905651	0.282949
S	-0.892158	1.657428	-1.971334
O	-1.745676	0.497670	-2.151649
O	-1.362337	3.010716	-2.195033
C	0.620045	1.397489	-2.861107
C	4.627170	0.053710	-0.381814
N	5.586965	-0.886403	-0.229303
C	6.806311	-0.414177	-0.673169
C	6.597021	0.852580	-1.113657
N	5.255631	1.121329	-0.924337

C	5.396605	-2.207920	0.338417
C	4.615030	2.362141	-1.312923
H	-2.209872	1.815787	2.578878
H	-2.482339	4.233840	3.102985
H	-4.831921	4.746405	-0.473108
H	-4.584499	2.319578	-0.986093
H	-3.931170	6.722585	0.766748
H	-4.809225	6.259565	2.240686
H	-3.047009	6.492423	2.308725
H	-2.316405	-3.817362	-0.355557
H	-3.232239	-5.908001	-1.358411
H	-5.476263	-5.891758	-2.435562
H	-6.814085	-3.792668	-2.514376
H	-5.894056	-1.694387	-1.508461
H	-0.718902	-0.393753	3.112101
H	-1.196948	-2.331519	4.595228
H	-0.427507	-4.615231	3.958013
H	0.863731	-4.945422	1.849384
H	1.384883	-2.997432	0.389541
H	0.926013	3.323512	-0.255177
H	-0.782014	3.625303	0.246299
H	0.333660	2.715745	1.331185
H	1.320670	2.213882	-2.619284
H	1.027488	0.410747	-2.582702
H	0.354931	1.421677	-3.932017
H	7.711913	-1.019072	-0.627924
H	7.279901	1.587799	-1.538983
H	5.987761	-2.314948	1.263651
H	4.329352	-2.344809	0.575545
H	5.710083	-2.978878	-0.385335
H	5.314693	3.199373	-1.158352
H	4.318660	2.333455	-2.376620
H	3.721817	2.520756	-0.686977

3b1

71

scf done: -2192.390039

N	-4.023197	0.043656	-0.076177
C	-2.962563	0.805235	0.241875
C	-3.528541	-1.143630	-0.315332
O	-2.201601	-1.190339	-0.185563
N	-1.834793	0.076962	0.188914
C	-3.051299	2.200606	0.608799
C	-2.059585	2.843812	1.365017
C	-2.208042	4.177433	1.712510
C	-3.335987	4.908908	1.310547
C	-4.327389	4.251869	0.567799
C	-4.198328	2.914773	0.226337
C	-3.472155	6.357591	1.651488
C	-4.232233	-2.358431	-0.652753
C	-3.552941	-3.583431	-0.745037
C	-4.261680	-4.732771	-1.069173
C	-5.637133	-4.663322	-1.301423
C	-6.312904	-3.445402	-1.206819
C	-5.615311	-2.290419	-0.879799
C	-0.426674	0.380379	0.039891
C	0.509092	-0.398707	0.624357
C	0.098401	-1.429172	1.597922
C	-0.681320	-1.113833	2.722197
C	-1.079827	-2.105225	3.615913

C	-0.719226	-3.434221	3.398292
C	0.063967	-3.760560	2.290520
C	0.482329	-2.766962	1.409983
Au	2.551535	-0.252540	0.211154
N	-0.223951	1.506068	-0.782697
C	0.727789	2.555548	-0.442769
S	-0.629723	1.370717	-2.424329
O	-1.830914	0.546159	-2.492057
O	-0.607817	2.717615	-2.966965
C	0.701838	0.440615	-3.147633
C	4.607402	-0.181823	-0.152518
N	5.426131	-1.215176	-0.456478
C	6.725607	-0.778351	-0.625900
C	6.714517	0.563488	-0.421461
N	5.409076	0.908296	-0.130872
C	5.022604	-2.601658	-0.584492
C	4.960687	2.264567	0.116207
H	-1.182517	2.286958	1.713995
H	-1.437170	4.668606	2.318571
H	-5.220895	4.806547	0.257381
H	-4.978839	2.406230	-0.348677
H	-3.064925	6.988520	0.837018
H	-4.529723	6.646258	1.783579
H	-2.918667	6.615660	2.571140
H	-2.475241	-3.629560	-0.551858
H	-3.740905	-5.693300	-1.140215
H	-6.190884	-5.573355	-1.557702
H	-7.391525	-3.399317	-1.388919
H	-6.125332	-1.324736	-0.799070
H	-0.967793	-0.070136	2.906925
H	-1.679318	-1.835236	4.492989
H	-1.036871	-4.214231	4.099231
H	0.362351	-4.801052	2.117021
H	1.111550	-3.025713	0.547570
H	1.698208	2.434887	-0.966780
H	0.305779	3.543867	-0.693759
H	0.924096	2.505113	0.641010
H	1.637501	1.015727	-3.050960
H	0.774271	-0.533800	-2.635974
H	0.441742	0.306010	-4.211324
H	7.539664	-1.461879	-0.867528
H	7.516954	1.300769	-0.449312
H	3.952249	-2.684242	-0.336535
H	5.184947	-2.954451	-1.617306
H	5.603690	-3.231437	0.110020
H	5.750642	2.822180	0.644674
H	4.727603	2.779948	-0.832542
H	4.056886	2.236792	0.745988

TS_{3b2}

71

scf done: -2192.358629

O	-3.136837	-0.089512	-1.242204
N	-2.198136	0.831918	-0.835145
C	-2.778357	1.470899	0.179112
N	-4.020874	0.995976	0.451148
C	-4.184577	0.041532	-0.423639
C	-0.450520	-0.180439	-0.474017
C	0.562616	0.376584	-1.059035
Au	2.186008	-0.712491	-0.167611

C	3.767669	-1.728527	0.670639
H	4.782641	0.563017	-0.085150
C	5.603256	-0.153119	0.087952
H	6.097138	-0.387898	-0.871456
H	6.339188	0.303843	0.769428
N	5.066290	-1.359390	0.690659
C	5.827785	-2.307325	1.346280
H	6.903864	-2.195268	1.478639
C	4.974492	-3.286434	1.744482
H	5.149494	-4.208905	2.298024
N	3.714853	-2.911120	1.321349
C	2.499684	-3.679419	1.524140
H	2.693519	-4.467891	2.267958
H	2.172407	-4.144722	0.578169
H	1.697746	-3.019703	1.896886
N	0.707936	1.394108	-1.965295
C	-0.316020	1.761102	-2.946571
H	-0.961325	2.587241	-2.600406
H	0.170858	2.068348	-3.888276
H	-0.938723	0.874180	-3.142263
S	2.114439	2.359526	-1.930150
O	1.697977	3.667513	-2.405803
O	2.726424	2.206242	-0.616204
C	3.179393	1.615020	-3.140227
H	4.097191	2.226240	-3.172662
H	2.674567	1.634993	-4.119992
H	3.406739	0.582141	-2.825026
C	-5.315202	-0.851216	-0.585101
C	-2.143580	2.538621	0.936645
C	-1.013220	-1.305279	0.235581
C	-1.417999	-1.169116	1.574862
C	-1.999990	-2.242482	2.241316
C	-2.190408	-3.455409	1.576887
C	-1.790940	-3.601383	0.246795
C	-1.206505	-2.532348	-0.422968
H	-1.268867	-0.208733	2.084288
H	-2.311898	-2.132798	3.285507
H	-2.656754	-4.296792	2.101668
H	-1.942297	-4.555110	-0.270675
H	-0.894130	-2.627940	-1.469928
C	-2.779490	3.024473	2.088404
C	-2.191949	4.035547	2.837327
C	-0.963268	4.595232	2.462157
C	-0.335010	4.103022	1.309125
C	-0.912127	3.093350	0.553694
H	-3.741300	2.594705	2.387800
H	-2.696517	4.405005	3.738568
C	-0.350298	5.708758	3.250612
H	0.628757	4.521528	0.993298
H	-0.395792	2.744830	-0.345460
H	0.753055	5.661110	3.231234
H	-0.637063	6.692009	2.828499
H	-0.684631	5.696973	4.302881
C	-5.284276	-1.886944	-1.530499
C	-6.373735	-2.741409	-1.649317
C	-7.490618	-2.567285	-0.830236
C	-7.522504	-1.537017	0.111041
C	-6.437910	-0.677888	0.236872
H	-4.404969	-2.017675	-2.170521
H	-6.354874	-3.550377	-2.387335
H	-8.347884	-3.242698	-0.927717

H	-8.401837	-1.403303	0.749968
H	-6.443310	0.137063	0.968525

3b2

71

scf done: -2192.395084

O	-0.842489	-1.618181	-1.401553
C	-1.745072	-2.313401	-0.714631
N	-1.345216	-2.632603	0.489309
C	-0.114699	-2.090826	0.609677
N	0.234981	-1.464636	-0.520508
C	-3.026821	-2.599271	-1.323529
C	0.673667	-2.185971	1.821692
C	-3.327510	-2.158608	-2.621733
C	-4.574614	-2.437608	-3.166533
C	-5.517800	-3.150544	-2.423729
C	-5.219415	-3.588598	-1.131765
C	-3.975854	-3.315585	-0.577733
C	0.256562	-3.118690	2.788957
C	0.961102	-3.258372	3.972962
C	2.090838	-2.470499	4.239209
C	2.485026	-1.527375	3.279666
C	1.797668	-1.383401	2.083949
C	2.865473	-2.647100	5.504582
C	1.371188	-0.756885	-0.993586
C	2.517099	-1.634576	-1.321926
C	1.246370	0.615293	-0.953064
C	3.815320	-1.300531	-0.903828
C	4.888679	-2.146174	-1.168954
C	4.685493	-3.350016	-1.842717
C	3.398560	-3.703602	-2.246840
C	2.325585	-2.855125	-1.988381
Au	-0.422637	1.453097	0.037627
N	2.185412	1.408542	-1.584670
S	2.360523	3.053559	-1.133594
C	2.958192	1.015406	-2.763548
O	2.015835	3.180654	0.276536
O	3.675251	3.449063	-1.607774
C	1.133048	3.907526	-2.096231
C	-2.062474	2.264345	1.021420
N	-3.254989	1.674451	1.267534
C	-4.085875	2.526508	1.968325
C	-3.391089	3.677960	2.157433
N	-2.154312	3.495931	1.570654
C	-1.119666	4.513684	1.533742
C	-3.592754	0.318353	0.880567
H	-2.582473	-1.601379	-3.199937
H	-4.814833	-2.099296	-4.179780
H	-6.499171	-3.369240	-2.858940
H	-5.963001	-4.149570	-0.556188
H	-3.720730	-3.652965	0.432707
H	-0.626840	-3.734391	2.592505
H	0.630965	-3.992982	4.717252
H	3.352304	-0.887537	3.480930
H	2.118544	-0.626016	1.362897
H	3.391526	-1.720809	5.794268
H	2.215417	-2.961319	6.340045
H	3.635898	-3.433542	5.380944
H	3.982826	-0.366495	-0.352226

H	5.893944	-1.866834	-0.833601
H	5.530590	-4.016509	-2.047825
H	3.228631	-4.648400	-2.775593
H	1.319901	-3.140157	-2.323748
H	3.997524	0.735074	-2.520267
H	2.454036	0.160292	-3.241319
H	2.988395	1.849887	-3.485050
H	1.233443	4.977425	-1.846010
H	1.345529	3.745589	-3.165690
H	0.133144	3.530239	-1.818268
H	-5.093552	2.238963	2.268492
H	-3.664988	4.608745	2.654092
H	-1.421340	5.341211	0.867771
H	-0.953064	4.911682	2.548509
H	-0.180934	4.067790	1.164890
H	-3.070566	-0.415756	1.520961
H	-4.680195	0.173310	0.981352
H	-3.308215	0.149369	-0.172815

TS_{4b1}

71

scf done: -2192.381146

N	-1.751734	-0.209419	-0.866388
O	-2.929491	-1.385157	-0.382618
C	-3.965760	-0.640756	-0.274498
C	-5.264482	-1.232214	0.028244
N	-3.805743	0.671611	-0.466147
C	-2.533696	0.879586	-0.784864
C	-0.464776	-0.511874	-0.598181
N	0.114475	-1.477524	-1.442777
C	0.351261	-1.195374	-2.846011
H	0.756577	-2.090242	-3.346211
H	-0.588174	-0.899964	-3.352471
H	1.099807	-0.385390	-2.952869
S	0.518698	-2.971931	-0.790767
O	1.748396	-3.415985	-1.439030
O	0.439146	-2.839797	0.658909
C	-0.795008	-4.045476	-1.316906
H	-0.823812	-4.062860	-2.418950
H	-0.566466	-5.050802	-0.924846
H	-1.738718	-3.661579	-0.895249
C	0.269538	0.144112	0.389060
C	-0.401076	0.892278	1.435349
Au	2.341067	-0.019465	0.307648
C	4.400467	-0.342326	0.285293
N	4.994128	-1.533950	0.519892
C	4.278467	-2.762445	0.827930
H	3.528277	-2.978213	0.047664
H	5.003119	-3.590232	0.873823
H	3.768568	-2.672683	1.802435
C	6.366514	-1.416433	0.446952
H	7.030007	-2.266484	0.606025
C	6.633486	-0.116794	0.156078
H	7.577243	0.407179	0.005487
N	5.413644	0.524385	0.061648
C	5.265662	1.935348	-0.231074
H	4.192142	2.169275	-0.305892
H	5.714407	2.543724	0.572739
H	5.758021	2.178783	-1.187810
C	-2.027144	2.219782	-1.069152

C	-1.535617	0.380533	2.097837
C	-2.178121	1.130300	3.075944
C	-1.717130	2.409868	3.391599
C	-0.585489	2.924251	2.754890
C	0.084695	2.161455	1.807567
H	-1.879941	-0.634493	1.863364
H	-3.045270	0.714235	3.600645
H	-2.232817	3.003738	4.154549
H	-0.214793	3.921801	3.015092
H	0.984568	2.550031	1.314119
C	-6.392721	-0.405100	0.132639
C	-7.630816	-0.964748	0.422941
C	-7.746403	-2.343575	0.607699
C	-6.624994	-3.169569	0.503774
C	-5.383788	-2.618002	0.215152
H	-6.279905	0.672998	-0.020020
H	-8.514916	-0.323642	0.504430
H	-8.724632	-2.781658	0.835438
H	-6.723345	-4.250348	0.649876
H	-4.496745	-3.255584	0.131166
C	-0.854916	2.454398	-1.803503
C	-0.411254	3.752111	-2.003764
C	-1.110173	4.848913	-1.475435
C	-2.282216	4.602400	-0.748828
C	-2.747179	3.309051	-0.556375
H	-0.289033	1.619652	-2.231842
H	0.500081	3.928262	-2.587946
C	-0.633326	6.245567	-1.714316
H	-2.840287	5.446629	-0.326248
H	-3.662455	3.121533	0.014227
H	-0.938301	6.926041	-0.900124
H	0.465113	6.289801	-1.818524
H	-1.063598	6.649317	-2.651913

4b1

71

scf done: -2192.413441

C	-3.617472	-0.814637	-1.890213
O	-3.618971	-1.558057	-2.849971
C	-4.649013	-0.897709	-0.815783
N	-2.700993	0.222108	-1.755034
C	-1.434173	0.063034	-1.779504
C	-5.585452	-1.936353	-0.874444
C	-6.547572	-2.069457	0.121206
C	-6.582300	-1.163669	1.182926
C	-5.653984	-0.124223	1.245036
C	-4.691002	0.009905	0.248363
N	-0.604569	1.149086	-2.013197
C	0.064312	1.810120	-1.150105
C	-0.031006	1.432801	0.272122
N	0.977905	2.760784	-1.586556
S	2.018150	3.483262	-0.451845
C	1.418557	2.702068	-2.975970
O	1.344878	3.286435	0.834288
O	3.367068	2.991748	-0.674435
C	1.945670	5.204858	-0.855079
C	-0.715054	-1.227434	-1.590192
C	-1.174908	-2.152674	-0.643552
C	-0.466256	-3.323151	-0.402127
C	0.713246	-3.614994	-1.101733

C	1.161457	-2.688492	-2.049535
C	0.466382	-1.505759	-2.286472
C	-1.170892	1.813473	1.026736
C	-1.403873	1.216224	2.290658
C	-2.485787	1.603026	3.062688
C	-3.347057	2.599056	2.590258
C	-3.142701	3.200917	1.342333
C	-2.067815	2.811152	0.563582
C	1.450911	-4.895010	-0.855431
Au	1.382446	-0.020496	0.706897
C	2.811748	-1.507603	0.931111
N	3.943979	-1.611629	0.200664
C	4.613497	-2.778010	0.509227
C	3.880070	-3.408808	1.463936
N	2.778342	-2.613014	1.706538
C	1.765444	-2.908184	2.700545
C	4.356628	-0.664383	-0.820750
H	-5.538530	-2.633568	-1.718201
H	-7.279422	-2.883549	0.070929
H	-7.342828	-1.266653	1.965597
H	-5.689069	0.593785	2.073613
H	-3.970439	0.835936	0.278662
H	0.531888	2.688765	-3.629010
H	2.024485	3.590043	-3.215553
H	2.020573	1.791485	-3.158861
H	2.562618	5.708698	-0.091500
H	2.373705	5.376093	-1.855194
H	0.896682	5.533634	-0.789874
H	-2.087383	-1.940078	-0.070562
H	-0.836434	-4.033976	0.348393
H	2.075288	-2.904029	-2.619069
H	0.835137	-0.790013	-3.031225
H	-0.705767	0.447033	2.644144
H	-2.664587	1.140018	4.038107
H	-4.199135	2.911822	3.204972
H	-3.832340	3.972543	0.985967
H	-1.905933	3.272077	-0.418355
H	2.452723	-4.886646	-1.319852
H	1.575459	-5.095061	0.226157
H	0.899151	-5.758926	-1.274165
H	5.553722	-3.051697	0.030313
H	4.047864	-4.344656	1.997560
H	1.467884	-3.967517	2.626363
H	2.148545	-2.710340	3.716630
H	0.884927	-2.273115	2.511524
H	5.438411	-0.773263	-0.996446
H	3.814270	-0.856789	-1.764225
H	4.148811	0.366084	-0.487113

TS_{4b2}

71

scf done: -2192.379040

N	-1.715325	-0.355617	-0.503859
C	-0.488852	-0.749076	-0.130192
C	0.295241	0.020667	0.757560
Au	2.374629	-0.132586	0.450609
C	4.415669	-0.338241	0.098211
N	4.996631	-1.062834	-0.885576
C	4.294596	-1.820631	-1.903977
H	4.513491	-2.897133	-1.798666

H	3.209586	-1.666640	-1.784279
H	4.603919	-1.482412	-2.907474
C	6.372345	-1.000617	-0.789683
H	7.024747	-1.519307	-1.492280
C	6.653497	-0.215675	0.282009
H	7.603472	0.097608	0.715252
N	5.441466	0.180281	0.811477
C	5.312946	1.026471	1.981388
H	5.742878	0.525577	2.865401
H	4.243684	1.221410	2.162021
H	5.835549	1.983852	1.816544
N	-0.192282	0.942914	1.632452
C	0.711235	1.976524	2.148903
H	1.457481	1.547757	2.843266
H	1.217547	2.458908	1.297001
H	0.139777	2.747328	2.690732
S	-1.556204	0.658519	2.703431
O	-1.020187	0.839296	4.041273
O	-2.171615	-0.590675	2.302136
C	-2.669354	2.004768	2.379524
H	-2.137965	2.962072	2.500483
H	-3.452983	1.912974	3.151482
H	-3.108521	1.901069	1.374391
O	-3.019453	-1.356575	-0.162228
C	-3.998642	-0.557883	-0.362267
C	-5.370401	-1.028566	-0.203022
N	-3.700573	0.688872	-0.736677
C	-2.372573	0.749147	-0.849215
C	-1.703529	1.952145	-1.352587
C	0.067714	-1.914689	-0.854741
C	-0.175447	-2.089336	-2.224426
C	0.355306	-3.182037	-2.904507
C	1.125790	-4.125571	-2.223186
C	1.356461	-3.972965	-0.856485
C	0.827202	-2.878424	-0.175426
H	-0.785643	-1.354397	-2.765275
H	0.162483	-3.300714	-3.976761
H	1.533591	-4.991213	-2.757514
H	1.937554	-4.723928	-0.308976
H	0.975898	-2.781101	0.907322
C	-6.437024	-0.174184	-0.517862
C	-7.743834	-0.618447	-0.358838
C	-7.988317	-1.910009	0.111550
C	-6.927810	-2.762052	0.425574
C	-5.618210	-2.325501	0.270335
H	-6.224007	0.832895	-0.890869
H	-8.580524	0.043944	-0.605334
H	-9.020185	-2.257529	0.235295
H	-7.126492	-3.773107	0.796467
H	-4.776592	-2.980473	0.519375
C	-0.373289	1.962546	-1.801237
C	0.191536	3.137030	-2.275958
C	-0.539644	4.334159	-2.316954
C	-1.867520	4.312230	-1.872522
C	-2.448629	3.140436	-1.407553
H	0.226762	1.045468	-1.794738
H	1.229892	3.130024	-2.630036
C	0.073790	5.587135	-2.854406
H	-2.458352	5.235861	-1.897661
H	-3.492484	3.131103	-1.077005
H	-0.406691	6.489348	-2.437592

H	1.156664	5.634442	-2.642788
H	-0.041890	5.636483	-3.954981

4b2

71

scf done: -2192.425423

N	-1.237361	0.047585	2.013612
C	-1.757823	-0.661442	1.085475
C	-1.380359	-0.443657	-0.345706
N	0.857307	0.893997	2.270374
C	-0.309174	1.062637	1.775085
C	-2.627501	-1.811368	1.396571
C	-3.270735	-1.869687	2.639377
C	-4.090630	-2.947378	2.947678
C	-4.263736	-3.984757	2.027827
C	-3.612639	-3.942891	0.796138
C	-2.797958	-2.857365	0.479030
Au	0.607216	-0.978229	-0.778637
N	-2.208437	0.058508	-1.213837
C	-1.828866	0.407289	-2.587279
S	-3.931794	0.615457	-0.840292
O	-4.056695	0.655172	0.600487
O	-4.114597	1.782080	-1.677952
C	-4.865533	-0.746115	-1.483332
C	-0.752283	2.203595	0.935816
C	-2.014044	2.778936	1.122959
C	-2.464583	3.769893	0.261096
C	-1.687538	4.200437	-0.822313
C	-0.417258	3.635846	-0.988831
C	0.051509	2.657532	-0.117109
C	-2.228420	5.209593	-1.785217
C	1.830261	1.886392	2.308997
C	3.192359	1.425577	1.908852
O	1.616576	3.015786	2.696632
C	3.512682	0.066864	1.789609
C	4.805246	-0.316604	1.439325
C	5.778345	0.652315	1.190019
C	5.463010	2.008020	1.305183
C	4.177524	2.392636	1.674378
C	2.582248	-1.472481	-1.181350
N	3.177250	-2.675879	-1.035185
C	4.505590	-2.605931	-1.402739
C	4.738534	-1.320893	-1.779268
N	3.544782	-0.645153	-1.641806
C	3.378180	0.780991	-1.853079
C	2.503072	-3.879000	-0.579519
H	-3.123350	-1.048199	3.348686
H	-4.602607	-2.982759	3.915374
H	-4.907242	-4.835692	2.277304
H	-3.732208	-4.764583	0.081429
H	-2.274560	-2.841297	-0.487291
H	-0.922775	-0.158391	-2.853848
H	-2.642020	0.157105	-3.287851
H	-1.632099	1.492715	-2.641073
H	-5.921714	-0.452890	-1.349909
H	-4.642439	-0.875094	-2.554220
H	-4.632748	-1.645451	-0.887754
H	-2.648341	2.439263	1.948379
H	-3.457693	4.210194	0.415748

H	0.216965	3.973265	-1.818613
H	1.050421	2.225681	-0.268467
H	-1.441252	5.614966	-2.444471
H	-3.006816	4.752912	-2.428190
H	-2.707290	6.055124	-1.258638
H	2.742674	-0.683169	2.005218
H	5.062353	-1.380653	1.374882
H	6.796554	0.348844	0.918420
H	6.230822	2.767777	1.120429
H	3.912169	3.449095	1.793854
H	5.163171	-3.474357	-1.368434
H	5.645736	-0.828987	-2.130714
H	4.193751	1.149252	-2.494833
H	2.413891	0.971484	-2.353081
H	3.405279	1.316987	-0.885745
H	3.251615	-4.671029	-0.424254
H	1.984665	-3.682037	0.373645
H	1.769765	-4.218881	-1.330458

TS_{5b1}

71

scf done: -2192.366490

C	-0.283266	0.822975	0.775342
N	1.119606	0.241610	-1.027034
C	2.158590	1.084766	-0.700769
N	1.623711	2.185854	-0.249772
C	0.285745	1.759495	-0.242508
C	0.387260	0.676281	2.031267
C	1.269483	1.650598	2.571424
C	1.897789	1.432074	3.787260
C	1.684562	0.237196	4.481466
C	0.811995	-0.732794	3.979404
C	0.153922	-0.505069	2.782956
C	1.023307	-1.148649	-1.131654
O	0.053058	-1.640847	-1.675512
C	2.090817	-2.006744	-0.541537
C	2.385808	-3.210900	-1.192365
C	3.380066	-4.049111	-0.699807
C	4.064751	-3.706651	0.467281
C	3.749337	-2.527557	1.142929
C	2.771961	-1.676322	0.636470
N	-0.567421	2.501929	-1.001684
C	-0.129499	3.029801	-2.288501
S	-2.101007	3.016571	-0.393970
O	-3.152978	2.511942	-1.257840
O	-2.066528	2.730495	1.035904
C	-1.995226	4.776223	-0.597517
C	3.589480	0.852658	-0.873239
C	4.085384	0.005548	-1.873192
C	5.448842	-0.232297	-1.971622
C	6.352675	0.360115	-1.077778
C	5.848548	1.226773	-0.098749
C	4.486504	1.480029	0.000466
C	7.816072	0.059469	-1.159996
H	1.438896	2.586237	2.031859
H	2.561281	2.196643	4.204588
H	2.196098	0.066072	5.435457
H	0.641541	-1.660853	4.534219
H	-0.539477	-1.254234	2.380344
H	1.830786	-3.470971	-2.100682

H	3.621736	-4.979725	-1.225129
H	4.846642	-4.368030	0.857466
H	4.271916	-2.265286	2.069857
H	2.539669	-0.749409	1.175097
H	-1.016066	3.180955	-2.927719
H	0.436901	3.972639	-2.184687
H	0.503782	2.271191	-2.776558
H	-2.911940	5.165717	-0.122056
H	-1.101312	5.144307	-0.069155
H	-1.987061	5.040808	-1.665846
H	3.398150	-0.465817	-2.585610
H	6.544198	1.712777	0.596415
H	4.098684	2.155479	0.772398
H	8.058158	-0.868723	-0.605938
H	8.141098	-0.096275	-2.204100
H	8.425238	0.869188	-0.721491
H	5.829274	-0.891913	-2.761271
Au	-1.967465	-0.304922	0.255886
C	-3.614842	-1.414066	-0.342263
N	-3.943933	-1.662834	-1.628758
C	-5.100106	-2.410926	-1.697726
C	-5.497614	-2.636097	-0.417657
N	-4.572314	-2.015458	0.397725
C	-3.197526	-1.163767	-2.772593
C	-4.630467	-2.024576	1.845187
H	-5.536648	-2.718777	-2.647919
H	-6.350263	-3.183173	-0.015363
H	-3.413390	-0.092307	-2.928897
H	-3.496465	-1.731147	-3.668108
H	-2.116814	-1.297904	-2.595009
H	-5.578121	-1.578892	2.191753
H	-3.789376	-1.428698	2.233394
H	-4.553381	-3.057438	2.225575

5b1

71

scf done: -2192.390075

C	-0.348605	0.804301	0.774153
N	1.249737	-0.049347	-0.760843
C	2.334027	0.837157	-0.604611
N	1.673851	1.934126	-0.396355
C	0.419337	1.150071	-0.487856
C	0.188916	1.062509	2.071423
C	1.081219	2.124436	2.382174
C	1.569524	2.275166	3.669476
C	1.207416	1.367235	4.669839
C	0.321326	0.322175	4.396175
C	-0.205697	0.191596	3.122294
C	0.956887	-1.405344	-0.958590
O	-0.082524	-1.738485	-1.485142
C	1.984151	-2.354628	-0.472818
C	2.216737	-3.526701	-1.201663
C	3.186395	-4.426704	-0.773277
C	3.897028	-4.177850	0.402824
C	3.635519	-3.033091	1.155616
C	2.686728	-2.116026	0.714931
N	-0.445292	1.547645	-1.564906
C	-0.040245	1.306545	-2.938801
S	-1.349523	2.925373	-1.232941
O	-2.574577	2.860289	-2.012010

O	-1.382179	2.982107	0.234294
C	-0.378381	4.298171	-1.801352
C	3.766385	0.601250	-0.660659
C	4.336110	-0.388350	-1.473730
C	5.712348	-0.563956	-1.490837
C	6.554611	0.230180	-0.698926
C	5.974664	1.226831	0.097280
C	4.599120	1.417891	0.116159
C	8.033381	0.002619	-0.691973
H	1.344425	2.843686	1.603612
H	2.236427	3.110880	3.906190
H	1.609290	1.487123	5.682440
H	0.030838	-0.376201	5.187600
H	-0.919090	-0.610621	2.896462
H	1.639587	-3.710823	-2.114972
H	3.387381	-5.333175	-1.354514
H	4.656786	-4.891340	0.741199
H	4.178350	-2.852673	2.089690
H	2.480651	-1.214723	1.306730
H	-0.825747	1.698914	-3.606919
H	0.927759	1.787500	-3.189332
H	0.026768	0.217625	-3.106298
H	-0.916235	5.208963	-1.487926
H	0.612193	4.233665	-1.320428
H	-0.303621	4.260705	-2.900144
H	3.702047	-1.016634	-2.109920
H	6.620131	1.864880	0.713315
H	4.150943	2.197046	0.744332
H	8.307213	-0.782240	0.040172
H	8.397192	-0.336741	-1.678064
H	8.586150	0.916090	-0.411131
H	6.151263	-1.334425	-2.136589
Au	-2.111979	-0.224300	0.420078
C	-3.902922	-1.112651	-0.133299
N	-4.293167	-1.217004	-1.423112
C	-5.535222	-1.808095	-1.507507
C	-5.924945	-2.081514	-0.233849
N	-4.908978	-1.645470	0.592789
C	-3.507642	-0.730907	-2.547021
C	-4.931321	-1.755365	2.037292
H	-6.033387	-1.981551	-2.461378
H	-6.830071	-2.546985	0.156094
H	-3.473009	0.373418	-2.540256
H	-3.972414	-1.079307	-3.482810
H	-2.478853	-1.125149	-2.477480
H	-5.816431	-1.237997	2.444292
H	-4.020403	-1.283239	2.437903
H	-4.957330	-2.815586	2.341702

TS_{5b2}

71

scf done: -2192.376423

C	0.758531	-1.948383	1.126541
N	0.998929	-1.063684	0.096305
C	2.293953	-0.661422	-0.166131
N	2.412341	0.627991	-0.025240
C	1.181209	0.919777	0.544750
C	0.277533	1.649412	-0.374310
Au	-1.546950	0.692423	-0.804603
C	-3.405115	-0.187029	-1.065488

N	-3.894108	-0.815196	-2.155654
C	-5.144273	-1.339588	-1.892174
C	-5.437492	-1.018212	-0.604889
N	-4.360342	-0.306660	-0.118480
C	-4.225140	0.162549	1.248399
C	-3.173461	-1.013977	-3.398295
H	-5.716541	-1.880243	-2.646039
H	-6.320435	-1.221316	0.001374
H	-3.500442	-0.466489	1.798085
H	-3.882903	1.210942	1.252611
H	-5.205594	0.105050	1.746389
H	-2.657277	-1.991060	-3.394394
H	-3.879178	-0.980685	-4.243864
H	-2.427495	-0.212518	-3.517510
N	0.632196	2.796744	-0.874120
C	-0.072171	3.450176	-1.979773
S	2.154438	3.710014	-0.353537
H	-0.664541	4.307234	-1.616213
H	0.669033	3.788825	-2.724726
H	-0.745023	2.718057	-2.451677
O	2.422368	3.272800	0.998925
O	3.085008	3.577419	-1.450935
C	1.537480	5.373711	-0.275360
H	2.374542	5.940828	0.169091
H	1.316845	5.759784	-1.281512
H	0.667056	5.401966	0.399632
O	1.594933	-2.280928	1.953445
C	-0.656672	-2.408414	1.229634
C	-1.431226	-2.647952	0.088995
C	-1.189040	-2.675884	2.496044
C	-2.722164	-3.157231	0.214089
H	-0.996683	-2.459228	-0.901145
C	-2.491108	-3.152293	2.622187
H	-0.559227	-2.504854	3.377152
C	-3.257273	-3.398089	1.479966
H	-3.317756	-3.372532	-0.682605
H	-2.908332	-3.352073	3.615823
H	-4.275786	-3.793532	1.577288
C	3.364606	-1.543165	-0.616256
C	3.099516	-2.868328	-0.985074
C	4.676574	-1.057511	-0.703312
C	4.130235	-3.692213	-1.416477
H	2.072047	-3.249903	-0.944390
C	5.700499	-1.888435	-1.135950
H	4.878240	-0.016945	-0.424609
C	5.447789	-3.220468	-1.493638
H	3.913756	-4.728044	-1.706070
H	6.725184	-1.501580	-1.200155
C	6.561395	-4.122872	-1.923892
H	7.381110	-3.559162	-2.403594
H	6.997617	-4.651335	-1.053376
H	6.210199	-4.897477	-2.628536
C	0.941112	0.944069	1.983931
C	1.968414	0.561441	2.860244
C	-0.303306	1.340674	2.506041
C	1.747733	0.564357	4.232309
H	2.943931	0.277138	2.453234
C	-0.517127	1.341181	3.877677
H	-1.115980	1.639649	1.830558
C	0.508557	0.950247	4.742207
H	2.552666	0.264842	4.911342

H	-1.488999	1.647127	4.280170
H	0.339009	0.950414	5.824737

5b2

71

scf done: -2192.395386

C	0.976145	-1.764101	1.387547
N	1.274164	-0.852897	0.351585
C	2.601497	-0.488646	0.031866
N	2.515175	0.801683	0.094022
C	1.104207	0.671783	0.492835
C	0.214968	1.239018	-0.591680
Au	-1.613285	0.304257	-1.008930
C	-3.511342	-0.526132	-1.186409
N	-3.969940	-1.424135	-2.083598
C	-5.254553	-1.818211	-1.762595
C	-5.600927	-1.137218	-0.638703
N	-4.519791	-0.346500	-0.305890
C	-4.437090	0.505541	0.866648
C	-3.193333	-1.980739	-3.175086
H	-5.808811	-2.533935	-2.369515
H	-6.524324	-1.133109	-0.059477
H	-3.684344	0.108951	1.573021
H	-4.158817	1.531113	0.570722
H	-5.420092	0.531006	1.362128
H	-2.675084	-2.902564	-2.853883
H	-3.862686	-2.218880	-4.017126
H	-2.446000	-1.241504	-3.503875
N	0.551440	2.358539	-1.166892
C	-0.098843	2.835825	-2.391878
S	1.917152	3.522407	-0.629097
H	-0.851435	3.611891	-2.169739
H	0.672930	3.235725	-3.071721
H	-0.589475	1.984294	-2.886481
O	2.053031	3.400689	0.804152
O	2.988018	3.351896	-1.585200
C	1.114443	5.086480	-0.919651
H	1.821167	5.810629	-0.477690
H	0.992829	5.289756	-1.992912
H	0.163116	5.114792	-0.364760
O	1.846417	-2.349150	1.987348
C	-0.468017	-1.991337	1.662415
C	-1.317094	-2.438707	0.645207
C	-0.936671	-1.907463	2.977869
C	-2.628942	-2.804825	0.945015
H	-0.929523	-2.547296	-0.376141
C	-2.260444	-2.226433	3.264585
H	-0.251692	-1.583832	3.770966
C	-3.105081	-2.683559	2.249327
H	-3.282597	-3.195778	0.154782
H	-2.631750	-2.143687	4.292055
H	-4.139569	-2.963845	2.482208
C	3.728462	-1.314481	-0.353192
C	3.611261	-2.693441	-0.565906
C	4.965009	-0.686210	-0.564600
C	4.716507	-3.427598	-0.976179
H	2.650115	-3.195930	-0.413209
C	6.062564	-1.430466	-0.970050
H	5.043879	0.395992	-0.409627
C	5.959917	-2.813801	-1.177969

H	4.618303	-4.507102	-1.144563
H	7.026941	-0.933625	-1.133360
C	7.156494	-3.617196	-1.580020
H	7.851263	-3.028521	-2.205195
H	7.725610	-3.947255	-0.688715
H	6.869714	-4.527044	-2.136312
C	0.734879	1.100043	1.892072
C	1.665855	0.923465	2.920668
C	-0.521153	1.636072	2.191400
C	1.336107	1.262160	4.229130
H	2.661586	0.526758	2.691977
C	-0.847282	1.982853	3.501632
H	-1.266543	1.787487	1.398698
C	0.078905	1.791891	4.523880
H	2.073693	1.120686	5.026584
H	-1.833824	2.405611	3.723348
H	-0.175258	2.062634	5.554771

TS_{6b1B}

71

scf done: -2192.376607

Au	2.019466	-0.506259	0.259170
C	3.975697	-1.199881	0.186647
N	4.778623	-1.566989	1.210638
C	6.007702	-1.981433	0.739451
C	5.963603	-1.869557	-0.613981
N	4.711710	-1.386907	-0.931618
C	4.234491	-1.150269	-2.283357
C	4.424833	-1.532888	2.616345
H	4.451921	-2.550528	3.041592
H	3.406836	-1.124890	2.716518
H	5.129335	-0.888693	3.168868
H	6.803079	-2.310134	1.408289
H	6.711877	-2.084508	-1.376860
H	3.637260	-0.223682	-2.308310
H	3.615548	-1.997672	-2.627149
H	5.102353	-1.043365	-2.953107
C	0.039549	0.101086	0.369473
C	-0.757440	0.300161	-0.852871
N	-0.201545	1.002886	-1.956402
N	-2.263478	0.363037	-0.706706
C	-2.198533	-1.019342	-0.771125
N	-0.892984	-1.175656	-0.969049
C	-3.199330	-2.052687	-0.731399
C	-2.753503	-3.386126	-0.653715
C	-3.668039	-4.425289	-0.645247
C	-5.046594	-4.172653	-0.731493
C	-5.479695	-2.841052	-0.820574
C	-4.576828	-1.789626	-0.818791
H	-4.936586	-0.759524	-0.877275
H	-6.553978	-2.630643	-0.884936
C	-6.030242	-5.296947	-0.754462
H	-3.315771	-5.460980	-0.569692
H	-1.677865	-3.587375	-0.592218
C	-0.558029	0.170622	1.704694
C	-3.083133	1.166609	0.120177
H	-6.988029	-5.009587	-0.286161
H	-6.257145	-5.592842	-1.797812
H	-5.639825	-6.192642	-0.240774
O	-4.004192	0.691482	0.737351

C	-2.725165	2.602172	0.158591
C	-2.498995	3.327895	-1.013492
C	-2.280218	4.702104	-0.939947
C	-2.237617	5.337196	0.300582
C	-2.455894	4.609019	1.471091
C	-2.728488	3.247738	1.399704
H	-2.535924	2.815952	-1.983738
H	-2.149989	5.289673	-1.856759
H	-2.048303	6.415052	0.354847
H	-2.431593	5.112697	2.443493
H	-2.934190	2.663861	2.305152
S	0.998923	2.161137	-1.640357
C	-0.126129	0.301670	-3.233002
C	0.604134	3.504893	-2.725915
O	0.775071	2.584563	-0.259201
O	2.298817	1.656365	-2.073265
H	0.093210	1.017310	-4.042092
H	0.646899	-0.490256	-3.225458
H	-1.107942	-0.150890	-3.451376
H	1.385832	4.258696	-2.530654
H	0.668993	3.170423	-3.772929
H	-0.388441	3.903115	-2.471992
C	-1.511619	-0.721387	2.216848
C	-2.007915	-0.552608	3.506845
C	-1.568735	0.503191	4.300929
C	-0.604116	1.381810	3.805757
C	-0.081797	1.210931	2.529165
H	-1.843891	-1.578717	1.622793
H	-2.747128	-1.263126	3.891990
H	-1.965654	0.633053	5.313592
H	-0.242424	2.210242	4.425328
H	0.675401	1.900212	2.139388

6b1B

71

scf done: -2192.388167

Au	2.072587	-0.546925	0.135473
C	4.125879	-0.851197	0.097665
N	4.925643	-1.294622	1.094362
C	6.237623	-1.371113	0.670063
C	6.251118	-0.964525	-0.625572
N	4.949020	-0.648353	-0.955678
C	4.513470	-0.191127	-2.263717
C	4.491316	-1.638508	2.433713
H	4.695799	-2.702847	2.640818
H	3.408197	-1.454993	2.512168
H	5.018831	-1.015876	3.176093
H	7.041252	-1.699849	1.328876
H	7.069797	-0.866430	-1.338488
H	3.789716	0.632612	-2.147163
H	4.043375	-1.018145	-2.824289
H	5.390440	0.170045	-2.823985
C	-0.018649	-0.295145	0.215982
C	-0.744585	0.570680	-0.718424
N	-0.234012	1.551346	-1.562175
N	-2.250810	0.429896	-0.574032
C	-2.087174	-0.887569	-0.844016
N	-0.724212	-0.886084	-1.072092
C	-2.950746	-2.009365	-0.969347
C	-2.351966	-3.235086	-1.343547

C	-3.126568	-4.366537	-1.504762
C	-4.520069	-4.316479	-1.321431
C	-5.110577	-3.092675	-0.964135
C	-4.349147	-1.951780	-0.788364
H	-4.827497	-1.016127	-0.490434
H	-6.195427	-3.046119	-0.814869
C	-5.355427	-5.533208	-1.535947
H	-2.656128	-5.315980	-1.786117
H	-1.269165	-3.269648	-1.508220
C	-0.636860	-0.589731	1.533414
C	-3.165916	1.060654	0.333269
H	-6.300048	-5.488544	-0.967169
H	-5.623795	-5.628396	-2.607014
H	-4.812521	-6.453770	-1.258861
O	-3.930431	0.396503	0.982890
C	-3.103912	2.533588	0.371955
C	-2.853904	3.290114	-0.778713
C	-2.960879	4.678113	-0.727737
C	-3.278150	5.310467	0.474244
C	-3.517493	4.557291	1.625604
C	-3.452339	3.171060	1.570695
H	-2.612469	2.788534	-1.724090
H	-2.802431	5.273528	-1.634250
H	-3.351199	6.403038	0.512223
H	-3.771526	5.057408	2.566169
H	-3.668809	2.559314	2.453766
S	1.005740	2.573240	-0.975596
C	-0.258733	1.289328	-2.996410
C	0.505999	4.181233	-1.528033
O	0.918579	2.547897	0.476670
O	2.242801	2.246673	-1.675788
H	-0.085320	2.220681	-3.560459
H	0.502916	0.541155	-3.287729
H	-1.261629	0.914854	-3.268665
H	1.320104	4.852571	-1.205402
H	0.421368	4.203839	-2.625972
H	-0.439456	4.448626	-1.030930
C	-1.023481	-1.882491	1.899808
C	-1.619023	-2.112143	3.139148
C	-1.812214	-1.059096	4.031622
C	-1.395560	0.225918	3.683161
C	-0.810876	0.463878	2.441984
H	-0.855538	-2.716636	1.206035
H	-1.932987	-3.126629	3.410076
H	-2.282648	-1.241285	5.004213
H	-1.534935	1.057349	4.384204
H	-0.478439	1.471769	2.160700

TS_{6b2B}

71

scf done: -2192.383777

Au	2.027486	-0.381149	0.036091
C	4.075733	-0.542944	-0.221517
N	4.900275	-1.472570	0.310168
C	6.204950	-1.245145	-0.080761
C	6.188300	-0.144740	-0.876375
N	4.873064	0.269373	-0.952139
C	4.426781	1.443145	-1.678046
C	4.491849	-2.571413	1.165872
H	4.776127	-3.533196	0.706618

H	3.398044	-2.541872	1.293026
H	4.972837	-2.482582	2.154591
H	7.024728	-1.890486	0.235089
H	6.990990	0.375208	-1.399309
H	4.616159	2.360143	-1.092579
H	3.344600	1.359003	-1.872089
H	4.962382	1.508443	-2.639475
C	-0.038712	-0.179659	0.339857
C	-0.744208	0.829374	-0.473957
C	-0.066788	2.012078	-1.056550
C	-0.168512	2.265058	-2.426092
C	0.419084	3.408041	-2.963602
C	1.110294	4.293489	-2.134846
C	1.224750	4.032285	-0.768717
C	0.640332	2.889275	-0.230178
H	0.724608	2.676971	0.844100
H	1.771629	4.724513	-0.119108
H	1.569741	5.193093	-2.559840
H	0.340864	3.609114	-4.037697
H	-0.710529	1.559529	-3.068261
N	-2.245409	0.775694	-0.369850
C	-2.150417	-0.453289	-0.956038
N	-0.817616	-0.466696	-1.195614
C	-3.070477	-1.511016	-1.232820
C	-2.506247	-2.763186	-1.557554
C	-3.329349	-3.839963	-1.838102
C	-4.726561	-3.699554	-1.833319
C	-5.277405	-2.442892	-1.529244
C	-4.471019	-1.361034	-1.222796
H	-4.920808	-0.394773	-0.979753
H	-6.367086	-2.321349	-1.534001
C	-5.613264	-4.865301	-2.122931
H	-2.888197	-4.814384	-2.078967
H	-1.415484	-2.871400	-1.562934
N	-0.700873	-0.731562	1.433341
C	-1.214360	0.115727	2.512963
H	-1.041373	1.175737	2.259428
H	-2.294277	-0.043211	2.686414
H	-0.653409	-0.083226	3.444881
S	-0.104331	-2.269901	1.943552
O	0.308546	-2.978950	0.741139
O	0.829817	-2.093134	3.048789
C	-1.597569	-3.001549	2.559610
H	-2.346405	-3.004767	1.750244
H	-1.950630	-2.446055	3.443084
H	-1.325802	-4.031430	2.846838
C	-3.206795	1.329357	0.518737
H	-6.541034	-4.553501	-2.634136
H	-5.103915	-5.623734	-2.742173
H	-5.917279	-5.363230	-1.180868
O	-4.086622	0.631164	0.961664
C	-3.037583	2.757840	0.853434
C	-2.556848	3.696118	-0.068617
C	-2.486660	5.040916	0.284008
C	-2.883377	5.450080	1.556353
C	-3.374391	4.519617	2.475455
C	-3.466263	3.179964	2.120803
H	-2.267110	3.382960	-1.077543
H	-2.121485	5.774062	-0.443705
H	-2.819267	6.508261	1.833613
H	-3.694907	4.846303	3.470515

H	-3.867408	2.438648	2.821728
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6b2B

71

scf done: -2192.389430

Au	2.000063	-0.491529	0.013418
C	4.051678	-0.791275	-0.096995
N	4.772911	-1.769238	0.495386
C	6.113039	-1.640248	0.187646
C	6.226519	-0.551281	-0.615621
N	4.951498	-0.046002	-0.779064
C	4.641086	1.147084	-1.542240
C	4.231299	-2.832705	1.321537
H	4.346509	-3.806391	0.815392
H	3.160349	-2.643868	1.500388
H	4.759349	-2.861076	2.289472
H	6.862591	-2.336824	0.563440
H	7.096741	-0.091984	-1.084970
H	4.952705	2.052783	-0.992722
H	3.553161	1.188216	-1.716309
H	5.161546	1.114339	-2.513717
C	-0.076922	-0.215116	0.153265
C	-0.698316	0.950251	-0.520949
C	0.038760	2.096222	-1.092893
C	-0.073106	2.393467	-2.453148
C	0.581176	3.507135	-2.974942
C	1.349176	4.319489	-2.139209
C	1.472452	4.015100	-0.782672
C	0.820726	2.901795	-0.259926
H	0.908512	2.654531	0.806471
H	2.078978	4.651291	-0.128613
H	1.861786	5.196117	-2.551262
H	0.495465	3.741957	-4.041615
H	-0.676661	1.745292	-3.101216
N	-2.191448	0.955123	-0.373205
C	-2.187556	-0.290483	-0.901367
N	-0.832238	-0.366216	-1.193356
C	-3.157396	-1.293928	-1.148668
C	-2.689987	-2.498102	-1.725099
C	-3.570292	-3.536504	-1.962400
C	-4.935692	-3.408050	-1.657036
C	-5.397480	-2.196520	-1.109963
C	-4.532088	-1.150081	-0.855179
H	-4.906937	-0.223258	-0.414655
H	-6.464245	-2.084357	-0.883966
C	-5.876519	-4.541162	-1.892757
H	-3.204222	-4.470137	-2.404882
H	-1.627506	-2.593761	-1.968099
N	-0.805567	-0.717001	1.296346
C	-0.574789	0.099694	2.484617
H	-0.983911	1.111870	2.310513
H	-1.099974	-0.331075	3.353665
H	0.503788	0.187380	2.728414
S	-0.567225	-2.394909	1.570580
O	-0.430714	-3.022957	0.262988
O	0.461318	-2.595102	2.586591
C	-2.141897	-2.845196	2.253890
H	-2.924306	-2.623394	1.508818
H	-2.315559	-2.295023	3.192340
H	-2.083049	-3.927676	2.457549

C	-3.009726	1.535525	0.651788
H	-6.903098	-4.187165	-2.090895
H	-5.547690	-5.177031	-2.732966
H	-5.925009	-5.190605	-0.996008
O	-3.820151	0.859730	1.232726
C	-2.741658	2.957587	0.931762
C	-2.349632	3.853783	-0.071179
C	-2.166277	5.198499	0.235253
C	-2.359330	5.647505	1.541324
C	-2.760992	4.759610	2.542430
C	-2.967473	3.420645	2.236773
H	-2.215925	3.506613	-1.101291
H	-1.871438	5.900157	-0.552731
H	-2.204265	6.705143	1.782278
H	-2.920598	5.119559	3.564373
H	-3.298811	2.711283	3.004070

TS_{6b1A}

71

scf done: -2192.371180

C	0.679950	-0.239790	1.735389
N	1.271327	0.197883	0.524795
C	2.598330	0.224815	0.047601
N	2.469912	0.806426	-1.104440
C	1.041474	0.901256	-1.005997
C	0.255253	-0.352119	-1.093361
Au	-1.790301	-0.499600	-0.630785
C	-3.781366	-0.725638	-0.083745
N	-4.320074	-1.780353	0.567458
C	-5.631971	-1.522040	0.910408
C	-5.916664	-0.275918	0.449466
N	-4.770348	0.191128	-0.160927
C	-4.628632	1.504029	-0.761125
C	-3.601502	-2.995227	0.903893
H	-6.250334	-2.251056	1.433754
H	-6.835055	0.309879	0.486545
H	-5.628313	1.935162	-0.926254
H	-4.049662	2.170142	-0.096992
H	-4.112998	1.415734	-1.731571
H	-2.989577	-3.314111	0.044355
H	-2.944335	-2.828615	1.776070
H	-4.325659	-3.789526	1.143480
C	0.897115	-1.555101	-1.605383
O	1.192361	-1.113755	2.392423
C	-0.591957	0.418389	2.118903
C	-1.519551	-0.340516	2.845467
C	-0.866869	1.758688	1.824926
C	-2.738941	0.215616	3.214963
H	-1.269518	-1.377789	3.100159
C	-2.077702	2.321576	2.221482
H	-0.117132	2.371151	1.313676
C	-3.020129	1.547013	2.898970
H	-3.474209	-0.385995	3.762193
H	-2.279448	3.377705	2.007828
H	-3.976088	1.990049	3.202338
C	3.846353	-0.223077	0.639888
C	3.980251	-1.387320	1.408742
C	4.987919	0.539225	0.337469
C	5.237002	-1.773994	1.858368
H	3.098349	-1.988165	1.643663

C	6.231319	0.150999	0.810373
H	4.874162	1.453234	-0.256937
C	6.378827	-1.012718	1.579650
H	5.337875	-2.694265	2.446892
H	7.114976	0.759643	0.582120
C	7.718692	-1.411490	2.112346
H	7.785128	-2.501473	2.275876
H	8.534401	-1.108210	1.432177
H	7.913802	-0.924043	3.087769
N	0.495415	2.133943	-1.237044
S	1.377655	3.549696	-0.721295
C	-0.828184	2.378754	-1.801144
H	-0.782553	3.267827	-2.450999
H	-1.122121	1.515508	-2.420202
H	-1.589508	2.555605	-1.019818
O	0.368913	4.593691	-0.671821
O	2.132163	3.197378	0.468812
C	2.486484	3.850678	-2.066812
H	3.056712	4.755375	-1.794495
H	3.144996	2.972628	-2.166317
H	1.890600	4.030068	-2.976913
C	0.565634	-2.804202	-1.038572
C	1.156152	-3.970007	-1.501987
C	2.044062	-3.918760	-2.580447
C	2.357251	-2.697178	-3.173668
C	1.812200	-1.518075	-2.675962
H	-0.143951	-2.840099	-0.200789
H	0.913919	-4.929938	-1.033877
H	2.492371	-4.842578	-2.962600
H	3.047384	-2.659463	-4.023178
H	2.081159	-0.560003	-3.130011

TS_{6b2B'}

71

scf done: -2192.371753

Au	2.186530	0.478786	-0.122481
C	4.248141	0.651856	0.079976
N	5.149004	0.571261	-0.925297
C	6.432167	0.743429	-0.446043
C	6.325586	0.931324	0.894735
N	4.978545	0.870962	1.196173
C	4.442680	1.014063	2.535051
C	4.802213	0.365900	-2.320553
H	4.370851	1.286120	-2.752023
H	4.067717	-0.451579	-2.409922
H	5.711934	0.097216	-2.880017
H	7.304618	0.712380	-1.098641
H	7.084353	1.096404	1.659609
H	4.868178	0.242584	3.199564
H	4.682069	2.012375	2.939316
H	3.348079	0.894010	2.492769
C	0.095146	0.292391	-0.437952
C	-0.756836	-0.318363	0.561194
N	-2.177519	-0.093727	0.292203
C	-1.987026	1.262426	0.089449
N	-0.685252	1.518939	0.041897
C	-0.356187	-0.729093	1.885720
C	-1.116729	-0.360603	3.012211
C	-0.718487	-0.762401	4.278017
C	0.415439	-1.567151	4.427697

C	1.158501	-1.960655	3.314136
C	0.787919	-1.531773	2.045174
H	1.345903	-1.854887	1.159856
H	2.030981	-2.610979	3.436524
H	0.717873	-1.896974	5.427964
H	-1.294223	-0.453956	5.156688
H	-2.010266	0.263186	2.885511
C	-3.007020	2.277626	0.121786
C	-4.332418	1.990003	0.488503
C	-5.277467	3.002615	0.514374
C	-4.935334	4.320959	0.175780
C	-3.607096	4.599132	-0.185697
C	-2.650817	3.598443	-0.204829
H	-1.613309	3.818301	-0.480731
H	-3.328577	5.625102	-0.454836
C	-5.954682	5.411835	0.227690
H	-6.310864	2.773905	0.800432
H	-4.622078	0.970761	0.765098
N	-0.321298	0.023009	-1.821052
C	0.143020	1.012853	-2.780714
H	1.250654	1.054971	-2.847829
H	-0.279413	0.802605	-3.777937
H	-0.234559	2.000328	-2.460894
S	-0.018095	-1.588559	-2.248166
O	1.303640	-1.755930	-2.842992
O	-0.377035	-2.357442	-1.050549
C	-1.236932	-1.884965	-3.503457
H	-1.207156	-2.972038	-3.689643
H	-0.958292	-1.341431	-4.420002
H	-2.224542	-1.569176	-3.128355
C	-3.069531	-0.912626	-0.479203
H	-5.755343	6.191194	-0.528644
H	-6.976690	5.023733	0.074838
H	-5.939735	5.910636	1.216909
O	-3.664442	-0.407167	-1.400359
C	-3.235576	-2.322212	-0.072903
C	-2.902854	-2.813826	1.194406
C	-3.118589	-4.153468	1.502292
C	-3.664301	-5.011246	0.548624
C	-4.016320	-4.524009	-0.711384
C	-3.812107	-3.185158	-1.016587
H	-2.494860	-2.148380	1.960576
H	-2.862274	-4.529804	2.498414
H	-3.826220	-6.067344	0.791752
H	-4.457965	-5.194270	-1.456639
H	-4.101860	-2.784761	-1.994306

6b1

71

scf done: -2192.476486

C	-0.158240	0.978052	0.282943
N	1.023611	0.258663	0.434729
C	1.437398	-0.145621	-0.829812
N	0.631110	0.288823	-1.761936
C	-0.366936	0.988012	-1.114606
C	-0.714094	1.875432	1.310307
C	0.126544	2.454132	2.269711
C	-0.380145	3.349152	3.206347
C	-1.730986	3.689751	3.192613
C	-2.572359	3.135126	2.229131

C	-2.069765	2.235709	1.295015
C	1.534927	-0.201293	1.718991
O	0.776560	-0.756591	2.468269
C	2.960725	0.055199	1.969286
C	3.581182	-0.688613	2.983277
C	4.940349	-0.535927	3.221876
C	5.681386	0.370393	2.460399
C	5.061912	1.137318	1.472336
C	3.702847	0.983632	1.224948
N	-1.159399	1.927992	-1.789149
C	-2.074976	1.480912	-2.828251
S	-0.349180	3.411132	-2.067875
O	-1.374130	4.419189	-2.268131
O	0.642399	3.521138	-1.005896
C	0.516249	3.167352	-3.604097
C	2.617939	-0.979197	-1.070265
C	2.934507	-2.087984	-0.276277
C	4.103000	-2.803835	-0.508734
C	4.983114	-2.440036	-1.535764
C	4.637807	-1.351219	-2.347258
C	3.470210	-0.632467	-2.125862
C	6.264722	-3.183076	-1.749451
H	1.200792	2.235414	2.273895
H	0.293488	3.793423	3.946845
H	-2.128098	4.396830	3.929052
H	-3.633007	3.407737	2.201667
H	-2.742475	1.814092	0.536508
H	2.981556	-1.400361	3.561356
H	5.429845	-1.126474	4.003538
H	6.755051	0.486994	2.645648
H	5.643145	1.862240	0.893024
H	3.214565	1.593004	0.454559
H	-2.531166	2.364641	-3.305020
H	-1.569906	0.860074	-3.596124
H	-2.892127	0.892023	-2.370639
H	1.109984	4.082173	-3.769748
H	1.169243	2.284726	-3.499533
H	-0.213877	3.037648	-4.419137
H	2.256830	-2.410385	0.524923
H	5.305114	-1.061474	-3.168418
H	3.217044	0.225691	-2.759431
H	7.088592	-2.722275	-1.169880
H	6.186509	-4.234328	-1.420424
H	6.570752	-3.171657	-2.810522
H	4.338518	-3.672410	0.118659
Au	-1.800074	-0.708407	-0.169798
C	-3.129385	-2.230664	0.154864
N	-3.135456	-3.454808	-0.410272
C	-4.180896	-4.204627	0.088058
C	-4.836917	-3.417404	0.981316
N	-4.173202	-2.208517	1.009002
C	-2.147810	-3.933515	-1.361609
C	-4.555530	-1.061655	1.816254
H	-4.365133	-5.228791	-0.235920
H	-5.715773	-3.610803	1.596075
H	-1.936412	-3.146499	-2.102985
H	-2.547448	-4.818928	-1.879280
H	-1.212580	-4.206426	-0.843318
H	-5.313167	-1.377168	2.549626
H	-4.978120	-0.266148	1.178417
H	-3.674954	-0.669754	2.351982

TS_{6b2A}

71

scf done: -2192.369348

C	-0.585716	0.529390	-1.773853
N	-1.248657	0.459186	-0.474270
C	-2.627560	0.562405	-0.040485
N	-2.504754	0.740388	1.229264
C	-1.071614	0.714548	1.218454
C	-0.507190	-0.516345	0.637639
Au	1.542321	-0.779396	0.140907
C	3.504929	-1.042422	-0.484805
N	3.961646	-1.974883	-1.348654
C	5.285512	-1.740817	-1.663542
C	5.659664	-0.632906	-0.971225
N	4.553110	-0.222989	-0.254382
C	4.497593	0.944467	0.605156
C	3.151180	-3.044747	-1.901076
H	5.844826	-2.387706	-2.339249
H	6.615198	-0.111623	-0.914665
H	5.515193	1.344342	0.735676
H	3.854048	1.722839	0.156285
H	4.093649	0.662865	1.591921
H	2.560489	-3.514655	-1.098224
H	2.465109	-2.653372	-2.673197
H	3.810957	-3.801669	-2.352883
N	-1.267650	-1.691494	0.850110
O	-0.938958	-0.209231	-2.653853
C	0.538196	1.476391	-1.889287
C	1.569858	1.155296	-2.786226
C	0.590864	2.673051	-1.166334
C	2.665930	1.998015	-2.913446
H	1.506357	0.221860	-3.358256
C	1.679065	3.528405	-1.314905
H	-0.233721	2.951406	-0.503083
C	2.721618	3.184417	-2.175482
H	3.481044	1.737438	-3.597728
H	1.709108	4.471079	-0.757237
H	3.582347	3.854177	-2.284716
C	-3.859402	0.427276	-0.788719
C	-3.943011	-0.130959	-2.073628
C	-5.041858	0.835171	-0.140607
C	-5.181818	-0.270896	-2.687553
H	-3.039833	-0.474439	-2.584974
C	-6.267302	0.693754	-0.768094
H	-4.977299	1.270118	0.863221
C	-6.361229	0.142017	-2.056222
H	-5.237620	-0.718710	-3.687184
H	-7.181124	1.016987	-0.254752
C	-7.685056	0.023860	-2.740278
H	-7.686322	-0.784430	-3.492155
H	-8.500454	-0.163654	-2.019378
H	-7.934829	0.963432	-3.271418
C	-0.347876	1.824221	1.834162
C	-1.088800	-2.797762	-0.077235
S	-1.622925	-2.087656	2.469043
H	-1.866928	-3.559772	0.095737
H	-1.210872	-2.411583	-1.105405
H	-0.094348	-3.277507	0.023406
C	-3.394633	-2.095659	2.539982

O	-1.151481	-3.446475	2.684949
O	-1.112709	-0.981254	3.272664
H	-3.660821	-2.412279	3.563028
H	-3.750788	-1.074306	2.329462
H	-3.771269	-2.826216	1.804921
C	-0.989679	3.068450	1.946569
C	-0.322594	4.151583	2.504095
C	0.977964	3.993005	2.987647
C	1.604403	2.748589	2.922853
C	0.946157	1.666404	2.348446
H	-2.016706	3.179948	1.581152
H	-0.822714	5.122965	2.577933
H	1.499824	4.844475	3.438661
H	2.609908	2.617817	3.337531
H	1.424769	0.679991	2.322666

TS_{6b1B'}

71

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Au	-2.606031	0.196253	0.010922
C	-4.620052	0.170256	-0.501271
N	-5.597930	0.996154	-0.065051
C	-6.812836	0.654134	-0.625564
C	-6.582932	-0.413821	-1.431591
N	-5.233313	-0.692663	-1.343968
C	-4.582960	-1.795276	-2.026086
C	-5.418512	2.105194	0.851440
H	-5.711894	3.051214	0.365681
H	-4.356387	2.159371	1.137923
H	-6.031732	1.955548	1.756223
H	-7.726794	1.206159	-0.406248
H	-7.255292	-0.995000	-2.062696
H	-4.644285	-2.720031	-1.425462
H	-5.073322	-1.963729	-2.998371
H	-3.524064	-1.543650	-2.196168
C	-0.543598	0.317391	0.494971
C	0.322090	-0.834868	0.518990
N	1.741354	-0.498196	0.493899
C	1.602156	0.389345	-0.540775
N	0.295616	0.413517	-0.793918
N	-0.019463	-2.135539	0.424585
C	2.572301	1.162027	-1.275531
C	3.749304	1.667238	-0.694400
C	4.594335	2.473890	-1.439866
C	4.312206	2.782674	-2.779333
C	3.128927	2.284864	-3.344691
C	2.259942	1.498398	-2.605463
H	1.336872	1.111767	-3.050158
H	2.888529	2.526109	-4.387057
C	5.260499	3.606436	-3.588531
H	5.498364	2.882901	-0.972895
H	3.987341	1.466719	0.355368
C	-0.264218	1.442969	1.439085
C	2.630722	-0.912497	1.513630
H	6.018619	2.961098	-4.074508
H	4.740693	4.156018	-4.392547
H	5.808215	4.331586	-2.961413
O	2.150069	-1.293693	2.554678
C	4.067335	-0.937783	1.184345
C	4.514350	-1.293415	-0.095747

C	5.880496	-1.337711	-0.356674
C	6.793273	-1.008315	0.645530
C	6.347745	-0.667147	1.924566
C	4.985700	-0.650768	2.202204
H	3.791491	-1.554809	-0.878975
H	6.236299	-1.626768	-1.351382
H	7.867722	-1.027493	0.431281
H	7.069792	-0.420064	2.710170
H	4.615546	-0.397800	3.202076
S	0.829793	-3.247053	-0.632296
C	-1.274105	-2.644158	0.978543
O	1.650415	-2.451935	-1.528356
C	1.860761	-4.154941	0.486838
O	-0.203015	-4.130139	-1.136407
H	-1.103668	-3.662040	1.369592
H	-1.573697	-1.995870	1.816819
H	-2.077756	-2.679495	0.222575
H	2.320004	-4.956926	-0.116493
H	2.634735	-3.492753	0.907309
H	1.227877	-4.587928	1.278338
C	-0.270852	1.195978	2.817213
C	-0.059026	2.236804	3.718049
C	0.157600	3.534724	3.254180
C	0.166430	3.783407	1.882200
C	-0.041955	2.744080	0.976864
H	-0.430229	0.172595	3.183963
H	-0.056083	2.029633	4.794338
H	0.324503	4.352735	3.963898
H	0.339464	4.799628	1.509448
H	-0.035418	2.938686	-0.103609

6b2

71

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N	0.533114	0.740386	1.824422
C	-0.381022	1.274266	1.004862
C	-0.196902	0.832915	-0.355867
N	1.052819	0.097469	-0.248238
C	1.377420	0.041278	1.066045
C	-1.384925	2.220373	1.487418
C	-1.187876	2.822449	2.738357
C	-2.096502	3.760454	3.217854
C	-3.213422	4.103829	2.457357
C	-3.423395	3.503412	1.213705
C	-2.516583	2.567642	0.729864
Au	-1.772508	-0.744252	-0.226567
N	-0.371982	1.710569	-1.448184
C	-0.913335	1.302698	-2.743267
S	0.711862	3.035425	-1.503106
O	1.357625	3.079387	-0.192872
O	1.507257	2.925096	-2.717253
C	-0.356562	4.446259	-1.638564
C	2.474167	-0.739825	1.625066
C	3.141467	-0.233915	2.749519
C	4.239357	-0.905586	3.268692
C	4.690290	-2.105229	2.700706
C	3.986686	-2.626541	1.606455
C	2.893552	-1.957824	1.072845
C	5.898131	-2.802791	3.241359
C	1.684833	-0.503337	-1.396756

C	3.138458	-0.313113	-1.516813
O	0.993529	-1.103471	-2.182855
C	3.807196	0.760348	-0.912024
C	5.189386	0.858564	-1.025999
C	5.903126	-0.106846	-1.736841
C	5.235475	-1.160843	-2.364766
C	3.854092	-1.257833	-2.265784
C	-3.205693	-2.214963	-0.206015
N	-4.257166	-2.293530	0.636953
C	-5.028196	-3.399065	0.340027
C	-4.434234	-4.018835	-0.713099
N	-3.315993	-3.274962	-1.033807
C	-2.407952	-3.603110	-2.118057
C	-4.542178	-1.330252	1.686564
H	-0.303038	2.547087	3.321042
H	-1.930762	4.229688	4.193640
H	-3.929575	4.841482	2.836369
H	-4.306364	3.764828	0.620142
H	-2.693178	2.092798	-0.243606
H	-1.801172	0.669701	-2.568518
H	-1.242648	2.194904	-3.303804
H	-0.186387	0.745726	-3.360356
H	0.309551	5.324019	-1.692159
H	-0.955605	4.373807	-2.560405
H	-0.992001	4.487336	-0.738313
H	2.797864	0.705622	3.195696
H	4.765195	-0.493158	4.138597
H	4.301098	-3.582880	1.170893
H	2.348151	-2.407488	0.233801
H	5.867973	-3.888056	3.040266
H	6.820813	-2.410096	2.770588
H	6.002836	-2.651090	4.330276
H	3.243111	1.535131	-0.378266
H	5.715009	1.699141	-0.560905
H	6.993700	-0.031062	-1.812914
H	5.799293	-1.908628	-2.932730
H	3.309913	-2.079434	-2.744976
H	-5.925623	-3.648372	0.906112
H	-4.703263	-4.922738	-1.259227
H	-2.031383	-4.631988	-1.993085
H	-2.927645	-3.521503	-3.087656
H	-1.558313	-2.901244	-2.101716
H	-5.335619	-1.732192	2.335187
H	-3.637053	-1.154574	2.290907
H	-4.878502	-0.372740	1.252377

Cartesian coordinates of C-Series

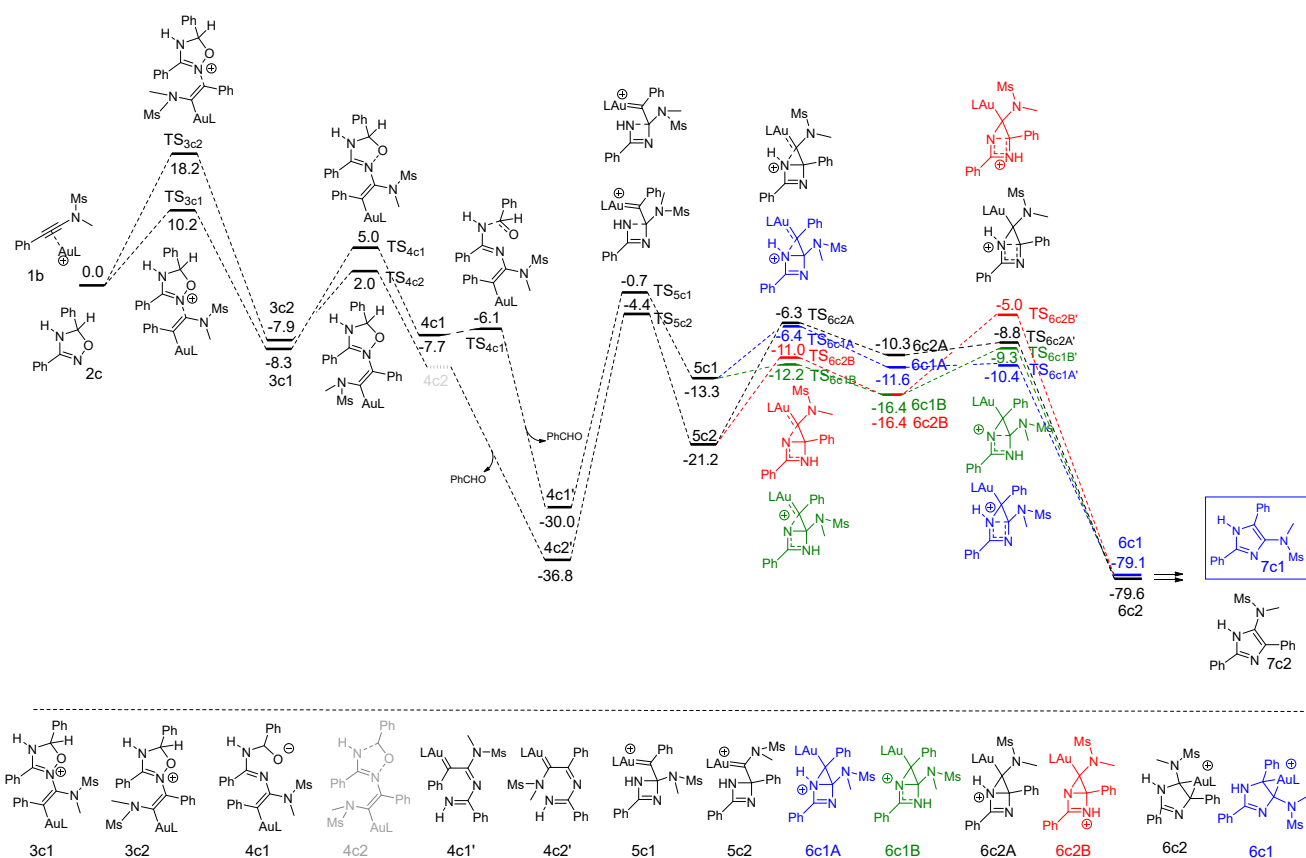


Figure S3. C-series reaction mechanism

41

scf done: -1429.958460

C	-1.695926	2.089645	-0.034247
N	-2.571859	2.227485	-1.054851
C	-3.215743	3.445743	-0.978289
C	-2.729658	4.075845	0.122128
N	-1.798637	3.227403	0.686854
C	-2.776430	1.259880	-2.117049
C	-1.070505	3.529812	1.904710
Au	-0.482158	0.456421	0.324310
C	0.661462	-1.320253	0.714498
C	1.690644	-1.128030	-0.014310
C	0.196963	-2.413218	1.560578
N	2.626030	-0.902472	-0.866610
S	2.385913	-1.544326	-2.530487
C	3.901925	-0.231976	-0.584999
O	3.725603	-1.713102	-3.051913
O	1.443734	-2.632251	-2.383502
C	1.593906	-0.164449	-3.313478
C	-0.848992	-2.230134	2.476485
C	-1.273350	-3.285313	3.278378
C	-0.668500	-4.536163	3.162795
C	0.364474	-4.733008	2.243689
C	0.798175	-3.679267	1.449760
H	-3.963846	3.752060	-1.709481
H	-2.967018	5.046052	0.558617
H	-2.637871	0.241773	-1.719832
H	-3.804130	1.356445	-2.501257
H	-2.065507	1.431090	-2.944681
H	-1.766934	3.606367	2.756698
H	-0.349878	2.720420	2.098835
H	-0.526651	4.482484	1.792671
H	4.022303	0.644103	-1.245629
H	3.889381	0.098642	0.464549
H	4.736247	-0.931415	-0.751619
H	1.385428	-0.483838	-4.349344
H	0.655098	0.056643	-2.776731
H	2.287221	0.692353	-3.310013
H	-1.326068	-1.245615	2.560599
H	-2.086396	-3.131917	3.996202
H	-1.007262	-5.367890	3.790501
H	0.834296	-5.717712	2.146122
H	1.599691	-3.830390	0.715941

2c

29

scf done: -724.316851

C	-1.774773	-0.804305	-0.711431
C	-2.642757	0.152695	-0.171436
C	-4.021930	-0.018799	-0.268865
C	-4.543349	-1.144542	-0.904194
C	-3.681186	-2.103103	-1.441706
C	-2.304525	-1.935648	-1.347798
C	-0.323689	-0.639883	-0.606736
N	0.280177	0.558956	-0.285060
N	0.510552	-1.613389	-0.746535
O	1.784323	-1.068775	-0.536013
C	1.697704	0.355543	-0.540160
C	2.613501	0.934990	0.500422

C	2.451735	0.579385	1.843304
C	3.300110	1.104587	2.812416
C	4.316278	1.991807	2.446245
C	4.481706	2.347799	1.109766
C	3.631172	1.816609	0.138773
H	-2.238947	1.028829	0.349459
H	-4.694261	0.732660	0.159913
H	-4.088458	-2.988153	-1.943283
H	-1.618906	-2.676622	-1.773167
H	1.650927	-0.117573	2.120304
H	3.171462	0.822991	3.863947
H	4.983260	2.406107	3.211223
H	5.278598	3.041713	0.818848
H	3.759871	2.090145	-0.916538
H	1.984631	0.746994	-1.547276
H	-5.628393	-1.277211	-0.982318
H	-0.142190	1.427019	-0.607258

TS_{3c1}

68

scf done: -2310.706364

N	-3.709882	0.866883	-1.158119
C	-2.886165	1.089986	-0.098697
C	-3.418628	-0.491783	-1.618763
O	-2.159106	-0.735599	-1.011688
N	-1.977203	0.176381	0.034333
C	-2.949728	2.274193	0.755675
C	-2.633611	2.179436	2.117040
C	-2.660155	3.318255	2.915375
C	-2.993006	4.554305	2.357849
C	-3.305598	4.650806	1.001582
C	-3.290663	3.513137	0.199445
C	-4.465666	-1.493665	-1.188992
C	-4.216109	-2.382395	-0.142115
C	-5.205402	-3.278123	0.262181
C	-6.445201	-3.289203	-0.376094
C	-6.694070	-2.405506	-1.427749
C	-5.704615	-1.513816	-1.836120
C	0.131783	0.524718	0.224552
C	0.642014	-0.650915	0.423256
C	0.008070	-1.915293	0.795682
C	-0.843275	-1.980263	1.909212
C	-1.438409	-3.186252	2.271353
C	-1.212610	-4.336369	1.514353
C	-0.369630	-4.278969	0.403638
C	0.253088	-3.082797	0.058309
Au	2.761447	-0.564635	0.141304
N	0.242018	1.830634	0.156126
C	0.643154	2.661886	1.297864
S	0.105437	2.622225	-1.401076
O	-0.841543	1.853487	-2.187462
O	-0.114672	4.024678	-1.095506
C	1.733183	2.404253	-2.067055
P	5.090540	-0.498074	-0.218813
H	-2.382023	1.201342	2.544191
H	-2.422936	3.242366	3.982220
H	-3.560527	5.621939	0.563799
H	-3.512975	3.585087	-0.871869
H	-3.234213	-2.377065	0.346067
H	-5.001442	-3.976649	1.082989

H	-7.221321	-3.994812	-0.058060
H	-7.663542	-2.417890	-1.938763
H	-5.895486	-0.828715	-2.674035
H	-1.024666	-1.074618	2.499307
H	-2.092282	-3.226056	3.150436
H	-1.689215	-5.282641	1.795082
H	-0.185555	-5.178960	-0.193924
H	0.928172	-3.039685	-0.805656
H	1.656746	3.074563	1.135156
H	-0.077040	3.483541	1.447564
H	0.656445	2.015787	2.189796
H	2.462389	2.880157	-1.390168
H	1.927933	1.323790	-2.180221
H	1.731718	2.906021	-3.049938
H	-3.278745	-0.514176	-2.717871
H	-3.011521	5.450658	2.987822
C	5.721436	-1.862255	-1.248023
C	5.625006	1.015578	-1.082965
C	6.100199	-0.551908	1.296385
H	5.120932	1.079592	-2.063969
H	5.348855	1.903983	-0.487488
H	6.720464	1.004161	-1.236033
H	5.515804	-2.828365	-0.754682
H	5.215310	-1.853853	-2.229426
H	6.811803	-1.752793	-1.398314
H	5.896307	-1.486465	1.848172
H	7.174979	-0.506015	1.039207
H	5.843423	0.302910	1.946370
H	-4.671485	1.204509	-1.143559

3c1

68

scf done: -2310.741157

N	-3.614583	1.162842	-0.660930
C	-2.559126	1.402161	0.100534
C	-3.438342	-0.081954	-1.416236
O	-2.153339	-0.507111	-0.958240
N	-1.670219	0.434853	-0.047439
C	-2.372966	2.573794	0.947964
C	-1.907639	2.432830	2.260917
C	-1.727335	3.565256	3.046955
C	-1.991114	4.830214	2.518909
C	-2.444853	4.968497	1.206792
C	-2.647042	3.840871	0.417590
C	-4.482751	-1.118594	-1.119017
C	-4.413491	-1.861344	0.063564
C	-5.398653	-2.802790	0.346884
C	-6.456004	-2.999135	-0.543978
C	-6.523814	-2.259630	-1.723878
C	-5.532677	-1.323040	-2.014760
C	-0.238715	0.453082	0.102158
C	0.432082	-0.677486	0.400998
C	-0.302258	-1.871454	0.857561
C	-1.039863	-1.843270	2.051754
C	-1.731369	-2.971073	2.492560
C	-1.712523	-4.144175	1.739348
C	-0.980221	-4.185280	0.551053
C	-0.269349	-3.067556	0.123526
Au	2.510608	-0.759399	0.167020
N	0.319889	1.730054	-0.119124

C	1.189560	2.377246	0.856911
S	0.292849	2.368039	-1.675483
O	-0.958631	1.931856	-2.292613
O	0.593238	3.787684	-1.551485
C	1.632085	1.576312	-2.532631
P	4.858415	-0.725361	-0.204203
H	-1.707266	1.434602	2.667406
H	-1.377614	3.461346	4.079303
H	-2.641331	5.963196	0.793691
H	-2.980254	3.938625	-0.622348
H	-3.570217	-1.718742	0.753708
H	-5.338107	-3.393097	1.268660
H	-7.229937	-3.741706	-0.318940
H	-7.347760	-2.420051	-2.427909
H	-5.571432	-0.749492	-2.949624
H	-1.051593	-0.925008	2.653650
H	-2.290930	-2.930621	3.434768
H	-2.259856	-5.029971	2.081664
H	-0.955489	-5.104352	-0.046043
H	0.314855	-3.106681	-0.805203
H	2.259254	2.338637	0.566168
H	0.888573	3.430657	0.998301
H	1.077190	1.838293	1.811581
H	2.577949	1.825921	-2.021388
H	1.457042	0.487276	-2.535657
H	1.629136	1.977082	-3.560554
H	-3.389870	0.141862	-2.501610
H	-1.839495	5.720792	3.138488
C	5.333516	-1.007335	-1.943344
C	5.576679	0.905871	0.190418
C	5.870620	-1.912322	0.739936
H	5.070796	1.684874	-0.409279
H	5.418682	1.133173	1.259957
H	6.660507	0.922243	-0.030526
H	5.004711	-2.012008	-2.262964
H	4.841745	-0.256909	-2.588524
H	6.430284	-0.926766	-2.062933
H	5.564253	-2.943558	0.490674
H	6.942200	-1.781249	0.498641
H	5.718124	-1.754044	1.822017
H	-4.486366	1.688138	-0.622775

TS_{3c2}

68

scf done: -2310.691220

O	-2.793702	-0.191362	-1.503251
C	-4.123277	0.319223	-1.574983
N	-4.066569	1.390767	-0.577590
C	-3.001155	1.109200	0.226848
N	-2.231973	0.196063	-0.278033
C	-5.171160	-0.720959	-1.266340
C	-2.719281	1.809550	1.478091
C	-4.870112	-1.848595	-0.496965
C	-5.873642	-2.763244	-0.182369
C	-7.178039	-2.557735	-0.632359
C	-7.479520	-1.436645	-1.405340
C	-6.476376	-0.523500	-1.724792
C	-3.193590	3.113788	1.668209
C	-2.908490	3.790860	2.850518
C	-2.154913	3.169720	3.845892

C	-1.684709	1.868442	3.660272
C	-1.964040	1.187095	2.480695
C	-0.142131	-0.297128	-0.117154
C	-0.337929	-1.637201	0.387680
C	0.596566	0.684099	-0.497946
C	0.098837	-1.969793	1.682241
C	-0.051248	-3.268583	2.160280
C	-0.658741	-4.240014	1.364409
C	-1.107720	-3.913821	0.082825
C	-0.941847	-2.623893	-0.409139
Au	2.519888	-0.340408	-0.182739
N	0.485933	1.939114	-1.012380
S	1.840912	2.983344	-1.029484
C	-0.741190	2.454164	-1.624002
O	1.297088	4.330008	-1.094238
O	2.720616	2.595960	0.066084
C	2.645634	2.614779	-2.567169
P	4.568907	-1.430119	0.120672
H	-3.842841	-2.019448	-0.152460
H	-5.633206	-3.648514	0.417348
H	-7.963886	-3.280476	-0.384938
H	-8.500533	-1.277112	-1.769896
H	-6.707310	0.353436	-2.344594
H	-3.770503	3.608759	0.878000
H	-3.275022	4.812964	2.993667
H	-1.100594	1.377922	4.446438
H	-1.618756	0.156762	2.336046
H	0.570275	-1.197800	2.303818
H	0.300207	-3.521515	3.166689
H	-0.783830	-5.259771	1.745324
H	-1.583407	-4.677200	-0.542944
H	-1.290502	-2.358948	-1.413575
H	-1.313531	1.607039	-2.032828
H	-1.357539	3.014696	-0.897855
H	-0.484284	3.133744	-2.453231
H	3.514381	3.290923	-2.635875
H	2.973343	1.561661	-2.556942
H	1.939460	2.810034	-3.390552
H	-1.933569	3.703289	4.776908
H	-4.274254	0.733335	-2.590049
C	5.953748	-0.303944	0.478149
C	4.529831	-2.601816	1.514292
C	5.117255	-2.417135	-1.307132
H	5.231265	-1.765110	-2.190700
H	6.085370	-2.903319	-1.083386
H	4.362863	-3.190554	-1.534973
H	3.746239	-3.359883	1.336180
H	5.509266	-3.104169	1.622528
H	4.289914	-2.060777	2.446760
H	5.731322	0.282971	1.386777
H	6.885112	-0.880471	0.631945
H	6.091631	0.395140	-0.365557
H	-4.936736	1.732955	-0.171017

3c2

68

scf done: -2310.738434

O	-2.865322	-0.317884	-1.366030
C	-4.089064	0.421715	-1.241560
N	-3.720212	1.409309	-0.220598

C	-2.534320	1.117513	0.305848
N	-1.993079	0.103437	-0.336970
C	-5.241792	-0.453317	-0.845733
C	-1.897330	1.838509	1.402519
C	-5.109926	-1.348350	0.222340
C	-6.185879	-2.147629	0.593920
C	-7.396662	-2.054869	-0.096809
C	-7.528905	-1.167102	-1.162409
C	-6.449170	-0.368683	-1.539222
C	-1.898538	3.238767	1.385717
C	-1.272917	3.934203	2.415524
C	-0.670534	3.237223	3.461939
C	-0.680840	1.840992	3.481526
C	-1.285979	1.135090	2.448802
C	-0.672559	-0.430667	-0.283016
C	-0.598680	-1.815171	0.253312
C	0.390878	0.371491	-0.587942
C	0.244245	-2.128099	1.333233
C	0.312436	-3.425690	1.835617
C	-0.476857	-4.434475	1.282528
C	-1.337522	-4.132384	0.228591
C	-1.397879	-2.836437	-0.282578
Au	2.348246	-0.384263	-0.335105
N	0.171001	1.645502	-1.124647
S	1.234536	2.908701	-0.739926
C	-0.821302	1.954774	-2.154036
O	0.474075	4.135202	-0.950952
O	1.820715	2.628561	0.564252
C	2.517642	2.837966	-1.967278
P	4.490519	-1.363101	-0.071242
H	-4.155987	-1.432258	0.760075
H	-6.081173	-2.851478	1.426849
H	-8.242697	-2.685952	0.197674
H	-8.475957	-1.098789	-1.708747
H	-6.543554	0.325603	-2.383736
H	-2.358623	3.782286	0.551745
H	-1.253974	5.028719	2.397943
H	-0.213770	1.298443	4.310035
H	-1.306302	0.039166	2.459164
H	0.843936	-1.333394	1.797205
H	0.977482	-3.645719	2.679164
H	-0.426975	-5.454634	1.679866
H	-1.965010	-4.916511	-0.210611
H	-2.068055	-2.614503	-1.121092
H	-1.165874	1.009835	-2.603098
H	-1.688734	2.523446	-1.769149
H	-0.363472	2.560365	-2.956312
H	3.208245	3.668215	-1.743975
H	3.036285	1.866646	-1.885638
H	2.066927	2.973207	-2.963845
H	-0.183965	3.788709	4.273861
H	-4.291015	0.923815	-2.207839
C	5.847943	-0.203270	0.301012
C	4.520581	-2.563770	1.302402
C	5.087295	-2.312996	-1.509284
H	5.175628	-1.647702	-2.386173
H	6.074133	-2.762960	-1.291066
H	4.365521	-3.113863	-1.748965
H	3.767773	-3.351290	1.116629
H	5.520713	-3.026499	1.397883
H	4.262685	-2.051585	2.246883

H	5.613264	0.360678	1.221134
H	6.798202	-0.752140	0.440628
H	5.960924	0.515739	-0.529926
H	-4.394267	2.031717	0.221796

TS_{4c1}

68

scf done: -2310.719099

O	-3.032147	-0.103258	-1.884266
C	-4.112264	0.266022	-1.207039
N	-3.612559	1.189061	-0.105507
C	-2.392915	0.937056	0.312926
N	-1.741637	-0.062757	-0.290738
C	-4.898748	-0.861930	-0.552505
C	-1.806541	1.692230	1.433416
C	-4.413775	-2.167601	-0.626714
C	-5.111640	-3.212162	-0.020779
C	-6.304073	-2.956020	0.655734
C	-6.801154	-1.653067	0.718469
C	-6.101158	-0.611032	0.113594
C	-2.154990	3.041711	1.595052
C	-1.554991	3.795142	2.598055
C	-0.619037	3.205576	3.447662
C	-0.283138	1.859828	3.295173
C	-0.868683	1.099294	2.288358
C	-0.494995	-0.247753	-0.666516
N	-0.108235	-1.592801	-0.887857
C	0.458054	0.792963	-0.815699
Au	2.394144	0.161049	-0.304928
C	0.091688	2.133146	-1.161610
P	4.399713	-0.964347	0.292566
H	-3.483620	-2.343217	-1.180168
H	-4.723651	-4.236469	-0.081536
H	-6.854895	-3.776620	1.129650
H	-7.744236	-1.449259	1.238491
H	-6.502335	0.411328	0.155639
H	-2.858036	3.522686	0.904900
H	-1.812744	4.853688	2.708382
H	0.442785	1.394565	3.970515
H	-0.600300	0.043442	2.169676
H	-0.146412	3.801439	4.236205
H	-4.808798	0.901781	-1.810190
C	4.251096	-1.741446	1.935027
C	4.684405	-2.372023	-0.830924
C	5.972499	-0.045861	0.337424
H	5.899574	0.785317	1.060767
H	6.798108	-0.718039	0.637380
H	6.189075	0.375080	-0.660112
H	4.835822	-2.008614	-1.862904
H	5.571745	-2.950509	-0.511788
H	3.787826	-3.020063	-0.806091
H	3.349813	-2.380839	1.940995
H	5.143610	-2.357846	2.152251
H	4.140625	-0.966811	2.714216
H	-4.231753	1.780483	0.449988
C	0.348930	-1.969767	-2.221723
S	0.261131	-2.611289	0.396867
H	0.181086	-3.047774	-2.389228
H	-0.260315	-1.416504	-2.957383
H	1.422586	-1.748054	-2.385022

C	-1.124686	-3.709598	0.481364
O	1.449769	-3.376556	0.027965
O	0.270875	-1.807144	1.617121
H	-0.916202	-4.436893	1.283651
H	-2.014024	-3.101015	0.717145
H	-1.237207	-4.222428	-0.488292
C	-1.048715	2.424162	-1.955580
C	-1.357539	3.737516	-2.278914
C	-0.562848	4.784134	-1.801963
C	0.565810	4.518989	-1.018624
C	0.904468	3.208829	-0.723838
H	-1.680054	1.602766	-2.320365
H	-2.226647	3.954220	-2.909340
H	-0.818363	5.819604	-2.053596
H	1.187611	5.343384	-0.654385
H	1.796796	2.985245	-0.125334

4c1

68

scf done: -2310.735894

N	-1.533063	2.272030	-0.071148
C	-2.243158	1.202084	-0.326701
C	-0.076065	2.384212	0.533043
O	0.282318	1.334907	1.208099
N	-1.759223	-0.035936	-0.242943
C	-3.606919	1.343280	-0.885816
C	-4.082716	0.395971	-1.800077
C	-5.357469	0.529524	-2.342590
C	-6.170633	1.596773	-1.962111
C	-5.707839	2.531483	-1.035152
C	-4.430183	2.408250	-0.499204
C	0.819199	2.745390	-0.649739
C	0.879018	1.938414	-1.793512
C	1.763775	2.237588	-2.827261
C	2.610779	3.345148	-2.727878
C	2.562614	4.150027	-1.591392
C	1.665837	3.851245	-0.562526
C	-1.166422	-0.826732	0.572225
C	-0.141009	-1.603686	-0.141953
C	-0.534291	-2.686006	-0.960691
C	-1.869479	-3.184783	-0.957733
C	-2.213128	-4.263619	-1.748479
C	-1.241719	-4.864760	-2.561104
C	0.077229	-4.397688	-2.583059
C	0.430822	-3.322886	-1.788444
Au	1.762729	-0.759980	0.080111
N	-1.354929	-1.055566	1.899516
C	-0.499840	-2.023184	2.584143
S	-2.380010	-0.092855	2.935573
O	-3.252841	0.678131	2.065058
O	-2.949517	-1.040129	3.878419
C	-1.220957	0.967891	3.736889
P	3.946989	0.116111	0.401868
H	-3.436755	-0.438232	-2.096014
H	-5.719562	-0.206155	-3.069039
H	-6.351916	3.359110	-0.718964
H	-4.087838	3.124449	0.257254
H	0.207467	1.073322	-1.885158
H	1.790933	1.605593	-3.723114
H	3.305508	3.581565	-3.542365

H	3.220519	5.023049	-1.507397
H	1.621396	4.491629	0.329393
H	-2.625158	-2.712864	-0.318745
H	-3.236713	-4.650542	-1.741413
H	-1.520662	-5.719443	-3.187468
H	0.820938	-4.883405	-3.221958
H	1.458381	-2.939626	-1.778884
H	0.492294	-1.588916	2.814834
H	-0.998114	-2.343512	3.511986
H	-0.366894	-2.920026	1.954572
H	-0.676157	0.374418	4.489632
H	-0.551114	1.352519	2.928733
H	-1.820425	1.756069	4.224018
H	-0.216197	3.327392	1.138583
H	-7.176254	1.697555	-2.385349
C	4.781120	0.681223	-1.115546
C	3.942894	1.576673	1.490074
C	5.127952	-1.039638	1.174365
H	3.293439	2.352687	1.044561
H	3.527029	1.303115	2.476012
H	4.969070	1.970232	1.615589
H	4.876308	-0.158126	-1.827111
H	4.179505	1.480043	-1.588020
H	5.787146	1.072939	-0.874238
H	5.261431	-1.924215	0.526806
H	6.106322	-0.545696	1.324654
H	4.735723	-1.375358	2.150671
H	-1.955596	3.162739	-0.337204

TS_{4c2}

68

scf done: -2310.723312

O	3.155485	0.196833	-1.726900
C	4.228593	-0.488286	-1.265866
N	3.657236	-1.440422	-0.250063
C	2.496543	-1.033077	0.229822
N	1.960471	0.024913	-0.344075
C	5.304033	0.346825	-0.597659
C	1.821732	-1.718258	1.344375
C	5.024042	1.638114	-0.146487
C	6.011360	2.378584	0.502346
C	7.280879	1.835291	0.699775
C	7.565745	0.548086	0.242588
C	6.579011	-0.191594	-0.406476
C	1.853629	-3.117178	1.408322
C	1.173862	-3.775332	2.429550
C	0.481325	-3.042910	3.392132
C	0.460173	-1.647897	3.334644
C	1.121069	-0.982431	2.309019
C	0.724327	0.503608	-0.475736
C	0.573090	1.965377	-0.223249
C	-0.365437	-0.366103	-0.744744
C	-0.194594	2.482572	0.830238
C	-0.283751	3.859488	1.029722
C	0.398167	4.737037	0.186511
C	1.180693	4.231239	-0.850401
C	1.270476	2.854724	-1.052065
Au	-2.297264	0.315529	-0.187967
N	-0.160715	-1.573919	-1.301674
S	-1.314446	-2.865608	-1.006340

C	0.921085	-1.952402	-2.221606
O	-0.575336	-4.085612	-1.284600
O	-1.890301	-2.641794	0.309336
C	-2.539149	-2.626944	-2.265014
P	-4.413460	1.216230	0.373052
H	4.027978	2.063015	-0.318798
H	5.789163	3.393045	0.853203
H	8.056225	2.421181	1.206707
H	8.564991	0.121311	0.386042
H	6.803857	-1.201298	-0.778044
H	2.383778	-3.696912	0.643252
H	1.183251	-4.869471	2.468690
H	-0.073784	-1.073758	4.099164
H	1.115247	0.112556	2.263613
H	-0.712813	1.802652	1.520428
H	-0.879890	4.249774	1.862832
H	0.326576	5.818997	0.345416
H	1.725828	4.914153	-1.511908
H	1.888955	2.450690	-1.862979
H	1.499503	-1.056047	-2.490853
H	1.594930	-2.702591	-1.776109
H	0.479582	-2.388450	-3.135165
H	-3.262692	-3.450770	-2.143175
H	-3.028504	-1.649701	-2.114100
H	-2.045608	-2.690622	-3.248357
H	-0.049483	-3.563663	4.196517
H	4.684078	-1.120436	-2.063581
C	-5.741716	-0.008414	0.609260
C	-4.373262	2.166409	1.928089
C	-5.071997	2.383866	-0.861219
H	-5.199996	1.870555	-1.830564
H	-6.047435	2.785027	-0.527982
H	-4.360481	3.217486	-0.997950
H	-3.637878	2.986150	1.839346
H	-5.370642	2.591096	2.148477
H	-4.065228	1.506916	2.758906
H	-5.457999	-0.715738	1.408295
H	-6.685081	0.498165	0.886209
H	-5.894111	-0.577613	-0.324784
H	4.247298	-2.078009	0.285091

4c2'

54

scf done: -1965.693535

N	-1.080458	-0.158991	1.759148
C	-0.772250	-0.901766	0.768089
C	-0.259459	-0.270420	-0.481611
N	0.092226	1.822248	1.896138
C	-1.024709	1.238779	1.676079
C	-0.756319	-2.372818	0.852409
C	-1.294931	-3.006602	1.978859
C	-1.303352	-4.393755	2.059434
C	-0.771002	-5.160841	1.019931
C	-0.227078	-4.536816	-0.101553
C	-0.219386	-3.146173	-0.185653
Au	1.787018	0.231884	-0.265561
N	-1.019904	0.017855	-1.488993
C	-0.586668	0.810477	-2.644845
S	-2.807379	-0.438759	-1.602185
O	-3.170130	-0.992418	-0.314032

O	-3.445152	0.739420	-2.151075
C	-2.742996	-1.746422	-2.795458
C	-2.315383	1.900330	1.352575
C	-3.536877	1.305744	1.694425
C	-4.736480	1.938993	1.382115
C	-4.729474	3.161315	0.710228
C	-3.517629	3.752785	0.351672
C	-2.317087	3.126406	0.672213
P	4.062921	0.755997	0.098798
H	-1.711499	-2.390913	2.783523
H	-1.730587	-4.886048	2.939938
H	-0.778831	-6.254444	1.087169
H	0.199237	-5.135184	-0.913861
H	0.230255	-2.663926	-1.064953
H	0.502817	0.951977	-2.578627
H	-0.830911	0.288682	-3.584672
H	-1.100867	1.785301	-2.625602
H	-3.789082	-2.084399	-2.896077
H	-2.373483	-1.364566	-3.759266
H	-2.114348	-2.556307	-2.389145
H	-3.539032	0.341355	2.213166
H	-5.687137	1.472510	1.663627
H	-3.507987	4.705719	-0.188908
H	-1.368492	3.587283	0.368381
H	-0.024071	2.841646	1.878444
H	-5.675333	3.654409	0.458866
C	4.325962	1.535753	1.723006
C	5.169651	-0.689937	0.075447
C	4.782047	1.913562	-1.108924
H	5.839341	2.118693	-0.856985
H	4.727319	1.476707	-2.121492
H	4.215245	2.861016	-1.101678
H	6.212170	-0.375544	0.269693
H	4.855054	-1.412039	0.849135
H	5.115458	-1.183229	-0.910980
H	5.397491	1.762617	1.876211
H	3.739564	2.469834	1.783083
H	3.977284	0.854855	2.519500

TS_{4c1'}

68

scf done: -2310.732662

N	-1.593680	2.306218	0.278342
C	-2.227970	1.252616	-0.117647
C	0.223189	2.473457	0.781048
O	0.635798	1.395761	1.263954
N	-1.607876	0.049324	-0.216210
C	-3.614790	1.302459	-0.644729
C	-4.020599	0.406424	-1.640167
C	-5.313600	0.469737	-2.153860
C	-6.214034	1.415605	-1.665383
C	-5.819188	2.299736	-0.660129
C	-4.525374	2.245536	-0.152802
C	0.768765	2.986826	-0.526003
C	0.896961	2.149520	-1.640945
C	1.464053	2.627438	-2.817955
C	1.923094	3.946253	-2.890217
C	1.796690	4.785585	-1.785759
C	1.213406	4.306851	-0.610209

C	-1.060549	-0.829008	0.523944
C	-0.080948	-1.609548	-0.266537
C	-0.556415	-2.621407	-1.130775
C	-1.913897	-3.054345	-1.106159
C	-2.336927	-4.070407	-1.940580
C	-1.424667	-4.670564	-2.819825
C	-0.085832	-4.266210	-2.865328
C	0.347012	-3.255519	-2.026864
Au	1.861911	-0.888421	-0.044038
N	-1.202342	-1.146813	1.851190
C	-0.311771	-2.140312	2.449152
S	-2.255992	-0.315300	2.950698
O	-3.254431	0.362842	2.140892
O	-2.670933	-1.316649	3.918042
C	-1.171930	0.849869	3.719501
P	3.977109	0.089237	0.433926
H	-3.306789	-0.332144	-2.022600
H	-5.620370	-0.225979	-2.942771
H	-6.529495	3.032258	-0.261327
H	-4.231616	2.919518	0.660886
H	0.528316	1.116278	-1.582110
H	1.550199	1.969160	-3.690533
H	2.375581	4.320120	-3.815998
H	2.151541	5.821386	-1.838161
H	1.108919	4.967589	0.260899
H	-2.623470	-2.582656	-0.415896
H	-3.377557	-4.408038	-1.917038
H	-1.766749	-5.474319	-3.481314
H	0.610496	-4.749479	-3.557280
H	1.391458	-2.921400	-2.036542
H	0.677816	-1.702777	2.685925
H	-0.779379	-2.529937	3.365951
H	-0.177958	-2.992848	1.760337
H	-0.560451	0.297539	4.452318
H	-0.533124	1.295882	2.928422
H	-1.815855	1.586996	4.228207
H	-0.020672	3.321868	1.474735
H	-7.233175	1.460940	-2.065520
C	4.308999	1.606701	-0.518962
C	3.990384	0.642615	2.170248
C	5.475863	-0.928434	0.239394
H	3.109466	1.291052	2.330071
H	3.911334	-0.230859	2.841954
H	4.918608	1.199171	2.398503
H	4.385459	1.369852	-1.595172
H	3.470314	2.314164	-0.376166
H	5.252157	2.072489	-0.176362
H	5.589609	-1.227488	-0.817485
H	6.369449	-0.358217	0.555043
H	5.389710	-1.840634	0.855641
H	-2.101232	3.186474	0.161213

4c1'

54

scf done: -1965.682154

N	-1.957423	3.202235	1.558996
C	-1.192938	2.190459	1.709293
N	-1.654198	0.894207	1.958070
C	-1.664738	-0.051349	1.092648
C	-1.109104	0.187653	-0.251462

N	-2.026803	-1.323297	1.492870
S	-2.265793	-2.553455	0.351254
C	-2.206083	-1.621705	2.906766
O	-2.054372	-1.896237	-0.942013
O	-1.464949	-3.701120	0.736365
C	-3.980853	-2.958397	0.510681
C	0.285510	2.357004	1.686657
C	0.842161	3.430521	0.980540
C	2.223101	3.596090	0.927781
C	3.061730	2.706298	1.602532
C	2.514256	1.640651	2.317028
C	1.132633	1.458236	2.348360
C	-1.813536	1.032232	-1.147702
C	-1.132638	1.621243	-2.243157
C	-1.796074	2.474525	-3.108214
C	-3.155315	2.735865	-2.910312
C	-3.857309	2.152578	-1.847374
C	-3.194333	1.315658	-0.970079
Au	0.874694	-0.445241	-0.463299
P	3.109250	-1.196443	-0.738111
H	-3.162788	-1.218652	3.284568
H	-2.175055	-2.714072	3.048980
H	-1.377639	-1.170589	3.477839
H	-4.176892	-3.740462	-0.242242
H	-4.169079	-3.351581	1.522603
H	-4.576646	-2.055333	0.302569
H	0.169965	4.126300	0.466073
H	2.651191	4.432362	0.363586
H	3.168143	0.949090	2.861576
H	0.703249	0.619141	2.909837
H	-0.066554	1.402075	-2.380607
H	-1.263235	2.939453	-3.943283
H	-3.681289	3.407284	-3.598102
H	-4.922688	2.363491	-1.712791
H	-3.738811	0.854353	-0.136285
H	-2.941110	2.905313	1.591670
H	4.148499	2.849699	1.576030
C	3.326460	-2.361587	-2.121570
C	4.288513	0.152979	-1.064573
C	3.782445	-2.064124	0.715403
H	4.828002	-2.372927	0.528499
H	3.751071	-1.395270	1.593680
H	3.170855	-2.957663	0.931796
H	5.313828	-0.248313	-1.169837
H	4.004323	0.677786	-1.993637
H	4.259981	0.877288	-0.230190
H	2.692963	-3.251529	-1.959555
H	3.018639	-1.879065	-3.065951
H	4.384438	-2.674388	-2.198475

Benzaldehyde

14

scf done: -345.064466

C	-4.891355	2.255582	-0.002960
O	-4.438512	2.790682	-0.987300
H	-4.726602	2.694415	1.018897
C	-5.684566	1.012755	-0.006702
C	-5.965219	0.359396	-1.214169
C	-6.156946	0.486893	1.200591
C	-6.713188	-0.811225	-1.210153

H	-5.584200	0.790608	-2.147148
C	-6.907116	-0.686458	1.204480
H	-5.930758	1.007340	2.140470
C	-7.183432	-1.332788	-0.000642
H	-6.935763	-1.326698	-2.151131
H	-7.278395	-1.100264	2.148513
H	-7.773552	-2.256514	0.000533

TS_{5c1}

54

scf done: -1965.635043

N	-0.186507	-1.791298	1.178599
C	-0.488365	-2.120266	-0.063229
N	0.608583	-1.965285	-0.840664
C	1.350784	-1.243511	0.086651
C	1.081535	0.111532	-0.374511
Au	-0.703626	1.061287	0.198166
P	-2.837129	1.913016	0.753970
C	2.001635	0.666614	-1.338845
C	-1.795824	-2.512941	-0.598006
C	-2.795420	-3.003778	0.252101
C	-2.064190	-2.346736	-1.963104
C	-4.051566	-3.318411	-0.256897
H	-2.582148	-3.158324	1.316900
C	-3.323606	-2.656173	-2.468163
H	-1.274858	-1.960680	-2.618048
C	-4.317201	-3.140539	-1.615806
H	-4.828647	-3.709516	0.408834
H	-3.533586	-2.519740	-3.534696
N	2.494794	-1.686139	0.652833
H	-5.307598	-3.386594	-2.015199
H	-0.941859	-1.601098	1.847867
C	-4.038969	0.551381	0.917154
C	-2.942869	2.819321	2.330432
C	-3.563713	3.034565	-0.483423
H	-2.291603	3.710090	2.294737
H	-3.985790	3.136301	2.517651
H	-2.604395	2.169321	3.156408
H	-3.613558	2.524205	-1.461359
H	-4.582162	3.336366	-0.175415
H	-2.932381	3.934366	-0.588746
H	-3.713619	-0.130176	1.724260
H	-5.045122	0.945431	1.154788
H	-4.081724	-0.024663	-0.026076
C	1.909653	2.046045	-1.631753
C	2.801948	2.652014	-2.504434
C	3.770485	1.881481	-3.149145
C	3.852369	0.505351	-2.911222
C	2.990674	-0.096593	-2.008097
H	1.128884	2.639138	-1.139776
H	2.732695	3.726986	-2.699632
H	4.462443	2.353318	-3.855421
H	4.597949	-0.098572	-3.438826
H	3.057878	-1.177067	-1.841888
S	3.320752	-0.615107	1.744839
C	2.672979	-3.117529	0.876308
C	4.897241	-0.407150	0.973042
O	2.581243	0.640091	1.694957
O	3.480396	-1.343477	2.988430
H	3.746308	-3.365564	0.902843

H	2.190609	-3.422190	1.821190
H	2.205661	-3.644730	0.029142
H	5.480181	0.236914	1.653322
H	5.380309	-1.392497	0.872530
H	4.750791	0.081894	-0.004306

5c1

54

scf done: -1965.655971

C	0.234894	-0.379766	0.501802
N	1.522850	0.489529	-1.269589
C	2.762036	0.590186	-0.630776
N	2.392972	1.056093	0.526702
C	0.998223	0.844136	0.072068
C	0.828849	-1.422470	1.270298
C	1.902625	-1.226717	2.181944
C	2.422660	-2.295910	2.891719
C	1.908369	-3.582403	2.700582
C	0.844387	-3.802180	1.820992
C	0.293769	-2.732157	1.137284
N	0.174612	2.028897	0.085780
C	0.529519	3.140505	-0.782879
S	-0.460956	2.406623	1.593167
O	-1.700588	3.140840	1.393737
O	-0.464429	1.127838	2.318883
C	0.727512	3.468282	2.372263
C	4.072656	0.259994	-1.158147
C	4.248269	-0.011267	-2.521043
C	5.512832	-0.333755	-3.003838
C	6.598983	-0.385453	-2.129268
C	6.426041	-0.115266	-0.769639
C	5.165289	0.206405	-0.281496
H	2.286100	-0.216994	2.343576
H	3.234892	-2.132956	3.607610
H	2.333177	-4.424354	3.258753
H	0.438650	-4.809914	1.687113
H	-0.553298	-2.887467	0.458105
H	-0.213003	3.943873	-0.645036
H	1.545727	3.531640	-0.574731
H	0.480893	2.806425	-1.831510
H	0.376084	3.626578	3.405516
H	1.702208	2.951874	2.355378
H	0.766005	4.427605	1.831557
H	3.393712	0.045034	-3.206207
H	7.282320	-0.160239	-0.088073
H	5.007113	0.413234	0.783417
H	5.654425	-0.543106	-4.069510
Au	-1.697520	-0.485053	-0.303913
P	-3.931536	-0.460543	-1.113279
H	1.192522	-0.311371	-1.818937
H	7.593828	-0.640149	-2.511594
C	-4.094789	0.065266	-2.850760
C	-4.822468	-2.047733	-1.025953
C	-4.970681	0.708214	-0.176575
H	-3.552096	-0.637906	-3.506934
H	-5.160799	0.089958	-3.144733
H	-3.657907	1.071694	-2.976129
H	-4.845025	-2.405140	0.018542
H	-5.858866	-1.924277	-1.391995
H	-4.304952	-2.801823	-1.644704

H	-4.522184	1.716831	-0.216388
H	-5.992459	0.741475	-0.598638
H	-5.021370	0.392339	0.880544

TS_{5c2}

54

scf done: -1965.637822

N	-0.224900	1.478165	0.827330
C	-1.057207	1.926476	-0.122039
N	-1.556733	0.899900	-0.802737
C	-1.226592	-0.084885	0.089310
C	-0.286725	-1.084783	-0.463382
Au	1.730493	-0.514739	-0.077619
P	3.945258	0.186040	0.328055
N	-0.651295	-2.116221	-1.159575
C	0.291902	-3.028815	-1.817572
S	-2.399819	-2.597791	-1.499585
H	0.037557	-4.074345	-1.577301
H	0.237539	-2.888134	-2.908771
H	1.304569	-2.799561	-1.452594
O	-3.203052	-1.409706	-1.312104
O	-2.331916	-3.288895	-2.770707
C	-2.691288	-3.746473	-0.183836
H	-3.709861	-4.132489	-0.363292
H	-1.956643	-4.565202	-0.242872
H	-2.640244	-3.203221	0.775562
C	-1.386383	3.328835	-0.411165
C	-0.579493	4.366441	0.072641
C	-2.522896	3.632951	-1.171588
C	-0.911941	5.692016	-0.190815
H	0.327132	4.131955	0.643814
C	-2.852474	4.958783	-1.435863
H	-3.146380	2.812354	-1.545196
C	-2.048917	5.988562	-0.943689
H	-0.276374	6.500510	0.187069
H	-3.744116	5.193300	-2.027879
C	-1.999574	-0.441157	1.297584
C	-3.299422	0.050961	1.457331
C	-1.464543	-1.322221	2.248332
C	-4.053450	-0.332064	2.562161
H	-3.717490	0.714194	0.691346
C	-2.223247	-1.700955	3.351745
H	-0.437258	-1.696126	2.135479
C	-3.520143	-1.208293	3.508581
H	-5.073902	0.048392	2.680806
H	-1.798829	-2.382270	4.097174
H	-4.119823	-1.511173	4.374044
H	-2.309534	7.032623	-1.151526
H	-0.081360	2.070296	1.656502
C	4.052617	1.996680	0.498382
C	4.660022	-0.476937	1.866313
C	5.144348	-0.238372	-0.974470
H	4.714325	-1.578341	1.808867
H	5.675773	-0.068045	2.021478
H	4.020182	-0.199685	2.722404
H	4.822509	0.204020	-1.933578
H	6.146780	0.148174	-0.711389
H	5.195240	-1.334966	-1.091948
H	3.400158	2.330053	1.325322
H	5.094670	2.304609	0.704958

H	3.707340	2.476892	-0.434493
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5c2

54

scf done: -1965.667921

N	0.847902	-1.120576	0.755988
C	2.010246	-1.364465	0.029082
N	2.275664	-0.176622	-0.433310
C	1.145729	0.307816	0.398332
C	0.043169	0.868060	-0.471160
Au	-1.849642	-0.041736	-0.192946
P	-3.944189	-1.079105	0.191919
N	0.272210	1.796594	-1.351351
C	-0.733659	2.219017	-2.335396
S	1.893909	2.638303	-1.659542
H	-1.166725	3.194462	-2.057571
H	-0.264365	2.278239	-3.331840
H	-1.532877	1.463280	-2.367549
O	2.662147	2.601632	-0.435269
O	2.367242	2.076516	-2.908422
C	1.359027	4.314946	-1.897297
H	2.305988	4.879426	-1.955716
H	0.794139	4.427916	-2.833504
H	0.787369	4.632276	-1.010162
C	2.701807	-2.628161	-0.169615
C	2.160080	-3.821782	0.322286
C	3.922090	-2.640965	-0.858812
C	2.837687	-5.021999	0.127695
H	1.198856	-3.809222	0.850135
C	4.593436	-3.842253	-1.053192
H	4.331464	-1.695673	-1.233167
C	4.052322	-5.031670	-0.558836
H	2.415354	-5.957240	0.510983
H	5.547528	-3.855481	-1.591313
C	1.463611	1.132359	1.621930
C	2.722322	1.033202	2.222027
C	0.484034	1.937534	2.209384
C	2.994383	1.729809	3.394698
H	3.499553	0.423209	1.747372
C	0.761629	2.641305	3.382191
H	-0.513341	2.020696	1.756724
C	2.015784	2.537679	3.977926
H	3.986025	1.650739	3.854444
H	-0.012894	3.272442	3.832237
H	2.235189	3.089462	4.898933
H	4.584690	-5.977370	-0.711145
H	0.763424	-1.391880	1.740879
C	-3.804217	-2.796148	0.784990
C	-4.966031	-0.234884	1.442110
C	-5.008868	-1.183307	-1.282845
H	-5.172221	0.800340	1.117673
H	-5.923172	-0.772022	1.579249
H	-4.425923	-0.201239	2.404599
H	-4.492747	-1.749706	-2.077828
H	-5.958891	-1.691002	-1.031328
H	-5.226707	-0.168123	-1.658426
H	-3.240456	-2.817801	1.734198
H	-4.809120	-3.229017	0.946537
H	-3.261157	-3.403358	0.039465

TS_{6c1A}

54

scf done: -1965.644633

H	0.856304	0.780142	1.465159
N	1.238698	0.256680	0.671642
C	2.576368	0.228870	0.192722
N	2.375893	0.473143	-1.063456
C	0.936224	0.612041	-0.733508
C	0.108899	-0.607813	-0.605649
Au	-1.853362	-0.366969	0.121826
P	-4.075350	-0.096452	0.907579
C	0.606833	-1.898328	-1.040090
C	3.764838	-0.102577	0.946578
C	3.680928	-0.388298	2.315808
C	5.004661	-0.136569	0.290954
C	4.833359	-0.710114	3.025077
H	2.710601	-0.361821	2.825272
C	6.151314	-0.456932	1.005688
H	5.050996	0.088473	-0.780547
C	6.065192	-0.743427	2.370984
H	4.771863	-0.935921	4.094796
H	7.121822	-0.486195	0.499087
H	6.971982	-0.996021	2.931779
N	0.273401	1.811187	-1.093966
S	0.893672	3.293080	-0.549045
C	-0.333878	1.785068	-2.421901
H	0.413962	1.597222	-3.219374
H	-1.100872	0.988607	-2.448409
H	-0.836299	2.747808	-2.605546
O	-0.164310	4.268726	-0.752359
O	1.414343	3.032777	0.788939
C	2.243824	3.690283	-1.629237
H	2.671730	4.635264	-1.254784
H	2.981684	2.872618	-1.588447
H	1.849630	3.828558	-2.649398
C	0.180681	-3.065803	-0.372552
C	0.610428	-4.315352	-0.791242
C	1.431648	-4.426371	-1.918149
C	1.831063	-3.286190	-2.613036
C	1.440166	-2.025916	-2.170660
H	-0.484516	-2.969106	0.494651
H	0.292206	-5.213772	-0.251946
H	1.752696	-5.415754	-2.262881
H	2.459417	-3.377952	-3.505344
H	1.758072	-1.133069	-2.717141
C	-5.072858	-1.621432	0.881037
C	-4.185237	0.495216	2.628010
C	-5.047706	1.106529	-0.055944
H	-6.094228	-1.416296	1.252780
H	-5.131748	-2.010190	-0.150779
H	-4.600056	-2.388745	1.519057
H	-6.066984	1.197433	0.363523
H	-4.552335	2.092927	-0.028549
H	-5.113892	0.775438	-1.107368
H	-5.244682	0.601659	2.927519
H	-3.686463	-0.222779	3.302690
H	-3.680510	1.473117	2.719462

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54

scf done: -1965.653913

N	-1.428449	0.214271	-0.913310
C	-2.715616	0.743391	-0.467407
N	-2.355817	1.555479	0.458449
C	-0.941893	1.277716	0.187218
C	-0.545096	-0.133107	0.304267
Au	1.425728	-0.699919	-0.288969
P	3.680190	-1.102218	-0.852922
C	-1.190280	-0.997930	1.321011
C	-4.005765	0.315220	-0.947840
C	-4.112822	-0.686287	-1.923607
C	-5.159952	0.911749	-0.414100
C	-5.369727	-1.094895	-2.355706
H	-3.211650	-1.150599	-2.341476
C	-6.410237	0.500155	-0.852908
H	-5.055490	1.694021	0.345841
C	-6.514461	-0.502224	-1.821816
H	-5.458592	-1.879257	-3.114375
H	-7.314012	0.959827	-0.439475
N	-0.107646	2.325497	-0.099054
H	-7.503583	-0.824112	-2.165983
H	-1.077330	0.122407	-1.871705
C	4.154620	-0.356218	-2.447123
C	4.777720	-0.297093	0.359818
C	4.256710	-2.827807	-0.946682
H	4.632314	-0.754651	1.354490
H	5.837147	-0.400207	0.058797
H	4.511570	0.773791	0.424257
H	3.693827	-3.368157	-1.727877
H	5.335897	-2.857732	-1.187139
H	4.084435	-3.330620	0.021205
H	3.917224	0.722876	-2.423723
H	5.237592	-0.489122	-2.629091
H	3.585688	-0.825281	-3.269168
S	1.357714	2.548782	0.770445
C	-0.575532	3.420569	-0.942356
H	0.295642	3.929616	-1.387387
H	-1.169409	3.003658	-1.773258
H	-1.197346	4.144826	-0.384792
C	1.095633	4.118016	1.552746
O	1.404727	1.524908	1.805627
O	2.437029	2.681569	-0.198012
H	1.984403	4.274252	2.187168
H	1.029128	4.914977	0.796619
H	0.184441	4.056850	2.169029
C	-1.186355	-0.605388	2.663996
C	-1.745548	-1.433624	3.635383
C	-2.321307	-2.651446	3.274007
C	-2.330725	-3.042660	1.934265
C	-1.761653	-2.223800	0.962195
H	-0.732430	0.354645	2.941253
H	-1.738821	-1.119214	4.685297
H	-2.765900	-3.298252	4.038737
H	-2.783020	-3.997716	1.643633
H	-1.757506	-2.535007	-0.091282

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54

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scf done: -1965.654478
N      -1.343208      0.222464      -1.315630
C      -2.574944      0.562282      -0.911264
N      -2.284019      1.612405      -0.108299
C      -0.860657      1.208271      -0.307476
C      -0.365236      0.035676      0.433665
Au      1.540090      -0.673021      -0.061952
P      3.749053      -1.354332      -0.580460
C      -1.179529      -0.585604      1.461133
C      -3.837073      -0.076311      -1.189342
C      -3.837344      -1.317143      -1.845756
C      -5.044315      0.514512      -0.786663
C      -5.041882      -1.962674      -2.092984
H      -2.882649      -1.763323      -2.146655
C      -6.245239      -0.136585      -1.039454
H      -5.041114      1.491180      -0.288415
C      -6.242189      -1.372602      -1.690050
H      -5.050278      -2.932659      -2.600931
H      -7.191378      0.319888      -0.730854
N      0.056990      2.198295      -0.703472
H      -7.191115      -1.883978      -1.886340
C      4.102768      -1.416520      -2.367492
C      4.992211      -0.207060      0.098629
C      4.244363      -2.992822      0.044767
H      4.919683      -0.196883      1.200664
H      6.011368      -0.518141      -0.198381
H      4.794012      0.814313      -0.272324
H      3.589223      -3.771274      -0.384354
H      5.294062      -3.205361      -0.231951
H      4.144817      -3.016722      1.144211
H      3.919670      -0.423796      -2.815223
H      5.155329      -1.708313      -2.541499
H      3.435389      -2.149201      -2.854582
H      -2.776628      1.918604      0.733350
S      1.011686      2.905370      0.493652
C      -0.178355      2.935794      -1.934279
H      0.752341      3.446382      -2.232536
H      -0.439289      2.212729      -2.724919
H      -0.998738      3.674221      -1.835549
C      0.243283      4.471236      0.816624
O      0.844909      2.066553      1.681779
O      2.332453      3.142714      -0.067842
H      0.827349      4.940236      1.625999
H      0.282746      5.095111      -0.090450
H      -0.795314      4.291144      1.141377
C      -1.794480      0.171676      2.477094
C      -2.550966      -0.458938      3.460544
C      -2.736562      -1.840096      3.421610
C      -2.130296      -2.602498      2.419131
C      -1.332096      -1.985991      1.465775
H      -1.612184      1.251201      2.535496
H      -3.001290      0.134776      4.263309
H      -3.347044      -2.331016      4.187568
H      -2.269068      -3.688624      2.395132
H      -0.835766      -2.576727      0.685576

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54

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scf done: -1965.662751
N      -1.269925      0.459449      -1.185164

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C	-2.525313	0.967302	-0.828276
N	-2.105667	1.972142	-0.086894
C	-0.723172	1.460807	-0.221710
C	-0.594309	0.026865	0.146539
Au	1.323452	-0.820559	-0.143117
P	3.588277	-1.454121	-0.407537
C	-1.480125	-0.572324	1.172751
C	-3.811384	0.400214	-1.083730
C	-3.916674	-0.631469	-2.032817
C	-4.934070	0.808005	-0.341367
C	-5.141198	-1.252509	-2.233633
H	-3.029285	-0.932101	-2.601097
C	-6.151438	0.175864	-0.545231
H	-4.844791	1.600497	0.410765
C	-6.252863	-0.850653	-1.489193
H	-5.234983	-2.055782	-2.971303
H	-7.029025	0.476783	0.035578
N	0.304819	2.348864	-0.526707
H	-7.217006	-1.346680	-1.645957
C	4.360000	-0.581479	-1.810432
C	4.576843	-0.931620	1.033178
C	4.015431	-3.208921	-0.656090
H	4.235378	-1.466867	1.936810
H	5.650380	-1.139845	0.866525
H	4.428806	0.152538	1.187961
H	3.532296	-3.584479	-1.575256
H	5.111880	-3.324876	-0.746595
H	3.655464	-3.806924	0.199474
H	4.205739	0.504434	-1.674257
H	5.443305	-0.800374	-1.858853
H	3.881303	-0.893123	-2.755820
H	-2.565450	2.611747	0.563394
S	1.589183	2.526675	0.569253
C	0.539857	2.703358	-1.921705
H	1.134755	3.628830	-1.988000
H	1.067400	1.893274	-2.461324
H	-0.434159	2.891880	-2.404181
C	1.597171	4.271891	0.878805
O	1.196698	1.848582	1.799747
O	2.836567	2.183941	-0.108558
H	2.433207	4.450851	1.575437
H	1.766805	4.819550	-0.061604
H	0.636989	4.547876	1.341385
C	-1.704154	0.065025	2.399239
C	-2.565788	-0.502415	3.337743
C	-3.215458	-1.704310	3.060119
C	-2.985227	-2.351293	1.844103
C	-2.115642	-1.794259	0.911371
H	-1.190777	1.010901	2.613787
H	-2.736296	0.005739	4.293883
H	-3.899090	-2.143009	3.795737
H	-3.485860	-3.300888	1.622753
H	-1.926384	-2.302629	-0.044097

TS_{6c2A}

54

scf done: -1965.646778

N	-1.259882	0.468925	-0.968054
C	-2.607954	0.710211	-0.520717
N	-2.370853	1.203565	0.643626

C	-0.923530	1.110997	0.363573
C	-0.386937	-0.261902	0.266139
Au	1.625849	-0.539347	-0.333713
P	3.909208	-0.789085	-0.927502
N	-1.102296	-1.282582	0.874791
C	-1.141485	-2.597482	0.255829
S	-1.674085	-1.118381	2.474378
H	-0.197696	-3.160811	0.402274
H	-1.989174	-3.171545	0.667380
H	-1.325187	-2.476472	-0.826557
O	-1.168098	0.157041	2.965999
O	-3.093455	-1.433709	2.513094
C	-0.785620	-2.407185	3.313222
H	-1.046882	-2.295524	4.379008
H	-1.105752	-3.396187	2.950854
H	0.293896	-2.243353	3.158940
C	-3.828594	0.307245	-1.179690
C	-3.808792	-0.254031	-2.463379
C	-5.042129	0.465091	-0.492525
C	-5.001359	-0.652739	-3.058343
H	-2.860505	-0.380098	-2.999240
C	-6.227968	0.065905	-1.093819
H	-5.032066	0.892118	0.516554
C	-6.207361	-0.490789	-2.375593
H	-4.991341	-1.091989	-4.061349
H	-7.177843	0.183889	-0.561770
C	-0.080087	2.322186	0.486195
C	-0.275812	3.413019	-0.363745
C	0.885006	2.381272	1.495670
C	0.510566	4.553403	-0.219903
H	-1.043819	3.368279	-1.146739
C	1.662030	3.527851	1.643025
H	1.009233	1.526812	2.171729
C	1.479159	4.610706	0.782752
H	0.364311	5.404906	-0.893322
H	2.415991	3.576625	2.436386
H	2.095224	5.509751	0.896322
H	-7.145128	-0.804920	-2.847190
H	-0.806476	0.643948	-1.870687
C	4.729503	0.805999	-1.252246
C	4.943612	-1.584721	0.344390
C	4.200835	-1.774024	-2.433034
H	4.571712	-2.605131	0.543621
H	5.993484	-1.639473	0.000260
H	4.897083	-1.003330	1.282064
H	3.675599	-1.314147	-3.288614
H	5.283640	-1.823903	-2.652789
H	3.811034	-2.797153	-2.289483
H	4.659231	1.449068	-0.356855
H	5.794249	0.646481	-1.505491
H	4.227507	1.318910	-2.091625

6c2A

54

scf done: -1965.652350

N	-1.302395	0.418802	-0.939730
C	-2.644962	0.656181	-0.458936
N	-2.389522	1.121211	0.712225
C	-0.947677	1.056642	0.407508
C	-0.410829	-0.300838	0.226088

Au	1.611702	-0.525262	-0.380602
P	3.911668	-0.690702	-0.928576
N	-1.092672	-1.364514	0.836109
C	-0.965973	-2.680930	0.226898
S	-1.308303	-1.309693	2.526640
H	0.065057	-3.078569	0.304399
H	-1.660042	-3.387193	0.710374
H	-1.248529	-2.598800	-0.837937
O	-0.780354	-2.560995	3.053197
O	-0.759931	-0.035315	2.976608
C	-3.066301	-1.314091	2.748225
H	-3.240847	-1.386716	3.835209
H	-3.465201	-0.372643	2.339163
H	-3.480856	-2.196784	2.233386
C	-3.871603	0.284359	-1.122657
C	-3.842549	-0.402622	-2.344010
C	-5.097254	0.600422	-0.515277
C	-5.036157	-0.778898	-2.950810
H	-2.884328	-0.650642	-2.815421
C	-6.284036	0.223485	-1.128862
H	-5.101787	1.144756	0.436161
C	-6.253081	-0.465286	-2.344804
H	-5.018354	-1.319324	-3.902897
H	-7.243364	0.467178	-0.660454
C	-0.135354	2.288787	0.524860
C	-0.518647	3.442625	-0.165097
C	0.984381	2.312021	1.362228
C	0.233982	4.607006	-0.044008
H	-1.408925	3.427955	-0.806500
C	1.728397	3.483157	1.489625
H	1.253810	1.413210	1.929383
C	1.358376	4.626940	0.782448
H	-0.060789	5.506768	-0.594797
H	2.602444	3.502940	2.149944
H	1.948088	5.545285	0.880370
H	-7.191954	-0.760038	-2.826429
H	-0.876712	0.626649	-1.849655
C	4.320993	-0.140533	-2.617720
C	4.941364	0.351028	0.157393
C	4.635722	-2.357636	-0.798877
H	4.817141	0.028499	1.206538
H	6.008054	0.273979	-0.124624
H	4.616009	1.403562	0.074099
H	4.118340	-3.044015	-1.491977
H	5.712348	-2.327579	-1.051081
H	4.512542	-2.738747	0.230056
H	3.992242	0.904425	-2.758085
H	5.411893	-0.205836	-2.788558
H	3.798757	-0.775892	-3.354685

TS_{6c2B}

54

scf done: -1965.653285

Au	1.427495	-0.520671	-0.130433
P	3.621150	-1.122272	-0.765502
C	4.307356	-2.569196	0.105029
C	-0.462417	0.158188	0.540660
C	-0.716786	1.612542	0.429380
C	0.354330	2.639819	0.428436
C	0.338274	3.651459	-0.534740

C	1.330528	4.627957	-0.532249
C	2.336004	4.598660	0.435641
C	2.349250	3.593411	1.402784
C	1.360038	2.612061	1.398737
H	1.368493	1.812333	2.151247
H	3.137301	3.571221	2.163613
H	3.117776	5.366599	0.434884
H	1.323145	5.416603	-1.292712
H	-0.452597	3.660300	-1.295143
N	-2.101540	2.013690	0.725528
C	-2.476246	1.309397	-0.342977
N	-1.243443	0.966873	-0.811052
C	-3.758282	0.840931	-0.793383
C	-3.783618	-0.096938	-1.839367
C	-4.995825	-0.644388	-2.239214
C	-6.177318	-0.253465	-1.604839
C	-6.155264	0.683448	-0.568006
C	-4.947845	1.233018	-0.158181
H	-4.926210	1.967218	0.655591
H	-7.087406	0.982898	-0.078146
H	-7.132312	-0.686199	-1.922769
H	-5.024731	-1.380374	-3.049235
H	-2.841011	-0.398465	-2.310405
N	-1.295812	-0.600462	1.337317
C	-1.822198	-0.181018	2.637590
H	-1.284874	0.721331	2.973604
H	-2.909121	0.024739	2.612141
H	-1.617938	-0.969957	3.383552
S	-1.330936	-2.294150	1.031186
O	-0.965232	-2.480806	-0.366240
O	-0.589181	-2.983187	2.080278
C	-3.059206	-2.648670	1.212593
H	-3.624222	-2.025614	0.498506
H	-3.377411	-2.476628	2.252546
H	-3.162716	-3.717707	0.960868
H	-2.573079	2.410917	1.537127
C	3.845804	-1.506499	-2.533151
C	4.809691	0.221437	-0.434680
H	5.343944	-2.762194	-0.229456
H	4.302245	-2.385538	1.193814
H	3.685076	-3.457439	-0.102841
H	3.217607	-2.371709	-2.808930
H	3.537511	-0.640335	-3.144696
H	4.906318	-1.743338	-2.740500
H	5.832633	-0.077801	-0.731057
H	4.513260	1.122444	-1.001327
H	4.797201	0.468514	0.642248

6c2B

54

scf done: -1965.661316

N	-1.315040	0.552075	-1.013370
C	-2.620830	0.795224	-0.569676
N	-2.322933	1.556285	0.461496
C	-0.899777	1.310303	0.211506
C	-0.556744	-0.124761	0.182007
Au	1.442374	-0.599944	-0.333869
P	3.710527	-1.034396	-0.892486
N	-1.372175	-1.020537	0.941236
C	-1.474872	-2.375763	0.417262

S	-1.345594	-0.858548	2.623715
H	-0.486471	-2.879674	0.365608
H	-2.167010	-2.959146	1.044833
H	-1.892916	-2.326895	-0.604013
O	-1.282019	0.573708	2.907540
O	-2.445573	-1.659496	3.138276
C	0.179872	-1.594603	3.158019
H	0.225925	-1.460232	4.251678
H	0.165113	-2.667812	2.905842
H	1.020319	-1.076654	2.663488
C	-3.846276	0.273007	-1.087363
C	-3.808844	-0.483928	-2.271761
C	-5.063097	0.493864	-0.418205
C	-4.983732	-1.026255	-2.773964
H	-2.852465	-0.629250	-2.786855
C	-6.231338	-0.051219	-0.928977
H	-5.085648	1.084362	0.504704
C	-6.189487	-0.809663	-2.103059
H	-4.965981	-1.617282	-3.695126
H	-7.182810	0.110371	-0.412606
C	0.073233	2.425323	0.221195
C	0.088058	3.356033	-0.820120
C	0.969362	2.547693	1.287758
C	1.007825	4.402296	-0.800963
H	-0.617877	3.246408	-1.652936
C	1.884554	3.597153	1.305781
H	0.935625	1.815364	2.103507
C	1.906105	4.521482	0.260170
H	1.026494	5.128535	-1.621141
H	2.587378	3.695023	2.140616
H	2.630515	5.343762	0.272279
H	-7.115544	-1.237484	-2.502618
C	4.051184	-1.002683	-2.683923
C	4.861346	0.193342	-0.187861
C	4.368268	-2.641635	-0.336555
H	4.771649	0.198598	0.913164
H	5.904366	-0.047351	-0.467334
H	4.604827	1.199949	-0.563986
H	3.786347	-3.462028	-0.792382
H	5.430319	-2.740665	-0.629786
H	4.285188	-2.720496	0.761713
H	3.765858	-0.019903	-3.098987
H	5.125346	-1.183082	-2.876648
H	3.454588	-1.782484	-3.189631
H	-2.826183	1.876578	1.290459

TS_{6c1A'}

54

scf done: -1965.653908

N	-1.434303	0.225377	-0.903922
C	-2.716195	0.755749	-0.447338
N	-2.352488	1.548722	0.493520
C	-0.939891	1.271154	0.219513
C	-0.550591	-0.144193	0.304822
Au	1.417214	-0.706461	-0.302874
P	3.677630	-1.072426	-0.870284
C	-1.195692	-1.025293	1.307703
C	-4.009513	0.347025	-0.936404
C	-4.124136	-0.638070	-1.927968
C	-5.159128	0.946233	-0.395832

C	-5.383942	-1.027382	-2.369313
H	-3.226540	-1.104965	-2.350712
C	-6.412348	0.553868	-0.843778
H	-5.048812	1.715577	0.376372
C	-6.524073	-0.431860	-1.828797
H	-5.478651	-1.798755	-3.140493
H	-7.312578	1.015843	-0.425205
N	-0.105017	2.322109	-0.047844
H	-7.515461	-0.738286	-2.180467
H	-1.086084	0.148041	-1.864449
C	4.162450	-0.205031	-2.398651
C	4.754852	-0.350724	0.411478
C	4.268850	-2.781897	-1.086335
H	4.602553	-0.881026	1.368315
H	5.818362	-0.422704	0.116195
H	4.477694	0.710433	0.550243
H	3.719295	-3.265908	-1.912674
H	5.350963	-2.785908	-1.315246
H	4.089829	-3.357200	-0.161113
H	3.909591	0.865821	-2.296628
H	5.249214	-0.310263	-2.576227
H	3.609606	-0.618845	-3.260372
S	1.379972	2.511882	0.797988
C	-0.571592	3.431210	-0.873697
H	0.299799	3.945612	-1.311963
H	-1.166334	3.028212	-1.710985
H	-1.191617	4.147434	-0.303937
C	1.160308	4.077257	1.600024
O	1.426409	1.478057	1.823216
O	2.446234	2.636028	-0.186364
H	2.070206	4.214971	2.208313
H	1.081762	4.883277	0.854733
H	0.268625	4.021475	2.244403
C	-1.179402	-0.660458	2.658381
C	-1.738386	-1.504071	3.616517
C	-2.325775	-2.709978	3.234340
C	-2.347241	-3.073582	1.886978
C	-1.778920	-2.239084	0.927831
H	-0.716076	0.290284	2.951952
H	-1.722195	-1.211291	4.672564
H	-2.770040	-3.369015	3.988749
H	-2.808715	-4.019099	1.580020
H	-1.784573	-2.528432	-0.131860

TS_{6c1B'}

54

scf done: -1965.647745

Au	-1.783728	-0.206164	0.159415
P	-3.975329	0.007329	1.033040
C	-4.468170	-1.348733	2.147629
C	0.204993	-0.489366	-0.558591
C	0.987577	0.591638	-1.108726
N	2.392948	0.251644	-1.219270
C	2.477702	-0.094031	0.070596
N	1.206148	-0.076212	0.534997
N	0.579730	1.846166	-1.418736
C	3.653740	-0.368409	0.852183
C	4.932446	-0.294562	0.274987
C	6.050698	-0.585992	1.043967
C	5.897081	-0.943825	2.385593

C	4.627881	-1.011238	2.966022
C	3.504842	-0.720894	2.204329
H	2.499772	-0.758001	2.639149
H	4.519884	-1.288226	4.019670
H	6.782371	-1.170189	2.990073
H	7.049505	-0.534105	0.599114
H	5.052993	-0.017621	-0.778359
C	0.410586	-1.879036	-1.061548
H	3.074107	0.708099	-1.820665
S	1.442876	3.237676	-0.814684
C	-0.763775	2.117691	-1.931490
C	0.775628	3.380319	0.821835
O	2.848085	2.875377	-0.727065
O	1.001655	4.351698	-1.630294
H	-1.460013	2.452017	-1.138869
H	-0.686829	2.894878	-2.708129
H	-1.155985	1.195615	-2.387498
H	1.281766	4.245204	1.283346
H	-0.309259	3.561915	0.749781
H	0.997109	2.447631	1.367780
C	0.148599	-2.168880	-2.406572
C	0.290989	-3.467795	-2.887942
C	0.691637	-4.494722	-2.031486
C	0.951680	-4.210470	-0.691355
C	0.814187	-2.910018	-0.207552
H	-0.167736	-1.362196	-3.082709
H	0.092286	-3.679415	-3.944997
H	0.803388	-5.516701	-2.410836
H	1.268685	-5.010387	-0.012144
H	1.018673	-2.686947	0.847788
C	-4.236689	1.521436	2.016061
C	-5.289696	0.059921	-0.229610
H	-5.499746	-1.190219	2.513903
H	-4.416041	-2.311088	1.608430
H	-3.777716	-1.391678	3.008498
H	-5.276610	1.562834	2.390939
H	-3.539681	1.534775	2.872560
H	-4.040818	2.410214	1.390005
H	-6.279860	0.164068	0.252440
H	-5.122186	0.916200	-0.906573
H	-5.270987	-0.868415	-0.827207

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54

scf done: -1965.648502

H	-1.050671	0.341087	-1.882513
N	-1.392318	0.132882	-0.941629
C	-2.696014	0.409236	-0.390674
N	-2.471494	0.913116	0.769087
C	-1.047152	0.981557	0.551112
C	-0.440019	-0.298678	0.178769
Au	1.595039	-0.431178	-0.444612
P	3.897657	-0.517665	-1.001949
N	-0.974324	-1.446948	0.866039
C	-3.942217	0.069248	-1.038533
C	-3.950938	-0.654890	-2.239490
C	-5.150931	0.458648	-0.438938
C	-5.162847	-0.995699	-2.830570
H	-3.007143	-0.962955	-2.704496
C	-6.356189	0.117057	-1.036086

H	-5.124639	1.031756	0.494550
C	-6.361632	-0.609100	-2.230677
H	-5.173592	-1.565247	-3.765636
H	-7.301554	0.418402	-0.572830
H	-7.314953	-0.874654	-2.700879
C	-0.395385	2.287897	0.593756
C	-0.812900	-2.729074	0.204724
S	-0.807975	-1.421308	2.544442
H	-1.351418	-3.514300	0.760670
H	-1.263783	-2.657792	-0.801729
H	0.252823	-3.021401	0.104704
C	-2.456640	-1.724805	3.115406
O	0.045998	-2.531596	2.950738
O	-0.438131	-0.050455	2.900254
H	-2.413876	-1.733862	4.217468
H	-3.093317	-0.904431	2.746127
H	-2.794021	-2.703584	2.737402
C	-1.134156	3.438295	0.272906
C	-0.532295	4.689377	0.319840
C	0.799755	4.806998	0.721556
C	1.529514	3.673051	1.079592
C	0.938739	2.415961	1.013092
H	-2.183970	3.344622	-0.025900
H	-1.107257	5.581689	0.051098
H	1.269858	5.795594	0.768539
H	2.565744	3.769499	1.421200
H	1.500541	1.527047	1.322564
C	4.277571	-0.393661	-2.780578
C	4.808801	0.866341	-0.239559
C	4.778510	-2.012910	-0.446018
H	5.372100	-0.400225	-2.940126
H	3.826588	-1.245570	-3.319311
H	3.855472	0.542395	-3.187066
H	5.882096	0.822122	-0.503688
H	4.384477	1.824551	-0.590089
H	4.700651	0.818152	0.859132
H	5.851627	-1.943987	-0.704838
H	4.672660	-2.121087	0.647765
H	4.342798	-2.904860	-0.929790

TS_{6c2B'}

54

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Au	1.515374	-0.470120	-0.438972
P	3.782725	-0.607869	-1.126082
C	4.730630	-2.002796	-0.432776
C	-0.494408	-0.254610	0.233774
C	-1.025748	1.052354	0.542098
N	-2.469314	1.051478	0.638808
C	-2.667799	0.298404	-0.454874
N	-1.460034	-0.031412	-0.940292
C	-0.357221	2.332759	0.491581
C	-1.071089	3.483999	0.107865
C	-0.438947	4.719215	0.071928
C	0.901362	4.825527	0.448841
C	1.610672	3.696553	0.866239
C	0.991000	2.454973	0.882876
H	1.534170	1.572182	1.239469
H	2.653015	3.790050	1.188875
H	1.396848	5.802554	0.428479

H	-0.993214	5.607901	-0.247020
H	-2.123668	3.393744	-0.180599
C	-3.933156	-0.042107	-1.059947
C	-5.137104	0.480420	-0.559697
C	-6.342703	0.106765	-1.138468
C	-6.350191	-0.781080	-2.216932
C	-5.154858	-1.296815	-2.723576
C	-3.945545	-0.927200	-2.150595
H	-2.995174	-1.316929	-2.532579
H	-5.171109	-1.988545	-3.572097
H	-7.303140	-1.071617	-2.672952
H	-7.283810	0.512122	-0.752987
H	-5.128651	1.190308	0.275340
N	-1.028222	-1.330911	1.072791
C	-0.862011	-2.662168	0.511714
H	0.205179	-2.947776	0.405886
H	-1.382675	-3.410910	1.132481
H	-1.334918	-2.666643	-0.486627
S	-0.595284	-1.166857	2.697853
O	0.613146	-1.928121	3.004508
O	-0.621064	0.274794	2.969250
C	-1.962367	-1.916738	3.540704
H	-1.754166	-1.792909	4.616570
H	-2.014787	-2.987783	3.290198
H	-2.884394	-1.387362	3.253812
H	-3.014530	1.165066	1.494541
C	4.066581	-0.711063	-2.924676
C	4.712674	0.874795	-0.607315
H	5.786204	-1.952801	-0.759524
H	4.687526	-1.968285	0.670278
H	4.289283	-2.957336	-0.769597
H	5.769473	0.807747	-0.927882
H	4.251062	1.774639	-1.052864
H	4.669907	0.970229	0.492776
H	5.150908	-0.712219	-3.144034
H	3.612959	-1.635908	-3.322663
H	3.594488	0.153092	-3.424677

6c1

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C	0.397711	0.987073	0.502809
N	1.714554	0.652272	0.944462
C	2.516276	0.503585	-0.112596
N	1.871530	0.764949	-1.254320
C	0.620370	1.106004	-0.917140
C	-0.347266	1.971463	1.346598
C	-0.273298	3.332589	1.023642
C	-0.913726	4.285691	1.813584
C	-1.619036	3.890216	2.949618
C	-1.676281	2.539903	3.293052
C	-1.047151	1.586864	2.494856
N	-0.223055	1.557288	-1.916596
C	0.325555	1.630412	-3.273463
S	-1.941455	1.523898	-1.844821
O	-2.391570	0.807139	-3.027828
O	-2.339526	1.061813	-0.522077
C	-2.373016	3.233197	-1.992533
C	3.909431	0.070022	-0.055202
C	4.548308	-0.214485	1.160658

C	5.878561	-0.619079	1.173684
C	6.583937	-0.743528	-0.023972
C	5.954596	-0.462630	-1.237158
C	4.624204	-0.059374	-1.254977
H	0.302107	3.651848	0.144139
H	-0.851066	5.346526	1.545348
H	-2.121778	4.638157	3.572962
H	-2.224422	2.222765	4.187257
H	-1.108077	0.523254	2.762109
H	-0.371430	2.179730	-3.923900
H	1.283618	2.170035	-3.240623
H	0.490628	0.624239	-3.697570
H	-3.475527	3.261150	-2.010763
H	-1.983256	3.763882	-1.108381
H	-1.966241	3.642241	-2.930745
H	4.015104	-0.123000	2.114234
H	6.506468	-0.560862	-2.178313
H	4.116165	0.161292	-2.199346
H	6.369498	-0.839094	2.127696
Au	-0.637130	-1.037036	0.369834
P	-1.773469	-3.072531	0.194352
H	1.950421	0.503537	1.923246
H	7.632013	-1.062673	-0.010705
C	-2.062612	-3.956370	1.758405
C	-3.427121	-2.795355	-0.516313
C	-0.979269	-4.291418	-0.898819
H	-2.613909	-3.305107	2.458855
H	-2.651884	-4.873421	1.570074
H	-1.096230	-4.231038	2.216318
H	-3.326974	-2.293524	-1.495628
H	-3.962003	-3.755036	-0.643791
H	-4.008376	-2.136355	0.153086
H	0.011350	-4.565180	-0.495478
H	-1.608093	-5.198425	-0.975180
H	-0.842990	-3.855332	-1.903896

6c2

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C	0.430011	0.911973	0.950600
N	1.689775	0.357005	1.208800
C	2.452420	0.511240	0.102595
N	1.808403	1.185003	-0.837439
C	0.569037	1.476912	-0.349862
N	-0.404418	1.336446	1.994623
C	-0.335831	2.384975	-1.076055
C	3.802952	-0.028325	-0.046193
C	4.490463	-0.607076	1.029885
C	5.777530	-1.104207	0.852293
C	6.391042	-1.026743	-0.398158
C	5.714072	-0.447704	-1.472409
C	4.427091	0.048965	-1.299367
H	4.034619	-0.663593	2.025266
H	6.194404	-0.384865	-2.454966
H	3.883124	0.503095	-2.134071
H	6.307560	-1.552288	1.699615
Au	-0.716000	-0.696809	-0.403290
P	-1.934564	-2.511573	-1.212553
H	1.890678	-0.211945	2.029569
H	7.404906	-1.418889	-0.535463

C	-2.581992	-3.521689	0.154122
C	-3.382513	-2.038707	-2.203972
C	-0.964785	-3.641224	-2.253722
H	-3.243566	-2.905118	0.788813
H	-3.153123	-4.381503	-0.243188
H	-1.745208	-3.890726	0.772964
H	-3.056461	-1.473311	-3.094286
H	-3.932649	-2.943352	-2.523866
H	-4.050341	-1.397779	-1.602052
H	-0.099040	-4.021591	-1.684236
H	-1.595309	-4.490856	-2.575983
H	-0.594968	-3.101485	-3.142754
C	-0.150735	2.661662	2.568380
S	-1.120293	0.177241	3.012455
H	-1.013381	2.981586	3.175217
H	0.756739	2.670019	3.200534
H	-0.029350	3.380712	1.740427
O	-0.996035	0.661644	4.378561
C	-2.835837	0.212143	2.564692
O	-0.559395	-1.120218	2.635572
H	-3.344548	-0.516299	3.218758
H	-3.222948	1.228122	2.747887
H	-2.941148	-0.075830	1.504700
C	0.108330	2.951138	-2.279361
C	-0.706844	3.825229	-2.992190
C	-1.976166	4.148722	-2.514166
C	-2.427169	3.591319	-1.317152
C	-1.616645	2.715998	-0.601751
H	1.108604	2.697758	-2.644205
H	-0.344996	4.261141	-3.930068
H	-2.616717	4.838589	-3.074855
H	-3.422937	3.841142	-0.934610
H	-1.986297	2.284708	0.335555

Tables of partial charges of crucial structures of B/C-Series

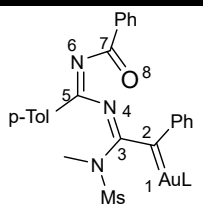
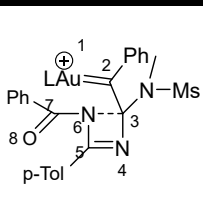
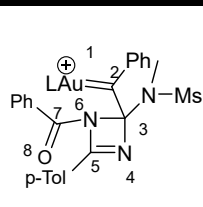
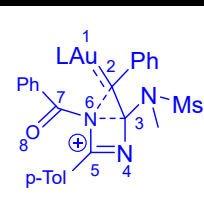
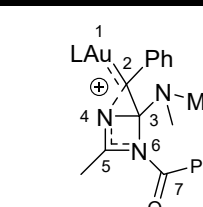
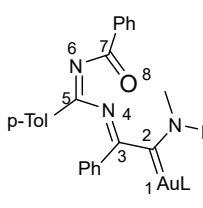
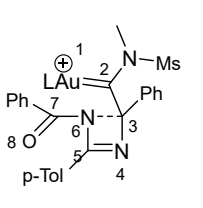
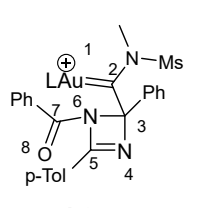
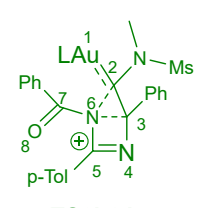
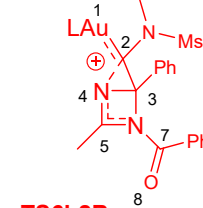
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<div style="display: flex; flex-wrap: wrap; justify-content: space-around;"> <div style="text-align: center;">  <p>4b2</p> </div> <div style="text-align: center;">  <p>TS5b2</p> </div> <div style="text-align: center;">  <p>5b2</p> </div> <div style="text-align: center;">  <p>TS6b2A</p> </div> <div style="text-align: center;">  <p>TS6b2B</p> </div> </div>										
	4b1	4b2	TS_5b1	TS_5b2	5b1	5b2	TS_6b1A	TS_6b2A	TS_6b1B	TS_6b2B
1-Au	0.120944	0.194652	0.145753	0.211691	0.114595	0.235655	0.206867	0.238972	0.144805	0.179897
2-C	0.894065	0.236744	0.907579	0.19533	0.955435	0.325304	0.762552	0.673092	0.806853	0.77089
3-C	1.185185	1.003198	1.414182	1.60575	0.853187	0.661227	1.155488	1.377783	0.763504	0.600618
4-N	-1.332222	-1.208757	-1.133197	-1.230472	-1.020151	-0.982092	-1.042689	-1.09442	-1.413728	-1.519344
5-C	1.537495	1.538158	1.152096	1.324972	1.224882	1.278928	1.221485	1.266385	1.775056	1.848884
6-N	-1.355262	-1.43594	-1.42201	-1.492785	-1.140083	-1.106504	-1.517246	-1.480617	-1.239887	-1.331464
7-C	1.62677	1.686675	1.449818	1.324283	1.552585	1.396078	1.508171	1.54265	1.531206	1.710358
8-O	-0.955994	-0.975795	-0.945551	-0.829415	-0.967732	-0.874619	-0.880036	-0.936137	-0.881069	-0.920224

Table S1. Values of partial charges for Series-B

	4c1	4c2	TS_5c1	TS_5c2	5c1	5c2	TS_6c1A	TS_6c2A	TS_6c1B	TS_6c2B
1-Au	0.098709	0.19294	0.162348	0.211666	0.088815	0.193403	0.13896	0.171871	0.127574	0.18835
2-C	0.916796	0.089538	0.939511	0.061567	1.070416	0.337279	0.876762	0.776936	0.932643	0.879914
3-C	1.263572	1.137719	1.407143	1.468532	0.815943	0.534177	0.900219	0.834716	0.848677	0.638202
4-N	-1.263664	-1.243767	-1.445964	-1.209881	-1.040223	-0.948257	-0.980906	-0.904711	-0.925783	-1.536372
5-C	1.209813	1.321927	1.419242	1.185547	1.176866	1.206591	1.168054	1.154241	1.398518	1.554621
6-N(NH)	-0.924369	-0.992448	-1.18242	-1.183294	-0.906437	-0.913927	-1.131005	-1.133475	-1.360403	-0.910495

Table S2. Values of partial charges for Series-C

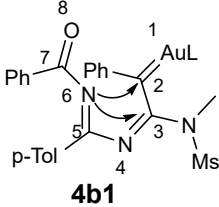
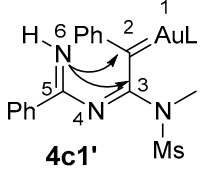
Alternative pathways of cyclization for 4b1			Alternative pathways of cyclization for 4c1		
1-Au	0.120944	 <p>4b1</p>	1-Au	0.098709	 <p>4c1'</p>
2-C	0.894065		2-C	0.916796	
3-C	1.185185		3-C	1.263572	
4-N	-1.332222		4-N	-1.263664	
5-C	1.537495		5-C	1.209813	
6-N	-1.355262		6-N(NH)	-0.924369	
7-C	1.62677				
8-O	-0.955994				

Table S3. Values of partial charges on the structures of alternative cyclization for Series-B/C

Energy diagrams of B/C-Series including alternative attack of N-4 of oxadiazole

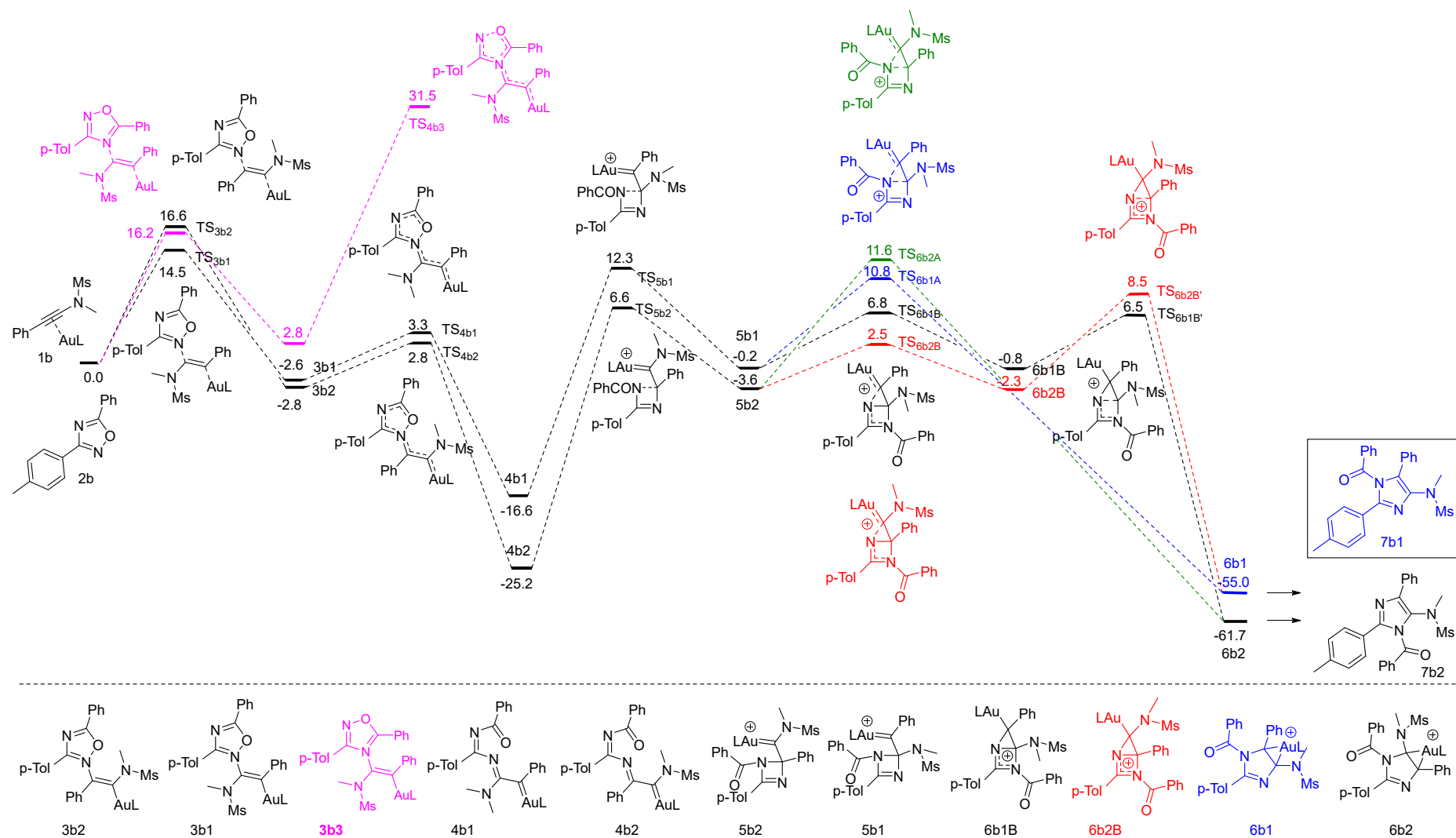


Figure S4. B-series reaction mechanism including the alternative path of nucleophilic attack of N-4 of 1,2,4-oxadiazole on ynamide

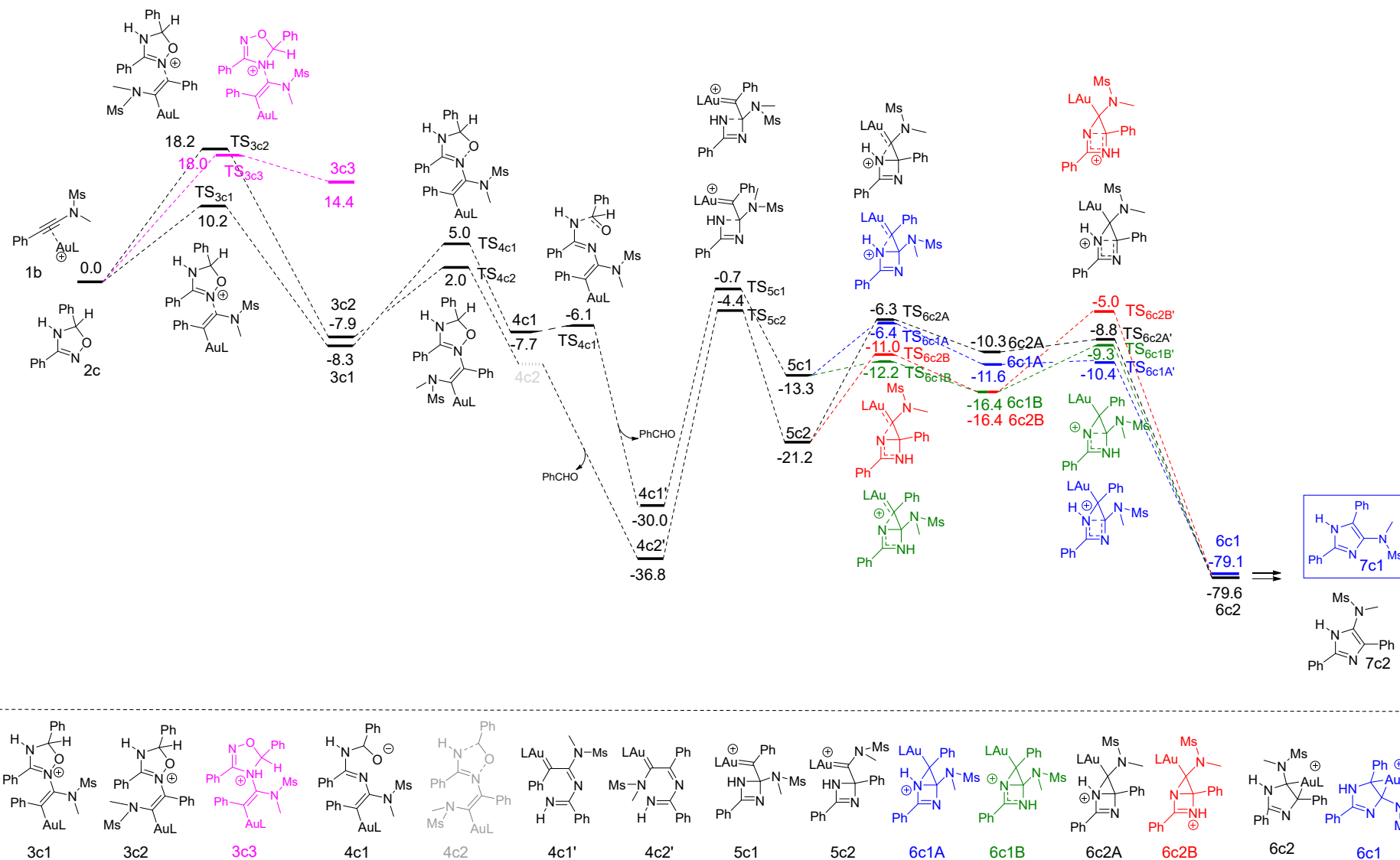


Figure S5. C-series reaction mechanism including the alternative path of nucleophilic attack of N-4 of 1,2,4-oxadiazole on ynamid