

Supporting Information

DFT Mechanistic Study of the Cyclopropanation of Styrene and Aryldiazodiacetate Catalyzed by Tris(pentafluorophenyl)borane

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Contents

SI1: Other Possible Pathways in Mechanism A of Activating N-bound boron.

SI2: Other Possible Pathways in Mechanism C of Activating O-bound boron.

SI3: Table of Energy Values.

SI4: Calculated Imaginary Frequencies of all Transition States Species.

SI5: Cartesian Coordinates.

SI1 Other Possible Pathways in Mechanism A of Activating N-bound boron.

We also calculated and considered another pathway of aryldiazodiacetate substrate **N-bound boron** activation mechanism: the mechanism by which styrene nucleophilic attack directly forms ternary rings, as shown in **Figure S1**. The free energy of transition state is 34.8 kcal/mol, so it is excluded by us.

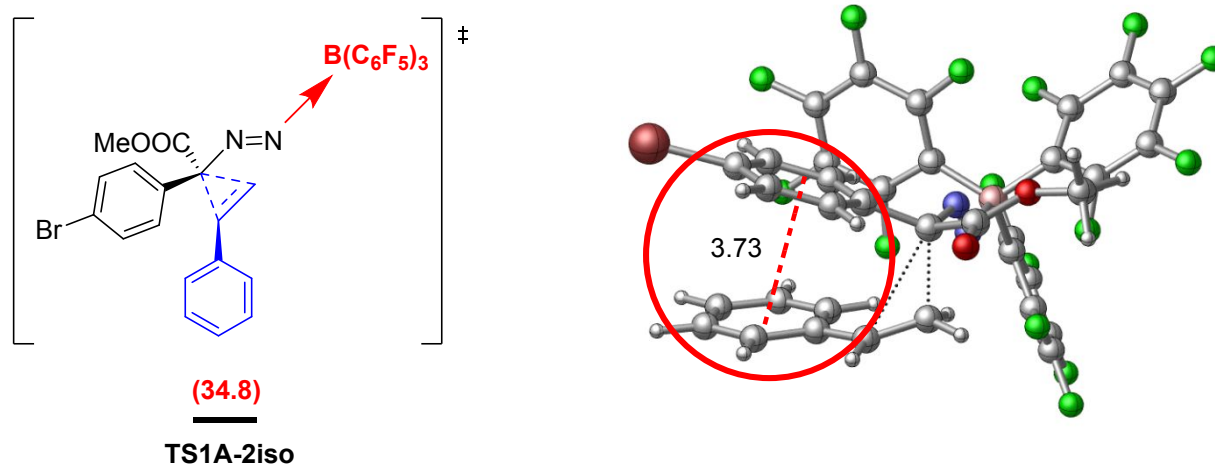


Figure S1. Other Possible Pathways in Mechanism A of Activating N-bound boron. Free energies are relative to **1a**, and are given in kcal/mol.

SI2 Other Possible Pathways in Mechanism C of Activating O-bound boron.

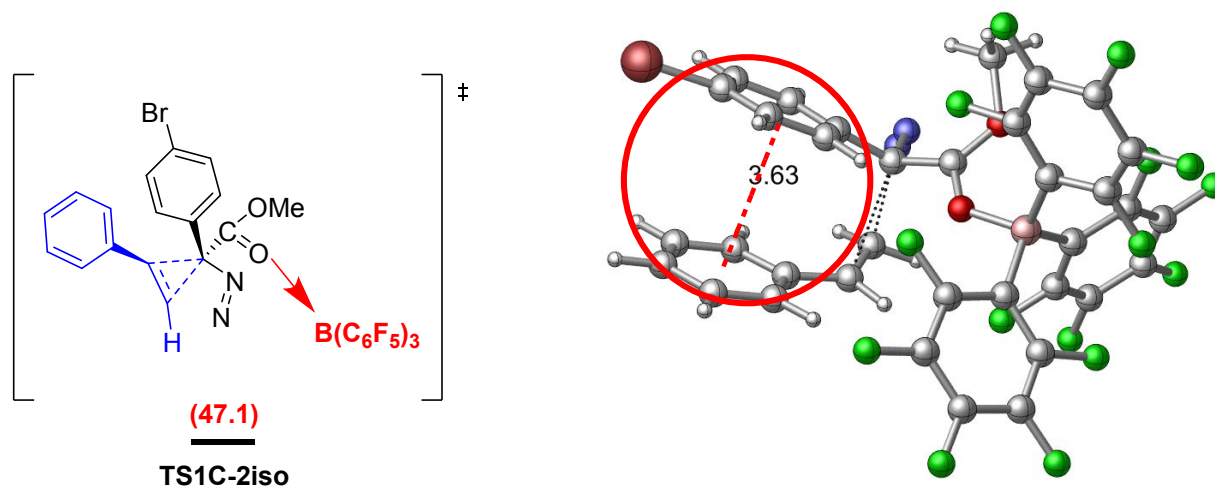


Figure S2. Other Possible Pathways in Mechanism C of Activating O-bound boron. Free energies are relative to **1a**, and are given in kcal/mol.

In the same way, we also calculated and considered another pathway of aryldiazodiacetate substrate O-bound boron activation mechanism: the mechanism by which styrene nucleophilic attack directly forms ternary rings, as shown in **Figure S2**. The transition state has a high free energy of 47.1 kcal/mol, so it is also excluded by us.

SI3 Table of energy values.

Table S1. Energies (in hartree) for the related TSs and intermediates by B3LYP-D3 method

Species	G	E ₀	E	H ₄₃₃	G ₄₃₃	E _(B3LYP-D3)
1a	0.107175	-3178.354328	-3178.341273	-3178.340329	-3178.396002	-3181.421806
2a	0.103009	-309.526929	-309.520265	-309.519321	-309.557834	-309.7467101
3a	0.228184	-3378.445973	-3378.428034	-3378.427090	-3378.495414	-3381.68512
3a-iso	0.227868	-3378.444201	-3378.426173	-3378.425229	-3378.493746	-3381.6823025
Cat-B(C₆F₅)₃	0.092584	-2208.097896	-2208.069025	-2208.068081	-2208.159098	-2208.9826472
N₂	-0.012840	-109.509597	-109.507237	-109.506293	-109.528046	-109.5600205
IN1A	0.226123	-5386.468058	-5386.425232	-5386.424288	-5386.546905	-5390.4128401
TS1A	0.356885	-5695.981161	-5695.931595	-5695.930651	-5696.066333	-5700.1606793

IN2A	0.362063	-5696.065205	-5696.016618	-5696.015674	-5696.150143	-5700.2250027
TS2A	0.349035	-5695.973394	-5695.923138	-5695.922194	-5696.061200	-5700.1320209
TS1A-N₂	0.219521	-5386.428270	-5386.384348	-5386.383404	-5386.509142	-5390.3717692
IN1D	0.097445	-3068.800092	-3068.788671	-3068.787727	-3068.839843	-3071.8256494
TS2D	0.221323	-3378.336924	-3378.317757	-3378.316813	-3378.387467	-3381.5796099
TS1B-N₂	0.220153	-5386.429695	-5386.385717	-5386.384772	-5386.509731	-5390.3727654
IN1B	0.221380	-5276.963114	-5276.922596	-5276.921651	-5277.036566	-5280.8648826
TS2B	0.350747	-5586.495364	-5586.448033	-5586.447089	-5586.576424	-5590.6122215
TS1C	0.354905	-5695.989373	-5695.939858	-5695.938914	-5696.075478	-5700.1497778
IN2C	0.358817	-5696.041784	-5695.992828	-5695.991884	-5696.127991	-5700.2029242
TS2C	0.351207	-5696.009540	-5695.959462	-5695.958518	-5696.096373	-5700.1720611
E-IN1C	0.225508	-5386.475440	-5386.432576	-5386.431632	-5386.554713	-5390.4241545
E-TS3C	0.219828	-5386.436565	-5386.393073	-5386.392129	-5386.517686	-5390.3854542
E-IN3C	0.215645	-5276.937119	-5276.895897	-5276.894953	-5277.014963	-5280.8407326
E-TS4C	0.341413	-5586.479339	-5586.430602	-5586.429658	-5586.566917	-5590.5989956
Z-IN1C	0.227466	-5386.484765	-5386.442013	-5386.441069	-5386.562165	-5390.4317374
Z-TS3C	0.220591	-5386.443503	-5386.400081	-5386.399137	-5386.523839	-5390.3900389
Z-IN3C	0.217450	-5276.947960	-5276.906967	-5276.906023	-5277.024515	-5280.8488882
Z-TS4C	0.343976	-5586.488999	-5586.440638	-5586.439694	-5586.574410	-5590.608066
TS5C	0.344003	-5586.485269	-5586.436858	-5586.435914	-5586.570742	-5590.6018467
TS1A-2iso	0.352797	-5695.987078	-5695.937165	-5695.936221	-5696.074586	-5700.1457944
TS1C-2iso	0.353654	-5695.966837	-5695.916922	-5695.915978	-5696.052601	-5700.1269347
TS1D-N₂	0.101362	-3178.302148	-3178.288413	-3178.287468	-3178.345261	-3181.3709229
TS1E	0.232558	-3487.862956	-3487.842984	-3487.842039	-3487.914436	-3491.1450655
TS1F	0.231806	-3487.839815	-3487.819585	-3487.818641	-3487.891082	-3491.1236934
Re1	0.071726	-415.843207	-415.834819	-415.833875	-415.876888	-416.0858823
IN1G	0.192404	-2623.977679	-2623.939955	-2623.939011	-2624.047998	-2625.0986094
TS1G-N₂	0.184360	-2623.913257	-2623.874594	-2623.873650	-2623.986342	-2625.0344411
Re2	0.068002	-508.080514	-508.070402	-508.069458	-508.116971	-508.3498452
IN1J	0.186970	-2716.203241	-2716.163441	-2716.162497	-2716.276889	-2717.3512076
TS1J-N₂	0.181547	-2716.154300	-2716.113813	-2716.112868	-2716.229095	-2717.2993322

Re3	0.081206	-604.387831	-604.376079	-604.375135	-604.426602	-604.7076985
IN1H	0.200137	-2812.504086	-2812.462825	-2812.461881	-2812.580461	-2813.7025008
TS1H-N₂	0.193414	-2812.444790	-2812.402370	-2812.401426	-2812.523032	-2813.6430887

G=Thermal correction to Gibbs Free Energy by B3LYP-D3 at the solvent phase.

E₀= Sum of electronic and zero-point Energies by B3LYP-D3 at the solvent phase.

E= Sum of electronic and thermal Energies by B3LYP-D3 at the solvent phase.

H₄₃₃= Sum of electronic and thermal Enthalpies by B3LYP-D3 at the solvent phase.

G₄₃₃= Sum of electronic and thermal Free Energies by B3LYP-D3 at the solvent phase.

E_(B3LYP-D3)= Single point energies calculated by B3LYP-D3 in the 1,2-Dichloroethane solvent.

SI4 Calculated imaginary frequencies of all transition states species.

Species	IF
TS1A	-238.86
TS2A	-737.55
TS1A-N ₂	-317.95
TS2D	-36.45
TS1B-N ₂	-293.98
TS2B	-217.61
TS1C	-401.87
TS2C	-265.84
<i>E</i> -TS3C	-358.96
<i>E</i> -TS4C	-71.58
<i>Z</i> -TS3C	-369.78
<i>Z</i> -TS4C	-47.28
TS5C	-138.73
TS1A-2iso	-423.50
TS1C-2iso	-500.16
TS1D-N ₂	-318.65
TS1E	-436.48
TS1F	-449.76

TS1G-N ₂	-293.79
TS1J-N ₂	-299.45
TS1H-N ₂	-127.97

SI5 Cartesian coordinates

21

1a SCF Done: E(RB3LYP) = -3178.50317690

C	-2.78305	1.24011	0.00001
C	-1.39694	1.09864	0.00076
C	-0.56203	2.231	0.00038
C	-1.16363	3.50395	-0.00076
C	-2.54716	3.64779	-0.00151
C	-3.3536	2.51079	-0.00113
H	-3.41577	0.35981	0.00031
H	-0.95829	0.11035	0.00163
H	-0.55492	4.4032	-0.0011
H	-2.99368	4.63546	-0.0024
C	0.90786	2.09673	0.00113
N	1.6286	3.20049	0.00088
N	2.22632	4.16835	0.00093
C	1.68094	0.84529	0.00177
O	1.20559	-0.27457	0.00184

O	3.01439	1.09063	0.00235
C	3.84803	-0.08103	0.00302
H	3.6587	-0.68833	-0.88591
H	4.87232	0.29105	0.00341
H	3.65787	-0.6879	0.89207
Br	-5.25482	2.70007	-0.0022

16

2a SCF Done: E(RB3LYP) = -309.66084258

C	-1.66068	2.0746	0.76429
C	-0.32802	2.17607	0.36132
C	0.36682	3.39731	0.44122
C	-0.32294	4.52016	0.94159
C	-1.65291	4.4198	1.34396
C	-2.32968	3.19698	1.25785
H	-2.17475	1.11953	0.69239
H	0.18715	1.29793	-0.02217
H	0.18271	5.47883	1.01713
H	-2.16571	5.29855	1.72686
H	-3.36723	3.12275	1.57279
C	1.7725	3.44344	0.00105

H	2.16322	2.49166	-0.36042
C	2.59232	4.50408	0.00057
H	2.25336	5.51486	-0.21382
H	3.65037	4.38807	0.21975

35

3a SCF Done: E(RB3LYP) = -3378.72359767

C	-2.90357	1.79899	-0.30929
C	-1.53089	1.77375	-0.53872
C	-0.63923	2.39215	0.3469
C	-1.15166	3.0268	1.48182
C	-2.52518	3.06386	1.72875
C	-3.38915	2.4509	0.82471
H	-3.58991	1.32611	-1.00215
H	-1.14335	1.27699	-1.42172
H	-0.47326	3.49888	2.1865
H	-2.91693	3.55936	2.60972
C	0.83407	2.36508	0.06965
C	1.46153	1.01038	0.22142
O	0.84835	-0.02666	0.363
O	2.81598	1.06157	0.14863

C	3.47676	-0.21193	0.22964
H	3.15281	-0.86673	-0.5839
H	4.54243	0.00318	0.14898
H	3.25315	-0.70141	1.18115
C	1.67621	3.59934	0.31786
C	1.4084	3.221	-1.10553
H	2.68075	3.45301	0.69734
H	1.1581	4.46457	0.71825
H	2.23946	2.73306	-1.60632
C	0.51286	3.97029	-2.03102
C	-0.44333	4.90177	-1.59764
C	0.6153	3.71526	-3.40725
C	-1.27054	5.55191	-2.51222
H	-0.55966	5.111	-0.53985
C	-0.20829	4.36786	-4.32419
H	1.35037	2.99628	-3.76091
C	-1.1573	5.28951	-3.87912
H	-2.00759	6.26482	-2.15391
H	-0.10819	4.15544	-5.38485
H	-1.80237	5.79836	-4.58937
Br	-5.27557	2.50768	1.14061

3a-iso SCF Done: E(RB3LYP) = -3378.72161421

C	-2.93874	2.46073	-0.47217
C	-1.57749	2.35925	-0.76516
C	-0.61818	2.33109	0.25207
C	-1.0512	2.39188	1.58434
C	-2.40503	2.49095	1.89531
C	-3.33937	2.52819	0.85962
H	-3.6757	2.48331	-1.26679
H	-1.26395	2.29428	-1.80271
H	-0.3189	2.34324	2.38247
H	-2.73377	2.53852	2.92715
C	0.84598	2.22508	-0.06506
C	1.50935	0.97002	0.43552
O	1.14687	0.35399	1.41678
O	2.60574	0.64529	-0.28021
C	3.43708	-0.37285	0.30303
H	2.87554	-1.30012	0.43876
H	4.26002	-0.51583	-0.39696
H	3.81394	-0.0352	1.27235

C	1.72108	3.49263	0.09749
C	1.42157	2.9474	-1.2659
H	1.13365	4.35759	0.40131
H	2.21926	2.4472	-1.80199
Br	-5.20115	2.67324	1.27699
H	0.72575	3.49955	-1.88879
C	3.08214	3.41536	0.719
C	4.24507	3.56861	-0.0438
C	3.20337	3.18292	2.09674
C	5.50403	3.48828	0.55377
H	4.16069	3.746	-1.11186
C	4.45997	3.09889	2.69634
H	2.30604	3.04927	2.69488
C	5.61529	3.25099	1.92508
H	6.39757	3.60823	-0.05242
H	4.53747	2.91147	3.76354
H	6.59457	3.18416	2.39024

34

Cat-B(C₆F₅)₃ SCF Done: E(RB3LYP) = -2208.25168232

B	-0.51919	1.19836	0.00026
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C	-1.28851	2.56234	-0.01632
C	-2.50655	2.74407	0.6576
C	-0.80665	3.68613	-0.70608
C	-3.19946	3.94921	0.66118
C	-1.48077	4.90146	-0.74058
C	-2.68315	5.03297	-0.04755
C	1.04661	1.18291	0.00311
C	1.78724	0.20182	-0.67423
C	1.8038	2.14929	0.68333
C	3.17709	0.17741	-0.69074
C	3.19377	2.14685	0.7046
C	3.8832	1.15539	0.00809
C	-1.31507	-0.15032	0.01371
C	-0.85842	-1.28276	0.7064
C	-2.533	-0.30891	-0.66611
C	-1.556	-2.48488	0.73816
C	-3.249	-1.50045	-0.67255
C	-2.75725	-2.59361	0.03925
F	-1.08889	-3.53151	1.42602
F	0.28851	-1.23402	1.40336
F	-3.43398	-3.74033	0.05164

F	-4.39756	-1.60755	-1.34791
F	-3.05022	0.70829	-1.37413
F	0.3426	3.61569	-1.39731
F	-3.04673	1.73685	1.36273
F	-4.34891	4.07835	1.33113
F	-3.33743	6.19259	-0.0625
F	-0.99036	5.9393	-1.42553
F	3.87169	3.08002	1.3802
F	1.19222	3.12253	1.37794
F	5.21476	1.14256	0.0103
F	1.15928	-0.75949	-1.37081
F	3.83913	-0.76873	-1.36407

2

N₂ SCF Done: E(RB3LYP) = -109.51520581

N	-1.26146	1.8599	0.
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N	-2.36677	1.8599	0.
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55

IN1A SCF Done: E(RB3LYP) = -5386.77302755

C	-2.4826	-1.08792	-1.38224
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N	-1.30437	-0.59015	-1.53743
N	-0.21813	-0.19196	-1.61338
C	-3.65849	-0.2033	-1.44403
C	-4.95362	-0.69232	-1.20711
C	-3.48102	1.16585	-1.72345
C	-6.04573	0.17181	-1.24644
H	-5.10654	-1.73988	-0.9877
C	-4.56906	2.02669	-1.7622
H	-2.49332	1.56923	-1.9178
C	-5.85009	1.52393	-1.52103
H	-7.04393	-0.20741	-1.0608
H	-4.42522	3.0793	-1.97632
C	-2.48023	-2.55642	-1.04194
O	-3.47279	-3.2077	-0.80725
O	-1.22497	-3.01237	-1.00215
C	-1.03483	-4.38061	-0.58671
H	0.0457	-4.50838	-0.55032
H	-1.47888	-4.53926	0.39853
H	-1.48986	-5.0618	-1.30913
B	0.78447	0.20073	-0.19058
C	2.24483	-0.21805	-0.73154

C	2.43889	-1.43192	-1.39814
C	3.66162	-1.85637	-1.89962
C	4.77884	-1.03961	-1.73464
C	4.64409	0.17496	-1.07147
C	3.39375	0.56395	-0.58689
C	0.09437	-0.72009	0.95198
C	-1.1995	-0.42168	1.40068
C	-1.92804	-1.22156	2.27687
C	-1.34821	-2.38982	2.76203
C	-0.05692	-2.72362	2.36406
C	0.63771	-1.89319	1.48614
C	0.54943	1.78327	0.05023
C	0.86821	2.31649	1.30171
C	0.67471	3.65204	1.63623
C	0.13347	4.52096	0.69003
C	-0.19563	4.0362	-0.57124
C	0.03191	2.69342	-0.86513
F	1.39109	-2.27216	-1.56327
F	3.77754	-3.03368	-2.52819
F	5.96753	-1.42371	-2.20656
F	5.71185	0.96436	-0.90277

F	3.35701	1.74991	0.04719
F	-1.83892	0.67688	0.93565
F	-3.17157	-0.88603	2.6373
F	-2.02557	-3.18878	3.58963
F	0.50275	-3.8549	2.81323
F	1.87614	-2.30288	1.16255
F	-0.32362	2.28996	-2.11372
F	-0.72608	4.85393	-1.4905
F	-0.06755	5.80642	0.99275
F	1.00172	4.1089	2.85052
F	1.4045	1.51767	2.24412
Br	-7.34472	2.7026	-1.56936

71

TS1A SCF Done: E(RB3LYP) = -5696.42321845

N	-0.21777	1.28639	0.6125
N	0.53257	0.36794	0.74763
B	1.66674	-0.11722	-0.2939
C	2.40022	1.08897	-1.11174
C	2.56223	2.39977	-0.66583
C	3.29455	3.36026	-1.36281

C	3.91767	3.01899	-2.55558
C	3.79951	1.71752	-3.03319
C	3.05847	0.79222	-2.30848
C	0.67037	-1.06325	-1.19902
C	0.28394	-2.34795	-0.81299
C	-0.69334	-3.09299	-1.4642
C	-1.34245	-2.554	-2.56726
C	-0.99265	-1.2803	-3.00005
C	-0.0184	-0.56288	-2.31039
C	2.83607	-0.87245	0.54933
C	3.51876	-2.00053	0.09317
C	4.59376	-2.56688	0.7733
C	5.03824	-1.991	1.9584
C	4.4029	-0.85258	2.44214
C	3.3382	-0.31591	1.72605
F	2.01026	2.81103	0.49425
F	3.40654	4.61023	-0.883
F	4.62848	3.92846	-3.23639
F	4.40018	1.36949	-4.18291
F	2.98949	-0.45768	-2.81895
F	0.81007	-2.9227	0.29399

F	-1.06255	-4.29473	-0.99154
F	-2.30536	-3.2424	-3.18961
F	-1.6258	-0.73551	-4.04956
F	0.19777	0.6944	-2.74756
F	2.7815	0.81447	2.22603
F	4.8259	-0.27809	3.5796
F	6.06999	-2.52521	2.62523
F	5.20524	-3.66194	0.29448
F	3.15349	-2.60659	-1.05488
C	-1.26205	1.75285	1.34223
C	-2.58058	1.71344	0.71782
C	-3.67231	2.47109	1.18388
C	-2.79632	0.80008	-0.33781
C	-4.93446	2.31749	0.61562
H	-3.53862	3.16887	1.99862
C	-4.05081	0.64151	-0.90774
H	-1.9812	0.19311	-0.71299
C	-5.11618	1.40188	-0.41999
H	-5.76758	2.90436	0.98584
H	-4.19611	-0.06843	-1.71415
C	-0.87155	2.66244	2.47033

O	-1.65472	3.31928	3.1306
O	0.44247	2.5956	2.69482
C	0.96286	3.39727	3.77458
H	2.03631	3.21014	3.77031
H	0.75415	4.45528	3.59509
H	0.521	3.08711	4.72532
Br	-6.8535	1.17615	-1.18312
C	-1.2712	-0.27317	2.84811
C	0.05504	-0.60859	2.59981
H	0.83507	-0.09097	3.14424
H	0.33364	-1.56293	2.17105
H	-1.47485	0.46415	3.61929
C	-2.42922	-1.00633	2.34528
C	-3.72515	-0.5704	2.68997
C	-2.30913	-2.10196	1.46587
C	-4.8537	-1.19013	2.15784
H	-3.83786	0.27445	3.36406
C	-3.43647	-2.72217	0.93506
H	-1.3302	-2.48182	1.20649
C	-4.71475	-2.26257	1.27062
H	-5.84301	-0.82877	2.42394

H -3.31099 -3.55782 0.25193

H -5.59515 -2.73798 0.84725

71

IN2A SCF Done: E(RB3LYP) = -5696.51220592

N -0.23708 1.15027 0.68377

N 0.39841 0.11393 0.92508

B 1.58791 -0.42489 -0.0636

C 2.12869 0.75175 -1.06022

C 2.50172 2.00725 -0.5738

C 3.06335 3.00905 -1.35939

C 3.30967 2.76285 -2.70476

C 2.99503 1.51634 -3.23055

C 2.43079 0.54316 -2.4094

C 0.74096 -1.6249 -0.80627

C 0.75909 -2.96797 -0.42389

C -0.09079 -3.93362 -0.96184

C -1.03307 -3.56359 -1.91356

C -1.10042 -2.2367 -2.32349

C -0.22011 -1.31372 -1.7741

C 2.89222 -0.89242 0.80239

C	3.83223	-1.72976	0.19339
C	5.03513	-2.10008	0.78103
C	5.35643	-1.60985	2.04353
C	4.47099	-0.75063	2.6796
C	3.28062	-0.39713	2.04636
F	2.34786	2.29463	0.73499
F	3.38508	4.19892	-0.82525
F	3.8548	3.70899	-3.48084
F	3.24307	1.25555	-4.52461
F	2.18988	-0.64477	-3.00393
F	1.58091	-3.39598	0.55793
F	-0.03312	-5.20453	-0.53836
F	-1.90542	-4.46021	-2.38944
F	-2.03714	-1.85309	-3.20275
F	-0.37544	-0.03458	-2.18453
F	2.49812	0.47518	2.72673
F	4.76757	-0.25771	3.89287
F	6.50738	-1.95819	2.63315
F	5.88886	-2.91684	0.14446
F	3.58679	-2.21647	-1.04249
C	-1.35226	1.33531	1.64613

C	-2.60776	1.77314	0.90967
C	-3.65901	2.43339	1.55704
C	-2.80987	1.29707	-0.39498
C	-4.9067	2.55521	0.94312
H	-3.53153	2.81167	2.56123
C	-4.05054	1.40764	-1.01681
H	-2.01248	0.79544	-0.92832
C	-5.10097	2.00536	-0.32246
H	-5.72389	3.03425	1.47017
H	-4.1982	0.9976	-2.00843
C	-0.85487	2.30487	2.74833
O	-1.57138	2.80818	3.58578
O	0.46865	2.41598	2.70904
C	1.11255	3.19089	3.74565
H	2.17165	3.11779	3.53484
H	0.78315	4.22466	3.69909
H	0.88795	2.77382	4.72467
Br	-6.85278	2.00482	-1.09554
C	-1.49936	-0.10909	2.35979
C	-0.10294	-0.67785	2.0934
H	0.58065	-0.46392	2.91174

H	-0.05676	-1.74077	1.86427
H	-1.63613	0.06551	3.43162
C	-2.67999	-0.91672	1.85627
C	-3.94291	-0.68805	2.42572
C	-2.58446	-1.80954	0.7841
C	-5.08103	-1.31017	1.91196
H	-4.03165	0.00169	3.26118
C	-3.71897	-2.44218	0.26999
H	-1.62401	-2.01425	0.33652
C	-4.97578	-2.18666	0.82702
H	-6.04248	-1.10415	2.35222
H	-3.61288	-3.12197	-0.57046
H	-5.8607	-2.6688	0.42749

71

TS2A SCF Done: E(RB3LYP) = -5696.41023532

N	0.60936	0.8392	0.30383
N	-0.30888	0.35728	-0.16315
B	-1.86424	-0.15812	0.3798
C	-2.45801	1.0157	1.32756
C	-2.12189	2.37018	1.33185

C	-2.79523	3.31685	2.10519
C	-3.86106	2.92136	2.9055
C	-4.24551	1.58172	2.91843
C	-3.54927	0.67224	2.13202
C	-1.37256	-1.53419	1.08132
C	-1.0334	-2.64816	0.30954
C	-0.45389	-3.80245	0.82089
C	-0.21456	-3.89193	2.18933
C	-0.54812	-2.81695	3.00775
C	-1.09696	-1.66328	2.44629
C	-2.83491	-0.2778	-0.91017
C	-3.75651	-1.31254	-1.09409
C	-4.66433	-1.3423	-2.15238
C	-4.6871	-0.29817	-3.07371
C	-3.8047	0.76737	-2.91712
C	-2.9293	0.76096	-1.83704
F	-1.11325	2.85087	0.57076
F	-2.42486	4.60337	2.07271
F	-4.51644	3.81723	3.64965
F	-5.27705	1.18858	3.67557
F	-3.96745	-0.61076	2.15457

F	-1.20418	-2.61837	-1.03505
F	-0.08512	-4.80206	0.00325
F	0.34232	-4.98922	2.70672
F	-0.31452	-2.88671	4.32281
F	-1.32943	-0.65111	3.29825
F	-2.1199	1.84286	-1.71309
F	-3.81077	1.78732	-3.78685
F	-5.54665	-0.31785	-4.09581
F	-5.51485	-2.36598	-2.28942
F	-3.80598	-2.34793	-0.23917
C	2.20381	1.22676	-1.36197
C	3.49864	1.14204	-0.65032
C	4.52816	2.06651	-0.89953
C	3.73369	0.12824	0.29488
C	5.76046	1.96132	-0.26088
H	4.36474	2.87748	-1.59944
C	4.95666	0.01582	0.94724
H	2.94954	-0.58456	0.52193
C	5.96794	0.93136	0.65625
H	6.55105	2.67237	-0.47049
H	5.12321	-0.77026	1.67449

C	1.64644	2.59993	-1.50653
O	2.03224	3.56227	-0.87266
O	0.62783	2.67514	-2.39826
C	-0.08613	3.92909	-2.42014
H	-0.91076	3.77646	-3.11517
H	-0.46615	4.154	-1.42218
H	0.56994	4.73565	-2.75448
Br	7.65774	0.77537	1.5301
C	1.68001	0.08597	-2.09566
C	0.25255	-0.06584	-2.39175
H	-0.35834	0.80587	-2.54808
H	-0.07045	-1.0111	-2.81331
H	1.47359	0.43046	-3.21234
C	2.4882	-1.19483	-2.12463
C	3.7695	-1.20477	-2.69049
C	1.9722	-2.37625	-1.58587
C	4.52395	-2.37598	-2.70054
H	4.18368	-0.28778	-3.09878
C	2.72848	-3.54907	-1.58776
H	0.97413	-2.38763	-1.17619
C	4.00833	-3.54995	-2.14267

H 5.51712 -2.37175 -3.13921

H 2.30514 -4.45077 -1.15598

H 4.60166 -4.4594 -2.14543

55

TS1A-N₂ SCF Done: E(RB3LYP) = -5386.72866268

C -1.9354 -2.87175 0.98616

N -0.51042 -1.57022 1.41744

N 0.36999 -1.01077 1.03223

C -3.12804 -2.07402 0.82036

C -4.24362 -2.14747 1.6889

C -3.19886 -1.19935 -0.288

C -5.37699 -1.37899 1.46027

H -4.22116 -2.84325 2.52085

C -4.31007 -0.39434 -0.50368

H -2.36264 -1.16672 -0.97664

C -5.39222 -0.4946 0.37533

H -6.23621 -1.44554 2.11808

H -4.3465 0.28381 -1.34723

C -1.8165 -3.86354 2.02912

O -2.61729 -4.79498 2.04264

O	-0.73451	-3.79168	2.83726
C	-0.55421	-4.92749	3.70072
H	0.3263	-4.69934	4.3016
H	-1.42845	-5.07277	4.34131
H	-0.39335	-5.83687	3.11514
B	1.95762	0.87568	-0.5885
C	2.60124	-0.32418	-1.35972
C	3.22805	-1.38685	-0.69079
C	3.77148	-2.48187	-1.3526
C	3.7212	-2.52969	-2.74492
C	3.11965	-1.49208	-3.45566
C	2.56885	-0.42334	-2.75815
C	2.62429	1.4166	0.7203
C	1.86719	1.87456	1.80871
C	2.43842	2.32907	2.99137
C	3.82765	2.35634	3.10891
C	4.62402	1.92008	2.05138
C	4.01557	1.45424	0.89098
C	0.63771	1.53387	-1.12405
C	0.37156	2.90495	-0.99088
C	-0.80043	3.50162	-1.44599

C	-1.77314	2.71241	-2.05634
C	-1.54925	1.34728	-2.21939
C	-0.3669	0.78681	-1.75495
F	3.29513	-1.39792	0.65005
F	4.34087	-3.48176	-0.67243
F	4.24614	-3.56627	-3.39515
F	3.07593	-1.53631	-4.79096
F	2.00038	0.54966	-3.49079
F	0.52414	1.85998	1.75247
F	1.67556	2.73998	4.00966
F	4.3928	2.79797	4.23126
F	5.95575	1.95076	2.16331
F	4.82901	1.04761	-0.09751
F	-0.23681	-0.54479	-1.90188
F	-2.48723	0.58342	-2.79992
F	-2.91085	3.25601	-2.48385
F	-1.00306	4.81387	-1.29868
F	1.27385	3.71548	-0.41678
Br	-6.92993	0.5896	0.08071

IN1D SCF Done: E(RB3LYP) = -3068.93728829

C	-0.56319	-1.07852	-0.69577
C	0.7094	-0.53709	-0.35588
C	0.94425	0.82805	-0.02405
C	1.81697	-1.42507	-0.33563
C	2.2106	1.27748	0.30844
H	0.11515	1.52762	-0.06806
C	3.08344	-0.99613	0.0365
H	1.63809	-2.46003	-0.60786
C	3.26732	0.35503	0.34876
H	2.39302	2.31891	0.54783
H	3.92291	-1.68068	0.07001
C	-1.7302	-0.24977	-0.61782
O	-1.99133	0.50499	-1.55348
O	-2.53171	-0.45261	0.44917
C	-3.78033	0.2627	0.41454
H	-4.30188	-0.0163	1.33015
H	-3.61225	1.34306	0.38579
H	-4.36667	-0.02425	-0.4625
Br	5.00066	0.96403	0.83268

TS2D SCF Done: E(RB3LYP) = -3003.20267797

C	2.54905	-0.36188	0.63767
C	1.1711	-0.66809	0.43359
C	0.66781	-1.3046	-0.73655
C	0.23822	-0.31574	1.44523
C	-0.68019	-1.59543	-0.87736
H	1.35375	-1.56709	-1.53689
C	-1.11728	-0.57699	1.30651
H	0.60736	0.17595	2.33915
C	-1.56043	-1.21444	0.14371
H	-1.05312	-2.08574	-1.7697
H	-1.8211	-0.286	2.07746
C	3.55283	-0.66979	-0.35538
O	4.01543	0.11888	-1.17441
O	4.13902	-1.90336	-0.26528
C	3.63873	-2.86174	0.68395
H	2.64999	-3.23249	0.39315
H	4.35151	-3.68894	0.67289
H	3.58646	-2.43617	1.69289
Br	-3.42236	-1.56316	-0.06781

C	1.89284	2.35881	-0.38823
C	2.75655	2.29078	0.64884
H	2.44655	2.43528	1.6794
H	3.81576	2.14768	0.46945
H	2.28424	2.16375	-1.38404
C	0.44216	2.50933	-0.2886
C	-0.35851	2.08796	-1.3688
C	-0.20096	2.994	0.87011
C	-1.74945	2.11656	-1.28433
H	0.12248	1.71215	-2.26834
C	-1.59084	3.0387	0.94649
H	0.39407	3.3451	1.70824
C	-2.37119	2.58998	-0.12519
H	-2.34945	1.76567	-2.11953
H	-2.06878	3.41915	1.84538
H	-3.45544	2.61375	-0.0586

55

TS1B-N₂ SCF Done: E(RB3LYP) = -5386.72988386

C	-0.23661	-0.15258	-1.72494
N	0.43952	1.44579	-2.65426

N	1.14439	2.29832	-2.54626
C	-1.67884	-0.07846	-1.70816
C	-2.35197	1.13637	-1.43909
C	-2.45908	-1.25475	-1.82974
C	-3.73063	1.18265	-1.2997
H	-1.78939	2.05721	-1.36626
C	-3.83542	-1.22025	-1.6411
H	-1.96739	-2.20386	-2.00329
C	-4.4672	-0.00241	-1.38431
H	-4.22695	2.12575	-1.10193
H	-4.41755	-2.1326	-1.70342
C	0.46881	-1.23472	-2.39486
O	0.36888	-2.36941	-1.94007
O	1.27272	-0.89539	-3.41464
C	2.14458	-1.94475	-3.88383
H	2.66225	-1.52355	-4.74496
H	2.85778	-2.21259	-3.102
H	1.56681	-2.82569	-4.17176
B	1.189	0.14973	0.92703
C	-0.07265	0.83472	1.57562
C	-0.65746	1.9903	1.04493

C	-1.84909	2.53302	1.50598
C	-2.48531	1.95151	2.59891
C	-1.91676	0.83356	3.20482
C	-0.7409	0.29783	2.68748
C	2.34306	1.02037	0.30254
C	3.15528	0.54633	-0.7388
C	4.14743	1.30342	-1.34796
C	4.39049	2.59782	-0.89254
C	3.63366	3.10977	0.15816
C	2.63783	2.32344	0.73113
C	1.3584	-1.40744	1.0475
C	2.60142	-2.01696	1.27226
C	2.76781	-3.39364	1.36456
C	1.65858	-4.22556	1.22285
C	0.40164	-3.66966	1.00332
C	0.27482	-2.28889	0.93542
F	-0.10169	2.60955	-0.01708
F	-2.4051	3.58074	0.88058
F	-3.62901	2.45856	3.05824
F	-2.50946	0.27969	4.26775
F	-0.25455	-0.78118	3.32143

F	2.9879	-0.70071	-1.21657
F	4.86995	0.79996	-2.35588
F	5.34392	3.33861	-1.45663
F	3.87137	4.3461	0.60915
F	1.96317	2.87399	1.75345
F	-0.96318	-1.81202	0.72119
F	-0.66487	-4.46265	0.85318
F	1.80332	-5.54933	1.29753
F	3.97577	-3.92603	1.58897
F	3.70786	-1.2667	1.42732
Br	-6.35424	0.04838	-1.14292

53

IN1B SCF Done: E(RB3LYP) = -5277.25794538

B	-0.07549	-0.02361	0.17611
C	-1.08561	-1.2726	0.47191
C	-2.03353	-1.17747	1.49363
C	-3.00905	-2.14241	1.72563
C	-3.07337	-3.25888	0.89612
C	-2.16822	-3.38333	-0.15362
C	-1.20715	-2.39419	-0.35028

C	1.38416	-0.45439	-0.51581
C	2.10055	0.3835	-1.38374
C	3.30664	0.02433	-1.97768
C	3.8659	-1.21938	-1.69193
C	3.20773	-2.08217	-0.81746
C	2.00582	-1.68503	-0.24266
C	-0.98247	1.00877	-0.71197
C	-1.13951	0.81567	-2.0886
C	-2.02504	1.54722	-2.87514
C	-2.82004	2.52431	-2.28154
C	-2.70954	2.74956	-0.91325
C	-1.81109	1.99128	-0.16417
F	-2.05016	-0.09331	2.29285
F	-3.88949	-2.00178	2.72599
F	-4.00451	-4.1976	1.09928
F	-2.2302	-4.44735	-0.96686
F	-0.37751	-2.56794	-1.40069
F	1.63123	1.60409	-1.71073
F	3.93092	0.85951	-2.81503
F	5.02518	-1.57627	-2.24326
F	3.74734	-3.26902	-0.524

F	1.4543	-2.54282	0.62868
F	-1.75129	2.2788	1.15431
F	-3.46155	3.69113	-0.32657
F	-3.67592	3.23976	-3.01867
F	-2.11924	1.3197	-4.19163
F	-0.41223	-0.12515	-2.72445
C	0.68343	0.53587	1.49562
C	1.04164	1.88224	1.85061
C	1.46034	2.18169	3.17907
C	0.9838	2.95343	0.92072
C	1.77926	3.47244	3.56075
H	1.48833	1.3971	3.9279
C	1.35136	4.23698	1.28292
H	0.6835	2.75849	-0.09689
C	1.73619	4.4956	2.60428
H	2.06453	3.69379	4.58239
H	1.32663	5.04141	0.55736
C	1.15606	-0.47998	2.51477
O	0.34247	-0.99998	3.23883
O	2.46295	-0.76555	2.66369
C	3.54641	-0.03483	2.06135

H	3.29242	0.36894	1.08135
H	3.84905	0.77841	2.72644
H	4.36163	-0.75119	1.95837
Br	2.20633	6.25631	3.10835

69

TS2B SCF Done: E(RB3LYP) = -5586.92717097

B	1.04642	0.33327	0.15351
C	2.44956	-0.53481	0.36568
C	3.26892	-0.84242	-0.73045
C	4.49034	-1.50488	-0.65931
C	5.00723	-1.84311	0.58501
C	4.29561	-1.47246	1.7179
C	3.07385	-0.80828	1.59398
C	0.18513	0.60851	1.55621
C	-0.42908	1.8273	1.87693
C	-1.22321	2.03196	3.00331
C	-1.4496	0.98363	3.88844
C	-0.85999	-0.24776	3.62714
C	-0.06448	-0.39654	2.4988
C	1.67174	1.75021	-0.4588

C	2.46372	2.508	0.42107
C	3.1777	3.64475	0.06005
C	3.13671	4.09115	-1.2584
C	2.3739	3.38299	-2.17583
C	1.67794	2.24745	-1.76007
F	2.92414	-0.44049	-1.98071
F	5.18076	-1.78402	-1.77571
F	6.17992	-2.47808	0.68897
F	4.80213	-1.72743	2.93274
F	2.56133	-0.3947	2.76715
F	-0.28761	2.91715	1.08882
F	-1.77245	3.23223	3.23709
F	-2.2214	1.15619	4.96585
F	-1.07204	-1.28795	4.44846
F	0.46212	-1.63002	2.33281
F	0.9461	1.65732	-2.74775
F	2.30517	3.78918	-3.45287
F	3.81477	5.18225	-1.6303
F	3.90425	4.31156	0.9662
F	2.56708	2.13952	1.71347
C	-0.26031	-0.50536	-0.68759

C	-1.49984	0.23472	-1.04761
C	-2.73647	-0.41834	-1.28849
C	-1.49702	1.63552	-1.21791
C	-3.88516	0.27089	-1.64867
H	-2.80631	-1.49287	-1.19976
C	-2.63801	2.34329	-1.57991
H	-0.6021	2.1984	-1.02476
C	-3.82808	1.65581	-1.80484
H	-4.80854	-0.26381	-1.83557
H	-2.59745	3.42079	-1.68808
C	-0.48394	-1.90951	-0.09277
O	0.23635	-2.86912	-0.26862
O	-1.58317	-1.95572	0.68765
C	-1.81914	-3.20379	1.3719
H	-1.04852	-3.35866	2.12716
H	-2.7977	-3.09305	1.83839
H	-1.8124	-4.03598	0.66435
Br	-5.38231	2.60578	-2.36142
C	-3.84746	-1.45586	-4.90944
C	-2.76818	-2.04527	-4.26873
C	-1.62805	-1.27954	-3.91751

C	-1.59186	0.09263	-4.27431
C	-2.67953	0.67733	-4.90543
C	-3.81051	-0.08827	-5.21239
H	-4.7229	-2.04593	-5.16109
H	-2.7979	-3.09877	-4.00367
H	-0.73146	0.69836	-4.02186
H	-2.66076	1.73517	-5.14506
H	-4.66465	0.3818	-5.69033
C	-0.6164	-1.88339	-3.10467
H	-0.77305	-2.92704	-2.83472
C	0.45654	-1.23374	-2.51558
H	0.7897	-0.28413	-2.89396
H	1.19853	-1.86235	-2.0497

71

TS1C SCF Done: E(RB3LYP) = -5696.43038290

B	1.89243	0.12427	0.04376
C	1.894	-0.60894	1.50418
C	0.91151	-1.43041	2.04702
C	1.04045	-2.09559	3.26505
C	2.21087	-1.95373	4.00059

C	3.23179	-1.14731	3.49976
C	3.05415	-0.50848	2.27754
C	2.10264	1.74444	0.05517
C	2.27046	2.42641	-1.15444
C	2.38066	3.81015	-1.25471
C	2.30029	4.58429	-0.09945
C	2.10794	3.95538	1.1255
C	2.01417	2.56483	1.17866
C	2.94694	-0.70672	-0.88707
C	4.2294	-0.27061	-1.22646
C	5.11919	-1.03039	-1.98543
C	4.74158	-2.29331	-2.43178
C	3.48025	-2.78007	-2.10251
C	2.63212	-1.99117	-1.33186
F	-0.27641	-1.63645	1.41013
F	0.04172	-2.86805	3.72383
F	2.35623	-2.58184	5.17313
F	4.36667	-0.99987	4.19553
F	4.07142	0.25732	1.83234
F	2.3237	1.73552	-2.31144
F	2.54881	4.40318	-2.44471

F	2.38454	5.91732	-0.17167
F	1.9717	4.68758	2.24205
F	1.74886	2.05044	2.39999
F	1.43511	-2.55136	-1.01284
F	3.09679	-3.99808	-2.51601
F	5.58161	-3.0322	-3.16565
F	6.33383	-0.55431	-2.29083
F	4.67362	0.93743	-0.83364
C	-1.70498	0.42397	-1.22428
C	-3.09543	0.74598	-0.89806
C	-3.61977	0.37893	0.35633
C	-3.97121	1.26785	-1.86628
C	-4.9735	0.52649	0.63332
H	-2.97162	-0.07354	1.09775
C	-5.32866	1.41471	-1.5953
H	-3.58874	1.56338	-2.83821
C	-5.82405	1.03608	-0.34785
H	-5.37031	0.21819	1.59303
H	-5.99671	1.81777	-2.3476
C	-0.58462	0.46424	-0.3374
O	0.51516	-0.06489	-0.69467

O	-0.65449	0.9809	0.88259
C	-1.25902	2.27202	1.14248
H	-2.2504	2.13872	1.57495
H	-0.58841	2.75141	1.85449
H	-1.32724	2.85722	0.22355
N	-1.37692	0.3621	-2.56667
N	-1.11275	-0.48966	-3.33992
C	-1.62263	-2.24309	-1.31869
C	-1.18766	-2.19772	-2.66013
H	-0.13512	-2.41958	-2.81252
H	-1.84056	-2.59625	-3.43316
Br	-7.6903	1.19289	0.01335
H	-0.85026	-2.25271	-0.56269
C	-2.9716	-2.48217	-0.8664
C	-3.18038	-2.83398	0.48768
C	-4.09934	-2.33394	-1.70466
C	-4.46507	-3.05547	0.97248
H	-2.3223	-2.92147	1.14811
C	-5.38143	-2.53062	-1.20757
H	-3.96653	-2.03289	-2.73916
C	-5.56973	-2.89797	0.12998

H -4.60839 -3.33652 2.01151

H -6.24011 -2.38989 -1.85657

H -6.57409 -3.05005 0.51332

71

IN2C SCF Done: E(RB3LYP) = -5696.48680792

B 1.88745 0.04849 0.14983

C 1.97073 -0.65241 1.61782

C 1.02533 -1.48579 2.20858

C 1.23482 -2.14928 3.41677

C 2.43888 -1.98505 4.08846

C 3.41709 -1.15988 3.5393

C 3.16613 -0.52845 2.32878

C 2.03875 1.67114 0.09977

C 2.04803 2.31862 -1.13806

C 2.08354 3.70028 -1.28808

C 2.09176 4.50567 -0.15393

C 2.06307 3.91073 1.10125

C 2.0335 2.52118 1.20446

C 2.90979 -0.77354 -0.82462

C 4.1495 -0.29899 -1.25455

C	5.02313	-1.04386	-2.04346
C	4.67295	-2.33253	-2.42814
C	3.45507	-2.85758	-2.01072
C	2.6173	-2.082	-1.21581
F	-0.18722	-1.70191	1.63269
F	0.28144	-2.94288	3.93194
F	2.65734	-2.61073	5.25309
F	4.58436	-0.98792	4.17937
F	4.14754	0.25504	1.82771
F	2.00909	1.58952	-2.27569
F	2.09969	4.26202	-2.5076
F	2.11278	5.83992	-0.27125
F	2.03176	4.67674	2.20457
F	1.94702	2.03246	2.45953
F	1.46397	-2.67384	-0.81614
F	3.10595	-4.10542	-2.3648
F	5.50069	-3.06164	-3.18901
F	6.19989	-0.52741	-2.43395
F	4.5705	0.93907	-0.92125
C	-1.77449	-0.08208	-1.1017
C	-3.13841	0.49504	-0.78423

C	-3.75157	0.22396	0.44731
C	-3.86886	1.16998	-1.76873
C	-5.08483	0.55795	0.67212
H	-3.19923	-0.29182	1.22559
C	-5.20387	1.5196	-1.55486
H	-3.41736	1.38762	-2.73123
C	-5.80587	1.18434	-0.34555
H	-5.55739	0.31068	1.61572
H	-5.77098	2.00373	-2.34084
C	-0.61762	0.31439	-0.19997
O	0.47488	-0.23659	-0.48996
O	-0.63735	1.11463	0.82225
C	-1.49255	2.28512	1.02684
H	-2.17859	2.04503	1.8636
H	-0.79155	3.0727	1.30873
H	-2.04802	2.5361	0.10076
N	-1.32145	0.35175	-2.48526
N	-1.0377	-0.5842	-3.2313
C	-1.76649	-1.69773	-1.1842
C	-1.20778	-1.90659	-2.60754
H	-0.22747	-2.40358	-2.59577

H	-1.86122	-2.49979	-3.26021
Br	-7.66867	1.55147	-0.09329
H	-1.04005	-2.07802	-0.47179
C	-3.09779	-2.34807	-0.88799
C	-3.29374	-2.95103	0.36344
C	-4.17471	-2.27408	-1.78181
C	-4.5495	-3.44619	0.72806
H	-2.46016	-2.99292	1.06311
C	-5.43121	-2.76485	-1.41943
H	-4.04257	-1.78773	-2.74605
C	-5.62323	-3.34369	-0.15938
H	-4.68771	-3.88368	1.70336
H	-6.26128	-2.66721	-2.10916
H	-6.59671	-3.67636	0.13165

71

TS2C SCF Done: E(RB3LYP) = -5696.44758027

B	-1.84301	0.19917	-0.05837
C	-1.90334	1.72257	-0.63339
C	-0.94153	2.33091	-1.43757
C	-1.08106	3.61462	-1.96348

C	-2.24101	4.33715	-1.70715
C	-3.24194	3.7636	-0.92545
C	-3.05512	2.48187	-0.41934
C	-2.10407	-0.0063	1.54558
C	-2.19282	-1.29958	2.06448
C	-2.25919	-1.59712	3.42151
C	-2.23101	-0.55425	4.34323
C	-2.12338	0.75338	3.8813
C	-2.0596	1.00052	2.51011
C	-2.77912	-0.72153	-1.03263
C	-4.08601	-1.09815	-0.71665
C	-4.89766	-1.83935	-1.57394
C	-4.4061	-2.23267	-2.8152
C	-3.11222	-1.87274	-3.17998
C	-2.3373	-1.12477	-2.29606
F	0.21833	1.69618	-1.75777
F	-0.10853	4.15168	-2.71725
F	-2.39491	5.56983	-2.20599
F	-4.36648	4.44757	-0.67419
F	-4.05257	1.96429	0.32677
F	-2.17043	-2.3707	1.22833

F	-2.32732	-2.86776	3.84447
F	-2.28124	-0.80821	5.65563
F	-2.04401	1.76556	4.75825
F	-1.87634	2.29012	2.16253
F	-1.09837	-0.78853	-2.73634
F	-2.62619	-2.241	-4.37572
F	-5.16897	-2.9487	-3.64983
F	-6.14152	-2.18223	-1.21243
F	-4.62625	-0.76276	0.47011
C	1.8315	-0.77996	0.13418
C	3.14143	-0.10463	0.22595
C	3.32714	1.14911	-0.38898
C	4.22559	-0.67895	0.91237
C	4.55295	1.8067	-0.32275
H	2.50186	1.60839	-0.92531
C	5.45557	-0.03324	0.98265
H	4.10184	-1.63935	1.39874
C	5.61158	1.20726	0.3614
H	4.68823	2.7689	-0.80324
H	6.28459	-0.48305	1.51662
C	0.65203	-0.01451	0.31713

O	-0.42505	-0.40146	-0.25225
O	0.55637	1.09511	1.03404
C	1.38187	1.39172	2.17915
H	2.22831	2.01112	1.88035
H	0.72253	1.94107	2.8521
H	1.73449	0.47256	2.64845
N	1.11304	-2.1167	2.24214
N	0.71617	-3.05895	1.77206
C	1.68771	-2.09044	-0.59833
C	0.57651	-3.00368	-0.29846
H	-0.43269	-2.62323	-0.22409
H	0.68555	-4.04154	-0.59915
Br	7.29597	2.09612	0.45215
H	1.17949	-1.75905	-1.55145
C	2.98787	-2.79172	-0.94247
C	3.74592	-2.3535	-2.03375
C	3.4598	-3.85434	-0.16392
C	4.96103	-2.96422	-2.34023
H	3.39028	-1.52032	-2.63397
C	4.67739	-4.46539	-0.46901
H	2.88426	-4.20087	0.68959

C	5.43076	-4.02065	-1.55642
H	5.54035	-2.61485	-3.18938
H	5.03564	-5.28717	0.14377
H	6.37804	-4.49541	-1.79348

55

E-IN1C SCF Done: E(RB3LYP) = -5386.78022101

B	1.39551	0.10783	-0.08113
C	1.28246	1.06089	-1.39975
C	0.22069	1.89982	-1.73208
C	0.24257	2.76033	-2.82927
C	1.37524	2.82544	-3.63034
C	2.47309	2.02787	-3.32099
C	2.40387	1.1817	-2.22198
C	1.78624	-1.45919	-0.33165
C	1.98229	-2.28911	0.77661
C	2.24693	-3.65058	0.68949
C	2.30497	-4.25047	-0.56447
C	2.08702	-3.47667	-1.6967
C	1.82193	-2.11407	-1.56187
C	2.34069	0.91572	0.97964

C	3.65195	0.5845	1.31506
C	4.42522	1.33067	2.20244
C	3.89233	2.47518	2.78363
C	2.5962	2.86093	2.46046
C	1.86048	2.08881	1.56785
F	-0.9134	1.93133	-0.99067
F	-0.81978	3.53441	-3.11039
F	1.41471	3.65228	-4.68538
F	3.58105	2.08949	-4.07834
F	3.49944	0.43454	-1.95367
F	1.9108	-1.77122	2.02433
F	2.43645	-4.38955	1.79524
F	2.55441	-5.56216	-0.67706
F	2.11439	-4.05012	-2.91162
F	1.57104	-1.45538	-2.71317
F	0.62154	2.53943	1.26714
F	2.07179	3.97332	3.00252
F	4.62055	3.20316	3.64223
F	5.67975	0.95351	2.50178
F	4.24584	-0.50711	0.78669
C	-2.05442	-0.87309	1.19522

C	-3.51841	-0.78219	1.01243
C	-4.04101	0.22805	0.18863
C	-4.39009	-1.62313	1.71896
C	-5.41831	0.39818	0.07323
H	-3.37282	0.89748	-0.34574
C	-5.76845	-1.44322	1.62617
H	-3.99488	-2.40968	2.35721
C	-6.26866	-0.42851	0.80888
H	-5.81742	1.1834	-0.55973
H	-6.43937	-2.08508	2.18655
C	-1.02391	-0.55522	0.24543
O	0.03186	-0.00025	0.68152
O	-1.10961	-0.79774	-1.03393
C	-2.03989	-1.75197	-1.61556
H	-2.97306	-1.24463	-1.8638
H	-1.53847	-2.09546	-2.52006
H	-2.21275	-2.58254	-0.92913
N	-1.57948	-1.01421	2.42959
N	-1.17094	-1.19643	3.46433
Br	-8.15825	-0.14305	0.71857

E-TS3C SCF Done: E(RB3LYP) = -5386.73751430

B	1.30362	0.10001	-0.05971
C	1.23398	1.05414	-1.38328
C	0.1646	1.86709	-1.75431
C	0.21039	2.74003	-2.84099
C	1.37143	2.83869	-3.59636
C	2.47363	2.06163	-3.25208
C	2.38211	1.20629	-2.16152
C	1.74758	-1.45813	-0.29135
C	1.9137	-2.2843	0.82345
C	2.19844	-3.6429	0.74738
C	2.30892	-4.24291	-0.50251
C	2.12317	-3.4719	-1.64269
C	1.83902	-2.11287	-1.51814
C	2.21401	0.91753	1.02845
C	3.53054	0.60769	1.36764
C	4.28846	1.35959	2.26302
C	3.73474	2.4906	2.85037
C	2.43362	2.85627	2.52411
C	1.71298	2.07826	1.62305

F	-1.00383	1.85945	-1.06735
F	-0.85797	3.49319	-3.1568
F	1.43212	3.67594	-4.6428
F	3.60724	2.15252	-3.96801
F	3.484	0.48208	-1.85697
F	1.78933	-1.76778	2.06882
F	2.35791	-4.37881	1.86076
F	2.57735	-5.55248	-0.60544
F	2.19767	-4.04685	-2.85563
F	1.61663	-1.45788	-2.67769
F	0.47047	2.51502	1.31713
F	1.891	3.95859	3.07023
F	4.44879	3.22515	3.71598
F	5.5489	1.00117	2.56259
F	4.15029	-0.46688	0.83304
C	-2.09801	-1.20936	0.93717
C	-3.48056	-0.87764	0.96208
C	-3.97345	0.27826	0.30095
C	-4.39799	-1.74377	1.60851
C	-5.3352	0.53636	0.25177
H	-3.27722	0.95681	-0.18254

C	-5.75654	-1.47257	1.59459
H	-4.02262	-2.62556	2.11822
C	-6.21041	-0.33846	0.90689
H	-5.71255	1.40806	-0.27072
H	-6.45854	-2.13185	2.09201
C	-1.06649	-0.68255	0.13904
O	-0.08834	-0.01697	0.62319
O	-1.0081	-0.99332	-1.14506
C	-1.9299	-1.93446	-1.74714
H	-2.91313	-1.47647	-1.87476
H	-1.49037	-2.16479	-2.71714
H	-2.00114	-2.83682	-1.13307
N	-1.33595	-0.90769	2.68187
N	-0.93814	-1.31578	3.63307
Br	-8.07684	0.02367	0.86421

53

E-IN3C SCF Done: E(RB3LYP) = -5277.23060857

B	1.26344	0.04737	-0.11641
C	1.24139	1.01405	-1.43694
C	0.18536	1.83255	-1.83392

C	0.26381	2.71357	-2.91213
C	1.44557	2.81393	-3.63463
C	2.53516	2.03151	-3.26439
C	2.41143	1.16977	-2.18163
C	1.76063	-1.49723	-0.34133
C	1.95016	-2.31858	0.77302
C	2.23938	-3.67621	0.69884
C	2.34418	-4.27912	-0.54955
C	2.15377	-3.50988	-1.69023
C	1.86326	-2.1522	-1.56743
C	2.12227	0.87858	1.0024
C	3.45383	0.61438	1.32689
C	4.19909	1.39397	2.20805
C	3.61707	2.50899	2.79796
C	2.29917	2.82796	2.49018
C	1.59018	2.02132	1.60391
F	-1.005	1.81836	-1.18413
F	-0.79365	3.47163	-3.25318
F	1.53675	3.65622	-4.67501
F	3.68777	2.1214	-3.94976
F	3.50483	0.44385	-1.85228

F	1.85285	-1.80043	2.01871
F	2.41104	-4.40664	1.81423
F	2.61572	-5.58844	-0.65074
F	2.23084	-4.08602	-2.90303
F	1.64565	-1.49887	-2.72873
F	0.33108	2.4172	1.31129
F	1.73098	3.91727	3.03695
F	4.32104	3.27292	3.64639
F	5.47536	1.07833	2.48879
F	4.10624	-0.4378	0.78684
C	-2.16223	-1.323	0.59057
C	-3.46359	-0.8936	0.77989
C	-3.96424	0.32828	0.21639
C	-4.37913	-1.76482	1.45412
C	-5.31005	0.62578	0.26846
H	-3.2692	1.00253	-0.2749
C	-5.72521	-1.46724	1.51383
H	-3.99563	-2.67943	1.89328
C	-6.17664	-0.28545	0.90118
H	-5.69849	1.53406	-0.17851
H	-6.42469	-2.1355	2.00242

C	-1.0964	-0.77087	-0.11964
O	-0.16794	-0.12207	0.48279
O	-0.91231	-1.06527	-1.39722
C	-1.95869	-1.73907	-2.139
H	-2.8478	-1.11414	-2.1902
H	-1.55301	-1.88087	-3.13475
H	-2.19287	-2.69865	-1.68042
Br	-8.03015	0.08543	0.90803

69

E-TS4C SCF Done: E(RB3LYP) = -5586.90833017

B	1.79905	0.07798	-0.02815
C	2.28604	1.62131	-0.26976
C	1.51628	2.76311	-0.05528
C	2.01829	4.0585	-0.18069
C	3.35173	4.2504	-0.51705
C	4.16569	3.14067	-0.72407
C	3.62189	1.86993	-0.58816
C	2.05307	-0.9725	-1.26097
C	1.77458	-2.32668	-1.06423
C	1.85195	-3.29067	-2.06298

C	2.21614	-2.90581	-3.34852
C	2.4845	-1.56685	-3.60323
C	2.39029	-0.63542	-2.57057
C	2.48064	-0.3814	1.39431
C	3.61499	-1.18572	1.50735
C	4.20486	-1.51562	2.72565
C	3.66412	-1.02249	3.90668
C	2.54284	-0.20348	3.84703
C	1.9898	0.10599	2.60785
F	0.20957	2.68249	0.29673
F	1.22203	5.12266	0.02674
F	3.85086	5.48975	-0.63998
F	5.45949	3.31028	-1.04645
F	4.45769	0.82424	-0.78631
F	1.39631	-2.76907	0.16052
F	1.5758	-4.5805	-1.80219
F	2.29466	-3.81426	-4.33215
F	2.81274	-1.17758	-4.84806
F	2.61802	0.64795	-2.92406
F	0.91829	0.93435	2.63186
F	2.01167	0.28901	4.97999

F	4.21757	-1.33226	5.08867
F	5.29088	-2.30694	2.76957
F	4.20891	-1.70586	0.41089
C	-1.93368	-0.28879	-0.48225
C	-3.15946	0.38507	-0.35229
C	-3.23889	1.75145	0.05238
C	-4.36986	-0.3035	-0.65627
C	-4.45962	2.39478	0.14456
H	-2.32327	2.28502	0.28856
C	-5.59594	0.33569	-0.56159
H	-4.31735	-1.33417	-0.98613
C	-5.62737	1.67595	-0.15912
H	-4.5162	3.43422	0.44747
H	-6.51273	-0.1928	-0.79613
C	-0.63591	0.18902	-0.63098
O	0.28889	0.00285	0.23907
O	-0.24672	0.71664	-1.79335
C	-1.17995	0.88497	-2.88074
H	-1.91124	1.66164	-2.64417
H	-0.5678	1.1915	-3.72908
H	-1.68491	-0.06166	-3.09865

Br	-7.308	2.5557	-0.02529
C	-2.74949	-1.76206	1.99689
C	-1.43348	-1.61872	1.7022
H	-0.88806	-2.29584	1.05458
H	-0.84424	-0.86682	2.21299
H	-3.18719	-1.06145	2.70716
C	-3.69122	-2.68952	1.39114
C	-5.05454	-2.58948	1.73942
C	-3.31304	-3.63424	0.41106
C	-6.01067	-3.40394	1.13379
H	-5.35704	-1.85887	2.48538
C	-4.26858	-4.44286	-0.1931
H	-2.27191	-3.72217	0.11668
C	-5.62049	-4.33071	0.16443
H	-7.05647	-3.31198	1.41313
H	-3.96573	-5.16351	-0.94762
H	-6.36203	-4.96497	-0.31346

55

Z-IN1C SCF Done: E(RB3LYP) = -5386.78963100

C	1.11668	1.16753	2.63834
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N	1.55514	1.9382	3.63211
N	1.96454	2.6104	4.44124
C	2.17117	0.6106	1.7525
C	3.05626	1.47203	1.0879
C	2.35037	-0.77522	1.65215
C	4.09806	0.95926	0.31819
H	2.92242	2.54693	1.16018
C	3.37968	-1.29896	0.87199
H	1.69811	-1.44497	2.19733
C	4.24889	-0.425	0.22094
H	4.77363	1.6286	-0.20165
H	3.50942	-2.37243	0.79227
C	-0.29513	0.90733	2.68868
O	-1.02515	0.40532	1.79661
O	-0.86269	1.24184	3.834
C	-2.31509	1.17183	3.90946
H	-2.55238	1.48228	4.92347
H	-2.75029	1.85654	3.18024
H	-2.65004	0.15445	3.71952
B	-1.0676	0.13071	0.25574
C	-0.16586	1.28631	-0.4491

C	-0.51682	2.62359	-0.24331
C	0.16872	3.69993	-0.792
C	1.28491	3.45449	-1.58708
C	1.68331	2.14364	-1.81097
C	0.96261	1.09522	-1.24326
C	-2.67048	0.22829	-0.09885
C	-3.60367	-0.4595	0.68285
C	-4.96862	-0.48667	0.41547
C	-5.45603	0.18082	-0.70272
C	-4.56687	0.85868	-1.52685
C	-3.20764	0.86555	-1.21817
C	-0.6616	-1.42239	-0.01141
C	-0.67947	-1.89806	-1.32396
C	-0.44377	-3.2215	-1.67119
C	-0.20311	-4.15302	-0.66468
C	-0.2067	-3.73619	0.65969
C	-0.45496	-2.39814	0.96042
F	-1.58988	2.919	0.52891
F	-0.22955	4.96277	-0.56672
F	1.97643	4.47342	-2.11449
F	2.79493	1.89493	-2.52249

F	1.46779	-0.13556	-1.45763
F	-3.19662	-1.17304	1.75978
F	-5.81354	-1.16149	1.21279
F	-6.76604	0.1639	-0.98506
F	-5.0226	1.49815	-2.61678
F	-2.4181	1.53198	-2.08738
F	-0.4511	-2.09178	2.2818
F	0.02186	-4.62308	1.64258
F	0.03035	-5.43662	-0.97072
F	-0.45737	-3.61134	-2.9559
F	-0.93768	-1.03535	-2.3327
Br	5.6972	-1.14183	-0.80495

55

Z-TS3C SCF Done: E(RB3LYP) = -5386.74443038

C	1.04642	1.3016	2.257
N	1.65734	1.97513	3.93581
N	2.14807	2.79677	4.50027
C	2.18073	0.70983	1.6276
C	3.09979	1.55348	0.95504
C	2.3849	-0.69115	1.58237

C	4.14744	1.02316	0.22123
H	2.94151	2.62625	0.98606
C	3.42712	-1.23053	0.84469
H	1.70398	-1.34047	2.11725
C	4.29406	-0.36933	0.16225
H	4.82573	1.66452	-0.32765
H	3.56662	-2.30335	0.78468
C	-0.22956	0.80186	2.58023
O	-1.08864	0.43941	1.71345
O	-0.64357	0.8642	3.84025
C	-2.0448	0.5681	4.07766
H	-2.15451	0.62129	5.15965
H	-2.67438	1.31195	3.58436
H	-2.2888	-0.42336	3.69764
B	-1.09879	0.12289	0.18367
C	-0.16396	1.24458	-0.54034
C	-0.47502	2.59385	-0.33822
C	0.26168	3.64907	-0.86565
C	1.38321	3.36652	-1.64174
C	1.73646	2.04032	-1.86917
C	0.96919	1.01581	-1.3187

C	-2.68866	0.22211	-0.19551
C	-3.62742	-0.46716	0.57781
C	-4.99413	-0.47227	0.31539
C	-5.47419	0.2228	-0.79131
C	-4.57719	0.90198	-1.60923
C	-3.21598	0.88504	-1.30458
C	-0.67641	-1.43811	-0.03565
C	-0.71182	-1.94929	-1.33618
C	-0.46289	-3.27933	-1.65319
C	-0.18413	-4.18033	-0.62627
C	-0.16159	-3.72709	0.68761
C	-0.42512	-2.38349	0.9543
F	-1.54452	2.92164	0.41424
F	-0.08771	4.92129	-0.63184
F	2.12654	4.35878	-2.14374
F	2.85821	1.75798	-2.55038
F	1.4531	-0.22873	-1.50635
F	-3.22414	-1.2024	1.64308
F	-5.8441	-1.14535	1.10552
F	-6.78329	0.23205	-1.0673
F	-5.02726	1.56583	-2.68291

F	-2.41672	1.55495	-2.15766
F	-0.3771	-2.03707	2.27162
F	0.10945	-4.57983	1.68771
F	0.06366	-5.46558	-0.90276
F	-0.49373	-3.70407	-2.92278
F	-0.9908	-1.11524	-2.35826
Br	5.70031	-1.10337	-0.87267

53

Z-IN3C SCF Done: E(RB3LYP) = -5277.24196518

C	0.99226	1.25711	2.04862
C	2.17324	0.66694	1.62292
C	3.15219	1.50822	1.00452
C	2.3857	-0.74952	1.60898
C	4.21945	0.96599	0.31536
H	3.00592	2.58235	1.03684
C	3.46383	-1.29511	0.94327
H	1.67594	-1.3905	2.11551
C	4.34803	-0.43165	0.27346
H	4.93008	1.60062	-0.20013
H	3.60982	-2.36852	0.90692

C	-0.2346	0.76867	2.49054
O	-1.23071	0.50218	1.72088
O	-0.45837	0.77299	3.7962
C	-1.79419	0.40675	4.23415
H	-1.76361	0.5266	5.31765
H	-2.54011	1.06879	3.79416
H	-2.0029	-0.62757	3.95976
B	-1.2047	0.17189	0.21711
C	-0.27067	1.30736	-0.5067
C	-0.61517	2.65531	-0.34012
C	0.11536	3.71635	-0.86147
C	1.26533	3.44759	-1.59634
C	1.65483	2.12634	-1.78955
C	0.89057	1.09586	-1.25063
C	-2.78918	0.23176	-0.1936
C	-3.71992	-0.45763	0.58881
C	-5.08439	-0.48049	0.32201
C	-5.57009	0.19374	-0.79291
C	-4.68012	0.86844	-1.61955
C	-3.32073	0.86916	-1.31265
C	-0.74634	-1.38265	-0.01512

C	-0.73996	-1.88226	-1.31963
C	-0.46995	-3.20436	-1.64555
C	-0.21292	-4.11453	-0.62353
C	-0.22765	-3.67488	0.69312
C	-0.50818	-2.33722	0.96953
F	-1.71715	2.9752	0.36738
F	-0.27054	4.98595	-0.66084
F	1.99607	4.44808	-2.10081
F	2.79178	1.85657	-2.4515
F	1.40658	-0.14141	-1.40698
F	-3.31286	-1.1704	1.66485
F	-5.93086	-1.15169	1.12133
F	-6.88189	0.18687	-1.06925
F	-5.13654	1.51368	-2.70623
F	-2.52358	1.53665	-2.17534
F	-0.49344	-2.00876	2.28915
F	0.02395	-4.53901	1.69073
F	0.05026	-5.39749	-0.90832
F	-0.46313	-3.61406	-2.92432
F	-0.99995	-1.04055	-2.34595
Br	5.75727	-1.18526	-0.74025

69

Z-TS4C SCF Done: E(RB3LYP) = -5586.91838556

C	0.96561	1.3024	1.27494
C	1.93943	0.49408	0.69567
C	2.90761	1.09495	-0.16816
C	1.96967	-0.92782	0.85574
C	3.80999	0.32421	-0.88008
H	2.90307	2.17261	-0.27938
C	2.8746	-1.69934	0.15589
H	1.25696	-1.39433	1.52568
C	3.78186	-1.06413	-0.71091
H	4.52653	0.78491	-1.54847
H	2.88332	-2.77772	0.26508
C	-0.19081	1.03758	2.00485
O	-1.35798	0.82414	1.49779
O	-0.14273	1.22244	3.31916
C	-1.3934	1.1612	4.05325
H	-1.10418	1.31501	5.0929
H	-2.06871	1.95377	3.72291
H	-1.86425	0.18716	3.91967

B	-1.78546	0.21888	0.15117
C	-0.78759	0.80216	-1.00563
C	-0.67405	2.18977	-1.1496
C	0.22429	2.81044	-2.00922
C	1.07488	2.02324	-2.77729
C	0.99303	0.63837	-2.68133
C	0.07055	0.05917	-1.81503
C	-3.34968	0.70125	0.01184
C	-4.22432	0.50859	1.08486
C	-5.57086	0.85818	1.05715
C	-6.10543	1.41383	-0.09965
C	-5.28246	1.60366	-1.20262
C	-3.93848	1.24292	-1.12986
C	-1.8173	-1.41559	0.26515
C	-2.36978	-2.13959	-0.79394
C	-2.53109	-3.51829	-0.79402
C	-2.13335	-4.24675	0.32403
C	-1.57573	-3.57651	1.40415
C	-1.43845	-2.18924	1.35738
F	-1.46382	2.99922	-0.41474
F	0.29424	4.14857	-2.08965

F	1.9797	2.59025	-3.58428
F	1.85089	-0.12568	-3.37549
F	0.12351	-1.28813	-1.73637
F	-3.78547	-0.06443	2.22989
F	-6.35754	0.65434	2.12803
F	-7.40039	1.75752	-0.15224
F	-5.79015	2.13063	-2.33016
F	-3.21808	1.44676	-2.25442
F	-0.86475	-1.63154	2.45753
F	-1.17428	-4.26551	2.48598
F	-2.27647	-5.57964	0.35094
F	-3.06008	-4.15306	-1.85295
F	-2.75298	-1.48035	-1.91161
Br	5.01253	-2.13264	-1.68307
C	6.65304	1.60984	0.77969
C	5.6877	2.44591	1.33686
C	4.71226	1.94199	2.2231
C	4.75721	0.56951	2.55192
C	5.72183	-0.26364	1.99548
C	6.66805	0.24893	1.09993
H	7.38847	2.01613	0.09063

H	5.66915	3.50139	1.07608
H	4.0318	0.15422	3.24401
H	5.73363	-1.3194	2.25149
H	7.41305	-0.40769	0.65971
C	3.66905	2.84387	2.71256
H	3.80331	3.89401	2.45482
C	2.54148	2.47712	3.35251
H	2.34644	1.45691	3.66403
H	1.80088	3.21413	3.64506

69

TS5C SCF Done: E(RB3LYP) = -5586.91474493

B	1.56026	-0.30651	-0.28591
C	1.80773	0.07252	-1.85429
C	0.91162	0.67937	-2.72971
C	1.24872	1.07131	-4.02526
C	2.54497	0.87435	-4.48677
C	3.48559	0.28891	-3.64164
C	3.10133	-0.08418	-2.35888
C	1.92374	-1.8333	0.15881
C	1.87866	-2.18214	1.51077

C	2.0726	-3.47271	1.99025
C	2.31653	-4.50037	1.08261
C	2.34903	-4.21181	-0.27731
C	2.14405	-2.90145	-0.71119
C	2.29325	0.88543	0.56077
C	3.48137	0.75868	1.28212
C	4.09348	1.82673	1.93952
C	3.52196	3.09431	1.87888
C	2.35219	3.27396	1.14687
C	1.78291	2.18386	0.49779
F	-0.37546	0.92807	-2.37061
F	0.33201	1.64048	-4.82491
F	2.88619	1.24559	-5.72711
F	4.74158	0.09893	-4.06888
F	4.04962	-0.63061	-1.5691
F	1.61882	-1.23255	2.44253
F	2.01851	-3.73648	3.30437
F	2.50193	-5.75367	1.51414
F	2.55457	-5.19851	-1.16291
F	2.13837	-2.72554	-2.04742
F	0.66475	2.44097	-0.22767

F	1.78468	4.49269	1.0695
F	4.09062	4.12757	2.5106
F	5.22562	1.64244	2.63188
F	4.10328	-0.42918	1.38397
C	-2.18321	-0.9812	0.30251
C	-3.24112	-0.08854	-0.03612
C	-2.99336	1.17124	-0.64727
C	-4.57959	-0.4092	0.31828
C	-4.03082	2.06071	-0.90311
H	-1.97581	1.45408	-0.88869
C	-5.61788	0.46462	0.05626
H	-4.76971	-1.36207	0.80224
C	-5.33037	1.70196	-0.54705
H	-3.83339	3.02634	-1.35231
H	-6.63984	0.21661	0.31858
C	-0.91408	-0.86689	-0.32207
O	0.04916	-0.1706	0.13764
O	-0.65547	-1.60912	-1.39145
C	-1.70102	-2.39752	-1.98834
H	-2.42314	-1.74641	-2.48777
H	-1.19627	-3.03102	-2.71632

H	-2.20512	-2.99711	-1.22406
C	-1.48665	3.66118	1.63025
C	-2.68098	4.37002	1.80038
C	-3.80322	3.73629	2.34421
C	-3.72783	2.40094	2.72513
C	-2.53425	1.6677	2.55786
C	-1.41454	2.32254	1.99928
H	-0.61457	4.14147	1.2015
H	-2.73749	5.41405	1.50634
H	-4.73299	4.28342	2.46668
H	-4.60156	1.90543	3.13988
H	-0.49543	1.77334	1.84144
Br	-6.74724	2.92955	-0.84353
C	-2.53283	0.25564	2.88414
H	-3.47385	-0.1196	3.28582
C	-1.56157	-0.66009	2.61225
H	-1.70219	-1.69375	2.90375
H	-0.563	-0.38142	2.3058

71

TS1A-2iso SCF Done: E(RB3LYP) = -5696.42738306

N	0.11643	1.21238	-0.64891
N	-0.65928	0.31032	-0.83351
B	-1.71411	-0.15109	0.27999
C	-2.60851	1.12409	0.76174
C	-2.93558	2.16625	-0.10546
C	-3.68687	3.2736	0.27737
C	-4.19834	3.34107	1.5688
C	-3.94687	2.29444	2.45335
C	-3.16979	1.21609	2.03631
C	-0.65019	-0.77232	1.37107
C	-0.07522	-2.03306	1.19096
C	0.98991	-2.51451	1.94881
C	1.54693	-1.70901	2.93557
C	1.01173	-0.44381	3.15769
C	-0.05178	0.00082	2.37264
C	-2.714	-1.24291	-0.39888
C	-3.36528	-2.19998	0.38165
C	-4.28007	-3.11614	-0.12931
C	-4.58489	-3.08911	-1.48806
C	-3.96978	-2.1465	-2.30536
C	-3.06129	-1.24568	-1.75035

F	-2.52224	2.14286	-1.39331
F	-3.9112	4.27885	-0.59229
F	-4.92725	4.39463	1.95541
F	-4.44359	2.34187	3.69703
F	-2.94892	0.24349	2.94045
F	-0.49041	-2.84503	0.18929
F	1.51139	-3.72973	1.70485
F	2.60623	-2.13238	3.63572
F	1.5514	0.35065	4.09
F	-0.44119	1.26908	2.59148
F	-2.52078	-0.34872	-2.60925
F	-4.25759	-2.10728	-3.61524
F	-5.46126	-3.96096	-2.00161
F	-4.86489	-4.02154	0.66745
F	-3.10305	-2.27732	1.7027
C	1.14537	1.66168	-1.48722
C	2.50487	1.37866	-0.91417
C	3.65559	2.01905	-1.39754
C	2.64551	0.36744	0.0484
C	4.91618	1.63746	-0.94419
H	3.56794	2.79608	-2.14702

C	3.90006	-0.01562	0.51257
H	1.77528	-0.14	0.43887
C	5.03116	0.61661	0.00158
H	5.80482	2.12547	-1.3276
H	3.98932	-0.80032	1.25513
C	0.87761	3.09031	-1.97223
O	1.54315	3.63779	-2.82526
O	-0.20047	3.59667	-1.38165
C	-0.69685	4.86249	-1.87113
H	-1.71883	4.92321	-1.50049
H	-0.0841	5.67691	-1.4776
H	-0.67206	4.88155	-2.96246
Br	6.75975	0.06416	0.58349
C	2.05892	0.02236	-3.46283
C	0.87032	0.68736	-3.1664
H	0.60033	1.48593	-3.84931
H	0.02514	0.12144	-2.74843
C	2.5603	-1.15391	-2.81312
C	3.92313	-1.4958	-2.98474
C	1.76265	-1.95384	-1.95608
C	4.47709	-2.56818	-2.29843

H	4.54306	-0.88814	-3.63782
C	2.31196	-3.04674	-1.30253
H	0.71783	-1.71249	-1.79541
C	3.67212	-3.34483	-1.45739
H	5.53102	-2.80049	-2.41211
H	1.69165	-3.64601	-0.64826
H	4.10386	-4.18209	-0.91718
H	2.73092	0.4899	-4.18077

71

TS1C-2iso SCF Done: E(RB3LYP) = -5696.40625435

B	-1.49333	-0.29864	0.20664
C	-1.50921	-1.11562	1.61449
C	-0.41215	-1.50396	2.37747
C	-0.52112	-2.12352	3.62171
C	-1.77843	-2.3574	4.16321
C	-2.90852	-1.97017	3.44759
C	-2.74888	-1.35747	2.21188
C	-2.27443	-0.9811	-1.05293
C	-2.34117	-0.28736	-2.26413
C	-2.91841	-0.79635	-3.42075

C	-3.46635	-2.0751	-3.39675
C	-3.41141	-2.81463	-2.22205
C	-2.81484	-2.2662	-1.08731
C	-1.94585	1.23588	0.53622
C	-3.19215	1.78408	0.23217
C	-3.54297	3.09878	0.53244
C	-2.62555	3.92727	1.16829
C	-1.3801	3.41654	1.51531
C	-1.07787	2.093	1.21423
F	0.85946	-1.31212	1.93699
F	0.58011	-2.49138	4.29718
F	-1.90384	-2.95135	5.35776
F	-4.13132	-2.18904	3.95695
F	-3.8744	-0.9926	1.55792
F	-1.80927	0.95611	-2.3596
F	-2.95004	-0.07343	-4.55191
F	-4.02972	-2.59026	-4.49734
F	-3.91693	-4.05896	-2.19309
F	-2.7668	-3.07357	-0.00724
F	0.13777	1.65284	1.61889
F	-0.47371	4.20598	2.11925

F	-2.93925	5.19871	1.44979
F	-4.75494	3.57448	0.20385
F	-4.13658	1.05045	-0.39198
C	1.96643	-0.59491	-1.5048
C	3.19545	-0.28207	-0.70016
C	3.06641	0.34808	0.54646
C	4.47741	-0.49614	-1.23045
C	4.19339	0.78126	1.2416
H	2.08955	0.54171	0.9687
C	5.60897	-0.07727	-0.5356
H	4.60933	-0.98705	-2.18881
C	5.45545	0.56899	0.69116
H	4.07951	1.28974	2.1921
H	6.59568	-0.24249	-0.95434
C	0.74597	-1.02153	-0.76167
O	-0.02544	-0.11686	-0.3491
O	0.36642	-2.26365	-0.63513
C	1.25572	-3.39043	-0.35946
H	1.30408	-3.48294	0.72635
H	0.77012	-4.25673	-0.80506
H	2.24587	-3.2411	-0.78496

N	2.2464	-1.62975	-2.52692
N	2.3756	-1.62203	-3.67968
C	1.34492	2.06545	-1.70586
C	1.4966	0.94848	-2.53011
H	0.5867	0.56765	-2.99184
H	2.36527	0.8797	-3.18926
Br	7.00641	1.18136	1.62828
H	0.35036	2.26051	-1.31594
C	2.39868	2.91474	-1.20718
C	2.11734	3.80499	-0.14128
C	3.72558	2.87482	-1.70183
C	3.11911	4.58642	0.42619
H	1.11053	3.85477	0.25952
C	4.72255	3.65715	-1.13112
H	3.97372	2.2149	-2.52709
C	4.42917	4.51229	-0.05962
H	2.88055	5.24832	1.25518
H	5.73718	3.59872	-1.51557
H	5.21443	5.11507	0.38907

TS1D-N₂ SCF Done: E(RB3LYP) = -3178.44662283

C	-2.04363	0.38273	0.65535
N	-2.61212	1.92641	-0.46158
N	-2.95131	2.98532	-0.45959
C	-0.63201	0.21815	0.39878
C	-0.07496	-0.97643	-0.11768
C	0.24918	1.27155	0.73578
C	1.29769	-1.11495	-0.27695
H	-0.73033	-1.80922	-0.34681
C	1.6181	1.16232	0.53349
H	-0.16626	2.18361	1.1527
C	2.13307	-0.03821	0.0345
H	1.72132	-2.03868	-0.65406
H	2.28529	1.98058	0.77835
C	-3.00794	-0.64233	0.33719
O	-2.89715	-1.73465	0.88935
O	-4.06094	-0.29522	-0.4354
C	-5.08544	-1.29952	-0.53724
H	-5.83859	-0.88003	-1.20444
H	-4.68081	-2.22711	-0.95125
H	-5.51796	-1.51247	0.44415

Br 4.01351 -0.21504 -0.21203

37

TS1E SCF Done: E(RB3LYP) = -3488.14699409

N -0.15301 1.11291 0.68976

N 0.62396 0.2546 0.91199

C -1.25606 1.62478 1.34302

C -2.53984 1.57573 0.64012

C -3.67232 2.28314 1.08777

C -2.69458 0.69647 -0.45119

C -4.91104 2.10518 0.47735

H -3.58263 2.95402 1.93082

C -3.92813 0.51306 -1.0619

H -1.84055 0.13898 -0.82122

C -5.03563 1.2143 -0.58575

H -5.77722 2.64914 0.83647

H -4.03307 -0.17692 -1.89095

C -0.9314 2.6055 2.40013

O -1.75276 3.17474 3.09964

O 0.40392 2.73724 2.58041

C 0.7874 3.5951 3.66752

H	1.87716	3.60095	3.66275
H	0.39551	4.60456	3.51909
H	0.4079	3.20783	4.61722
Br	-6.74447	0.93965	-1.39633
C	-1.20159	-0.24551	2.88533
C	0.11733	-0.6244	2.58159
H	0.91846	-0.20363	3.18276
H	0.32001	-1.6255	2.21535
H	-1.36686	0.46893	3.68547
C	-2.38743	-0.9608	2.42395
C	-3.65769	-0.55826	2.8832
C	-2.32939	-1.99361	1.46594
C	-4.8184	-1.16018	2.408
H	-3.7241	0.25485	3.60088
C	-3.4911	-2.6042	1.00159
H	-1.37021	-2.31491	1.07209
C	-4.74188	-2.18694	1.46354
H	-5.78619	-0.81975	2.76406
H	-3.42187	-3.3983	0.26349
H	-5.64791	-2.65194	1.08706

TS1F SCF Done: E(RB3LYP) = -3488.12288841

N	-0.22431	1.84166	-0.3643
N	-1.23971	1.31765	-0.1701
C	0.91737	1.65401	-1.24987
C	2.12547	1.21391	-0.45712
C	3.41643	1.33632	-0.98994
C	1.96009	0.53102	0.75804
C	4.51056	0.76353	-0.34439
H	3.56096	1.84274	-1.93424
C	3.04861	-0.0369	1.41401
H	0.9762	0.42627	1.20197
C	4.31776	0.07109	0.84688
H	5.49929	0.83541	-0.78163
H	2.9103	-0.56925	2.34798
C	1.07235	2.88844	-2.12227
O	1.95439	3.02348	-2.94422
O	0.06178	3.75962	-1.96119
C	0.09322	4.90181	-2.84002
H	-0.7808	5.49509	-2.5741
H	1.0118	5.4736	-2.68747

H	0.0435	4.58262	-3.88413
Br	5.80525	-0.76273	1.70715
C	1.47639	-0.02026	-3.24252
C	0.42355	0.34042	-2.37817
H	-0.44357	0.80867	-2.85111
H	0.09397	-0.38861	-1.63217
C	2.52108	-0.96651	-2.95962
C	3.62778	-1.06139	-3.84016
C	2.526	-1.80838	-1.81894
C	4.68796	-1.92148	-3.58009
H	3.64762	-0.4304	-4.72522
C	3.59079	-2.66028	-1.55969
H	1.70161	-1.76745	-1.11569
C	4.68267	-2.72284	-2.43364
H	5.52726	-1.96425	-4.2689
H	3.57765	-3.27603	-0.66487
H	5.51611	-3.38577	-2.22232
H	1.58437	0.55192	-4.15969

14

Re1 SCF Done: E(RB3LYP) = -415.94861405

C	-6.41406	3.0625	0.
O	-5.95931	1.81704	-0.28908
O	-5.72615	4.0639	0.04566
C	-7.85116	3.06965	0.25041
N	-8.55293	1.96928	0.18304
N	-9.15444	1.00517	0.12273
C	-4.53903	1.7003	-0.54881
H	-4.21071	2.5801	-1.10693
H	-8.37598	3.9807	0.49578
C	-3.74967	1.54123	0.7409
H	-2.69132	1.38022	0.51039
H	-3.83359	2.44117	1.35466
H	-4.11016	0.68332	1.31592
H	-4.45403	0.81544	-1.18384

48

IN1G SCF Done: E(RB3LYP) = -2624.24040218

C	1.19745	1.08417	2.27581
O	1.1941	1.17726	3.58395
O	0.35101	0.33336	1.70752
C	2.17771	1.85939	1.59987

N	3.07595	2.50516	2.31426
N	3.87023	3.03953	2.91317
C	0.15286	0.45903	4.3415
H	-0.79649	0.60103	3.82138
H	2.26363	1.94235	0.52873
C	0.51277	-1.00639	4.5055
H	-0.24825	-1.48636	5.13082
H	0.54416	-1.5201	3.53877
H	1.48345	-1.11807	5.
H	0.13676	0.9908	5.29616
B	0.02657	0.06144	0.20428
C	-0.87367	1.29373	-0.37287
C	-1.3331	2.39819	0.34202
C	-2.20355	3.34751	-0.1941
C	-2.65603	3.20724	-1.49888
C	-2.23258	2.11508	-2.25138
C	-1.3701	1.19272	-1.67504
C	1.45263	-0.23177	-0.53743
C	1.99255	0.45518	-1.62413
C	3.22329	0.13505	-2.19642
C	3.97252	-0.91046	-1.67348

C	3.48268	-1.61994	-0.58052
C	2.25139	-1.2675	-0.04347
C	-0.94595	-1.25868	0.24999
C	-1.99651	-1.33967	1.16788
C	-2.88272	-2.41091	1.23618
C	-2.75361	-3.46088	0.33389
C	-1.74254	-3.41458	-0.61721
C	-0.87273	-2.32693	-0.64601
F	-0.95338	2.62361	1.6241
F	-2.60831	4.39373	0.54504
F	-3.48924	4.11272	-2.02957
F	-2.66303	1.96419	-3.51427
F	-0.99662	0.14294	-2.44106
F	1.36138	1.52222	-2.16043
F	3.6959	0.84076	-3.23612
F	5.15938	-1.22583	-2.20671
F	4.19985	-2.62943	-0.06267
F	1.82309	-1.99223	1.01591
F	0.06435	-2.3615	-1.61709
F	-1.61245	-4.41567	-1.50367
F	-3.59935	-4.49973	0.37472

F -3.86724 -2.43263 2.15014

F -2.21571 -0.33201 2.04578

48

TS1G-N₂ SCF Done: E(RB3LYP) = -2624.17070181

C -3.47656 1.23437 0.

O -3.39293 1.5358 1.27583

O -4.4413 0.49978 -0.38697

C -2.38091 1.58117 -0.87376

N -1.3251 2.83185 0.30889

N -0.33562 3.09577 0.73381

C -4.44374 1.03573 2.1769

H -5.39643 1.07997 1.64995

H -2.5436 2.38358 -1.58976

C -4.11404 -0.3649 2.6576

H -4.87796 -0.68658 3.37247

H -4.1056 -1.07284 1.82573

H -3.14264 -0.39075 3.1587

H -4.4338 1.76402 2.98883

B -4.72776 0.2586 -1.90049

C -5.61107 1.50769 -2.48494

C	-6.03365	2.63599	-1.78181
C	-6.87768	3.60796	-2.31973
C	-7.33847	3.47144	-3.62335
C	-6.94245	2.36532	-4.3718
C	-6.10197	1.42278	-3.79185
C	-3.22673	0.06169	-2.55933
C	-2.69889	0.74866	-3.66931
C	-1.49982	0.40585	-4.28276
C	-0.77171	-0.68074	-3.80316
C	-1.24049	-1.40131	-2.70561
C	-2.43825	-1.02452	-2.12039
C	-5.65753	-1.08652	-1.91888
C	-6.73216	-1.2025	-1.03116
C	-7.593	-2.29595	-0.99794
C	-7.40499	-3.33787	-1.90089
C	-6.3631	-3.26169	-2.81871
C	-5.52308	-2.14953	-2.81338
F	-5.62654	2.86748	-0.50689
F	-7.24267	4.67034	-1.58812
F	-8.14536	4.39468	-4.15621
F	-7.3702	2.22294	-5.63264

F	-5.73762	0.37579	-4.5626
F	-3.30706	1.84618	-4.14766
F	-1.03297	1.11182	-5.31828
F	0.3815	-1.01495	-4.37665
F	-0.53392	-2.4347	-2.2356
F	-2.84924	-1.74824	-1.06712
F	-4.54269	-2.14825	-3.74131
F	-6.17428	-4.25451	-3.69833
F	-8.22013	-4.39794	-1.88846
F	-8.59997	-2.34858	-0.11425
F	-6.9958	-0.21133	-0.1483

15

Re2 SCF Done: E(RB3LYP) = -508.18497265

C	-4.83594	0.92187	0.
O	-5.73398	1.92227	-0.09661
O	-5.07157	-0.26258	-0.07054
C	-3.47207	1.45975	0.20515
N	-3.29701	2.76965	0.26031
N	-3.17736	3.89518	0.30396
C	-7.12017	1.52641	-0.29586

H	-7.14082	0.6643	-0.96578
C	-7.80231	1.22061	1.02663
H	-8.85959	0.99804	0.85003
H	-7.3461	0.35097	1.50549
H	-7.74111	2.07559	1.70593
H	-7.56984	2.3868	-0.79536
C	-2.33207	0.63066	0.34569
N	-1.38969	-0.04302	0.46286

49

IN1J SCF Done: E(RB3LYP) = -2716.46385887

C	-1.35513	-0.31461	2.36098
O	-1.44499	0.06699	3.60692
O	-0.36197	0.00923	1.67214
C	-2.46372	-1.12953	1.90773
N	-3.54003	-1.13763	2.69226
N	-4.47203	-1.10603	3.32186
C	-0.37894	0.93173	4.17364
H	0.56583	0.65929	3.69483
C	-0.74156	2.38991	3.97175
H	0.01382	3.01347	4.46306

H	-0.77593	2.6611	2.90768
H	-1.71724	2.61391	4.42293
H	-0.36173	0.63473	5.22501
C	-2.46211	-2.04145	0.83368
N	-2.46229	-2.824	-0.02108
B	0.07828	0.0043	0.14375
C	-1.24239	0.44058	-0.70202
C	-1.89302	1.63378	-0.37067
C	-3.01728	2.11632	-1.02637
C	-3.54596	1.3844	-2.08578
C	-2.93662	0.19368	-2.45997
C	-1.80359	-0.24887	-1.77863
C	1.27156	1.1245	0.12619
C	1.4336	2.09318	-0.86524
C	2.49363	2.99713	-0.88758
C	3.45968	2.94807	0.10965
C	3.35175	1.99049	1.11232
C	2.28136	1.10219	1.09177
C	0.74942	-1.4371	-0.19554
C	0.85892	-2.52998	0.66046
C	1.5447	-3.69709	0.32861

C	2.16322	-3.79951	-0.91026
C	2.08405	-2.73249	-1.80089
C	1.39434	-1.58782	-1.42479
F	-1.4156	2.39483	0.64277
F	-3.58914	3.27346	-0.65805
F	-4.63298	1.82194	-2.7319
F	-3.44449	-0.52575	-3.47227
F	-1.28842	-1.41528	-2.20702
F	0.55565	2.19843	-1.88457
F	2.59003	3.91059	-1.86718
F	4.48475	3.81047	0.10372
F	4.28373	1.92314	2.07698
F	2.26135	0.17225	2.07688
F	1.34422	-0.57807	-2.32228
F	2.67329	-2.81932	-3.00389
F	2.82383	-4.91492	-1.24826
F	1.60968	-4.71927	1.19702
F	0.27404	-2.52662	1.88415

49

TS1J-N₂ SCF Done: E(RB3LYP) = -2716.41064204

C	-6.32031	3.14062	0.
O	-6.45806	3.28436	1.29498
O	-5.26751	3.54154	-0.56268
C	-7.45437	2.66521	-0.75195
N	-8.78074	2.36814	0.6758
N	-9.80151	2.52533	1.07786
C	-5.38716	3.98264	2.03624
H	-4.43136	3.71793	1.58537
C	-5.6375	5.47844	2.03121
H	-4.85741	5.97067	2.62031
H	-5.60304	5.87982	1.01581
H	-6.60623	5.71855	2.47737
H	-5.46345	3.54868	3.03355
C	-7.54276	1.4632	-1.43622
N	-7.703	0.47967	-2.05496
B	-4.83998	3.50163	-2.09432
C	-6.20495	3.89994	-2.90845
C	-6.8522	5.11297	-2.60872
C	-7.95874	5.59398	-3.29032
C	-8.4764	4.84718	-4.34859
C	-7.88443	3.63491	-4.68908

C	-6.77246	3.18857	-3.97764
C	-3.6617	4.63648	-2.14918
C	-3.52597	5.59895	-3.15166
C	-2.48757	6.5284	-3.18949
C	-1.51672	6.51419	-2.19402
C	-1.59768	5.565	-1.17976
C	-2.64828	4.65218	-1.18536
C	-4.18356	2.04094	-2.41183
C	-4.1102	0.94452	-1.5538
C	-3.44356	-0.23904	-1.86804
C	-2.80586	-0.3594	-3.09665
C	-2.85294	0.70457	-3.99442
C	-3.52856	1.86435	-3.63494
F	-6.39307	5.87561	-1.59344
F	-8.53158	6.75434	-2.94891
F	-9.54238	5.28581	-5.01651
F	-8.38848	2.90872	-5.6912
F	-6.28767	1.99474	-4.34435
F	-4.41759	5.67336	-4.15995
F	-2.41831	7.4318	-4.17577
F	-0.51576	7.40014	-2.21147

F	-0.66606	5.53162	-0.21616
F	-2.64483	3.7389	-0.1838
F	-3.55568	2.86124	-4.54422
F	-2.25021	0.60192	-5.18545
F	-2.16181	-1.48577	-3.41753
F	-3.41479	-1.25467	-0.9947
F	-4.71765	0.96142	-0.33782

17

Re3 SCF Done: E(RB3LYP) = -604.50780763

C	-3.89844	2.1875	0.
O	-4.9098	3.09454	0.00002
O	-4.05382	0.98956	0.00008
C	-2.59376	2.87709	-0.00014
N	-2.59376	4.19683	-0.00016
N	-2.59378	5.32895	0.00014
C	-1.28908	2.1875	-0.00017
O	-1.13369	0.98957	-0.00011
O	-0.27772	3.09455	-0.00015
C	1.04413	2.52817	-0.00013
H	1.19814	1.91213	-0.88905

H	1.72481	3.37888	-0.00035
H	1.19827	1.91251	0.88904
C	-6.23164	2.52816	0.00016
H	-6.38587	1.91245	-0.88896
H	-6.38557	1.91217	0.88913
H	-6.91233	3.37887	0.00041

51

IN1H SCF Done: E(RB3LYP) = -2812.78059785

O	1.12005	0.72987	-0.45797
B	-0.15071	-0.02508	0.10218
C	-1.10494	-0.60015	-1.09193
C	-2.18395	-1.41181	-0.73648
C	-1.05179	-0.2604	-2.44154
C	-3.1247	-1.89142	-1.63834
C	-1.973	-0.71755	-3.38344
C	-3.01821	-1.53851	-2.98034
C	-1.02877	1.14105	0.83042
C	-1.69823	0.98901	2.04481
C	-1.27435	2.34692	0.16893
C	-2.52063	1.97046	2.59281

C	-2.08383	3.3553	0.68395
C	-2.71234	3.16523	1.90966
C	0.5176	-1.1423	1.08958
C	0.63757	-2.50124	0.7967
C	1.15546	-0.74178	2.26659
C	1.30159	-3.40768	1.62114
C	1.82311	-1.61191	3.12107
C	1.89627	-2.96156	2.79435
F	-0.0692	0.53978	-2.92622
F	-1.85933	-0.36583	-4.67558
F	-3.91453	-1.98555	-3.87175
F	-4.13038	-2.68291	-1.23081
F	-2.34162	-1.77104	0.55794
F	-0.74114	2.5693	-1.05138
F	-2.27733	4.49794	0.00324
F	-3.50184	4.11997	2.42263
F	-3.13161	1.77028	3.77323
F	-1.57918	-0.14707	2.76467
F	0.12795	-3.0188	-0.34148
F	1.3868	-4.70513	1.28054
F	2.54021	-3.81933	3.59752

F	2.40135	-1.1629	4.24769
F	1.14688	0.55905	2.63148
C	1.99049	0.21173	-1.20924
O	1.80593	-1.0272	-1.58802
C	2.32357	-1.62051	-2.80916
H	2.35625	-0.87964	-3.60614
H	3.30037	-2.06281	-2.62522
H	1.60708	-2.40016	-3.04813
C	3.15836	0.99139	-1.51967
C	3.3152	2.437	-1.16727
O	2.39015	3.17946	-0.92957
O	4.61891	2.766	-1.15719
C	4.91446	4.15038	-0.86335
H	6.00046	4.20333	-0.79579
H	4.54759	4.78993	-1.66887
H	4.45332	4.44255	0.08072
N	4.24215	0.37374	-1.97029
N	5.19106	-0.08865	-2.36161

51

TS1H-N₂ SCF Done: E(RB3LYP) = -2812.71644626

O	-6.38281	3.875	0.
B	-7.68348	3.09834	0.58699
C	-8.62434	2.5255	-0.62272
C	-9.7398	1.75982	-0.26556
C	-8.54568	2.82196	-1.98195
C	-10.68757	1.29479	-1.16993
C	-9.46783	2.37552	-2.92843
C	-10.55114	1.60787	-2.52017
C	-8.51831	4.29655	1.31068
C	-9.15716	4.18857	2.54812
C	-8.73406	5.50562	0.64083
C	-9.9202	5.21215	3.10721
C	-9.48281	6.55514	1.16603
C	-10.08122	6.40631	2.41312
C	-6.98705	1.9908	1.56426
C	-6.90046	0.62323	1.28651
C	-6.32953	2.38559	2.73603
C	-6.26744	-0.29476	2.12293
C	-5.68485	1.50431	3.59862
C	-5.65643	0.14778	3.29036
F	-7.52456	3.57033	-2.48101

F	-9.31528	2.6874	-4.22455
F	-11.44904	1.17319	-3.41147
F	-11.72655	0.55778	-0.75686
F	-9.92871	1.43871	1.03033
F	-8.21958	5.69514	-0.59228
F	-9.64424	7.69483	0.47765
F	-10.80982	7.39994	2.9357
F	-10.50061	5.05377	4.30552
F	-9.06121	3.05994	3.27717
F	-7.41567	0.10932	0.15071
F	-6.22299	-1.5952	1.79726
F	-5.03545	-0.71714	4.09935
F	-5.08104	1.95008	4.7097
F	-6.28755	3.68767	3.08213
C	-5.51995	3.46089	-0.81096
O	-5.4888	2.18204	-1.12392
C	-5.08044	1.69837	-2.42609
H	-5.09474	2.5094	-3.15401
H	-4.08828	1.25217	-2.34952
H	-5.8112	0.9322	-2.68303
C	-4.6576	4.42652	-1.43256

C	-4.21756	5.64889	-0.81874
O	-5.15081	6.4247	-0.67791
O	-2.93686	5.86712	-0.55511
C	-2.63163	7.19223	-0.04529
H	-1.54784	7.21693	0.04812
H	-2.98093	7.9528	-0.74549
H	-3.10755	7.33686	0.92596
N	-2.78282	3.36019	-1.55171
N	-1.76214	3.16718	-1.93049