

SUPPORTING INFORMATION

Understanding the Cooperative NHC/LA Catalysis for Stereoselective Annulation Reactions with Homoenolates. A DFT study.

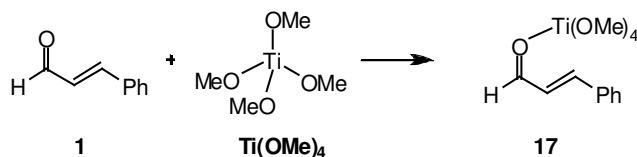
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Table S1. Total (E, in a.u.) and relative (ΔE , in kcal/mol) energies involved in the formation of the complex **17** using different computational levels.



	B3LYP/6-31G**		B3LYP/LanL2DZ		B3LYP/6-311++G**		MPW1B95/6-31G**	
	E	ΔE						
1	-422.988325		-422.913013		-423.084860		-422.786579	
Ti(OMe)₄	-1310.16898		-518.821870		-1310.324990		-1310.033520	
	-1733.15731		-941.734882		-1733.409850		-1732.820100	
17	-1733.16666	-5.9	-941.737111	-1.4	-1733.419400	-6.0	-1732.835550	-9.7

Table S2. B3LYP/6-31G** Total enthalpies (H, in a.u.) and free energies (G, in a.u.) computed at 298.15 K and 1 atm in DCM of the stationary points involved in the equilibria between complexes LA–NHC **16** and **18** and LA–enones **17** and **19**.

	H	G
1	-422.848885	-422.894198
5	-304.682758	-304.721600
16	-1614.698385	-1614.777931
17	-1732.855651	-1732.935742
18	-4006.750558	-4006.837772
19	-4124.870625	-4124.963779

Table S3. B3LYP/6-31G** Total enthalpies (H, in a.u.) and free energies (G, in a.u.) computed at 298.15 K and 1 atm in DCM of the stationary points involved in the formation of the extended Ti(IV)–Breslow intermediate **21** and Breslow intermediate **23**.

	H	G
5 + 1 + Ti(OMe)₄	−2037.539068	−2037.627557
MC1	−2037.547073	−2037.647050
TS1	−2037.532326	−2037.635000
20	−2037.564395	−2037.663548
TS2	−2037.543046	−2037.642240
21	−2037.555253	−2037.655067
5 + 1	−727.534464	−727.595682
MC2	−727.534157	−727.601562
TS3	−727.524259	−727.585367
22	−727.534838	−727.598080
22 + MeOH	−843.228689	−843.303390
TS4	−843.203914	−843.273662
23	−727.543272	−727.606503

Table S4. B3LYP/6-31G** Total enthalpies (H, in a.u.) and free energies (G, in a.u.) computed at 298.15 K and 1 atm in DCM of the stationary points involved in the stereoselective LA assisted C–C bond-formation steps.

	H	G
21 + 2	–2691.371223	–2691.495349
14 + MeOH	–2691.397742	–2691.531546
14	–2575.712761	–2575.834920
TS5	–2575.706706	–2575.822279
15	–2575.725271	–2575.843922
24	–2691.420613	–2691.547157
25	–2575.701566	–2575.821594
TS6	–2575.701542	–2575.816819
26	–2575.723121	–2575.841573
23 + 2	–1381.381753	–1381.474060
27	–1381.385942	–1381.488032
TS7	–1381.372280	–1381.465660
28	–1381.397696	–1381.491495
29	–1381.386107	–1381.484325
TS8	–1381.376787	–1381.469527
30	–1381.397745	–1381.490612

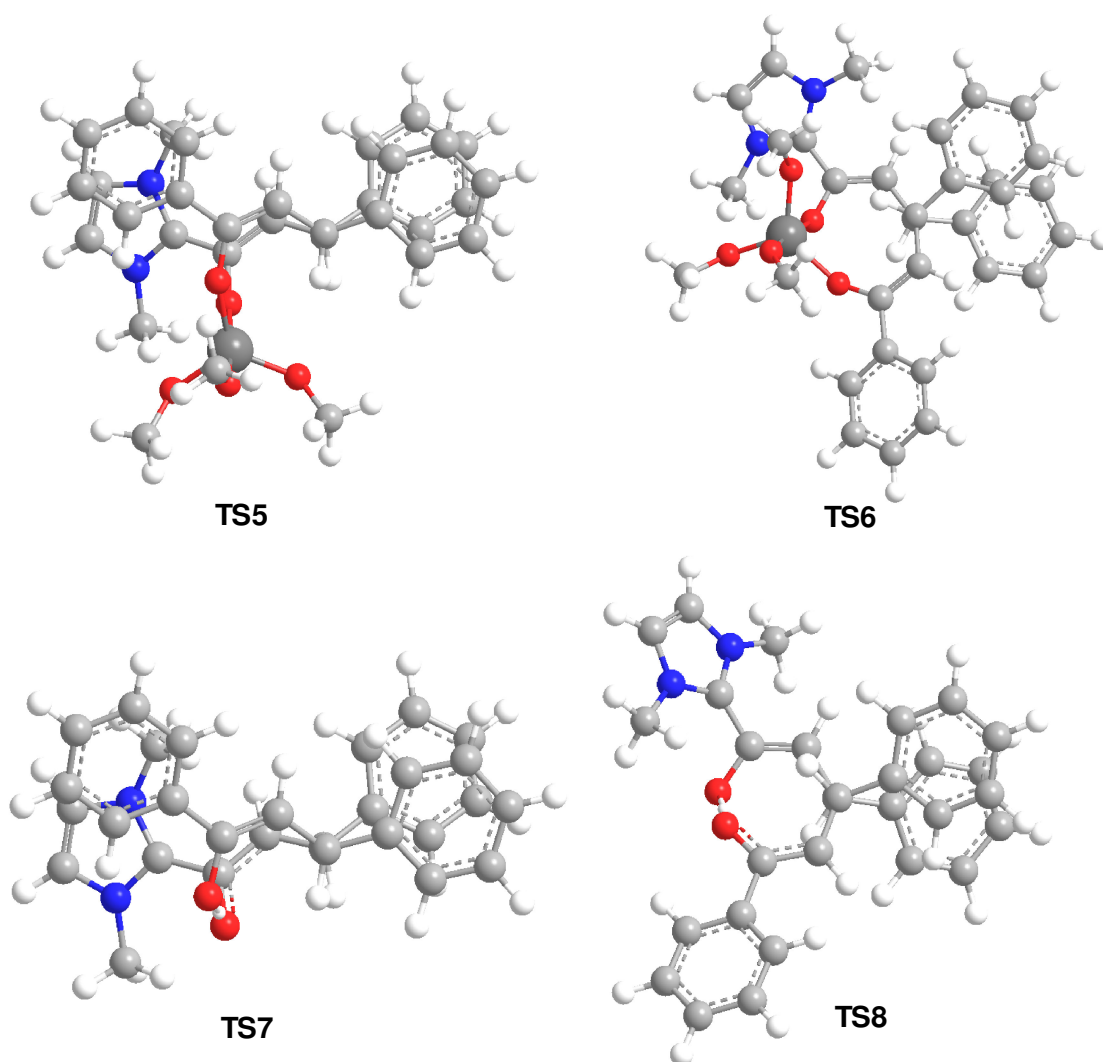


Figure S1. Top view of the sandwich parallel **TS5** and **TS7**, associated with the *cis* reactive channels, and the twisted **TS6** and **TS8**, associated with the *trans* reactive channels.

Complete citation for reference 19.

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J., J. A. ; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A *Gaussian 03*, Revision C.02, Gaussian, Inc., Wallingford CT, 2004.

B3LYP/6-31G** computed total energies, unique frequency imaginary, and cartesian coordinates of the stationary points involved in the NHC and the cooperative NHC/LA catalysis for stereoselective annulation reactions with homoenolates.

1

E (RB+HF-LYP) = -422.988324561 A.U.

O	-4.36915800	0.39503700	-0.00175700
C	-3.36209000	-0.29092600	0.00039400
C	-1.99741700	0.24154200	-0.00124000
C	-0.93353800	-0.58821600	0.00204000
H	-1.90567800	1.32414000	-0.00525100
H	-1.14237000	-1.65932600	0.00545600
H	-3.42602400	-1.40369300	0.00387500
C	0.48618700	-0.23961400	0.00127200
C	1.43861800	-1.27518200	-0.00017600
C	0.94781700	1.09130500	0.00180000
C	2.80332700	-0.99639600	-0.00156100
H	1.09764800	-2.30725000	-0.00040400
C	2.30991000	1.36918900	0.00052400
H	0.23611700	1.91052100	0.00361800
C	3.24338800	0.32755500	-0.00126500
H	3.52170400	-1.81057100	-0.00279300
H	2.64830500	2.40099400	0.00106300
H	4.30634400	0.54934500	-0.00223600

2

E (RB+HF-LYP) = -654.056912804 A.U.

C	-1.18266700	-0.94924300	0.02074400
C	0.08117700	-0.17292900	-0.02837500
C	1.26672300	-0.80822300	0.06149900
H	1.21731800	-1.88931600	0.18324400
H	0.02947700	0.90181500	-0.16028900
O	-1.17206100	-2.17866700	0.05336800
C	2.60723000	-0.22726500	0.01429700
C	2.84964800	1.14908900	-0.16505400
C	3.71549400	-1.08365100	0.15134700
C	4.14838500	1.64337900	-0.20428600
H	2.01580600	1.83503500	-0.27629400
C	5.01699700	-0.58864700	0.11264100
H	3.54425300	-2.14781700	0.28920100
C	5.23802900	0.77732100	-0.06548100
H	4.31554900	2.70730800	-0.34428700
H	5.85718800	-1.26803400	0.22072100
H	6.25101100	1.16735800	-0.09669300

C	-2.49311300	-0.21444600	0.01279300
C	-3.65684400	-0.96666500	-0.21534000
C	-2.61241600	1.16471500	0.24305000
C	-4.90578300	-0.35486200	-0.22886300
H	-3.54890300	-2.03342000	-0.37835500
C	-3.86590300	1.77655500	0.23968100
H	-1.73513100	1.76805500	0.44954500
C	-5.01338300	1.02030000	-0.00156900
H	-5.79733700	-0.94682800	-0.41395300
H	-3.94596100	2.84325600	0.42710200
H	-5.98822200	1.49935100	-0.00939900

14

E (RB+HF-LYP) = -2576.33154582 A.U.

C	-0.84695800	-0.61268900	-1.42965400
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C	1.59810700	-0.37225600	-1.62327600
C	1.65420100	0.54953300	1.48390800
C	0.72085500	-0.42136400	1.72823400
C	-0.67886600	-0.23118400	1.52356600
C	-1.64380600	-1.22878600	1.88685400
O	-1.16335100	0.94517600	1.18183900
N	-2.93944100	-0.97041200	2.26378700
N	-1.50717600	-2.59973200	1.91753800
C	-3.58433200	-2.16524400	2.53458600
C	-3.50613700	0.34305700	2.59038700
C	-2.70562800	-3.17141000	2.32148200
C	-0.37574600	-3.36676300	1.42295700
H	1.04348000	-1.37730000	2.12581700
H	1.28749200	1.52400400	1.17213100
H	1.46356700	0.69918100	-1.51343400
H	0.56138000	-2.22026500	-1.73727400
O	-1.01485900	0.65816600	-1.32882200
H	-4.61335800	-2.19015800	2.85340600
H	-4.50995000	0.17194500	2.98362000
H	-3.54316500	0.99124900	1.71561000
H	-2.89824000	0.82819700	3.35778600
H	-2.82473400	-4.23964800	2.39662800
H	0.38508200	-3.51094600	2.19650300
H	0.06973600	-2.83909100	0.57739400
H	-0.73624600	-4.34267400	1.09375900
C	3.08634600	0.45372100	1.72187200
C	3.86918500	1.62587600	1.63771000
C	3.75658200	-0.74932000	2.03621200
C	5.24094300	1.60346800	1.87409900
H	3.37727100	2.56513900	1.39777600
C	5.12620900	-0.77038900	2.27309300

H	3.19887600	-1.67993300	2.08319400
C	5.88019100	0.40509400	2.19755300
H	5.81254100	2.52548600	1.80946000
H	5.61379100	-1.71178400	2.51199000
H	6.95002200	0.38392300	2.38287500
C	2.96503300	-0.82662300	-1.82091200
C	3.31455000	-2.17740200	-2.04152700
C	4.00863900	0.12273800	-1.80438500
C	4.63820200	-2.55266400	-2.23819100
H	2.54130400	-2.93907700	-2.06866700
C	5.33365700	-0.25473700	-1.99787700
H	3.76555100	1.16615100	-1.62731600
C	5.65719700	-1.59464000	-2.21790100
H	4.88005100	-3.59785100	-2.41073800
H	6.11595400	0.49801500	-1.97284100
H	6.69037000	-1.89173700	-2.37142500
C	-2.05454100	-1.47144200	-1.49862100
C	-3.31498000	-0.91017900	-1.20329000
C	-2.01057200	-2.83319200	-1.86552000
C	-4.47048600	-1.68428300	-1.25038500
H	-3.37558300	0.13511400	-0.92509100
C	-3.17004300	-3.60190300	-1.91400600
H	-1.06991600	-3.29709200	-2.14110000
C	-4.40789400	-3.03539900	-1.59955400
H	-5.42853900	-1.22829600	-1.01605600
H	-3.10833600	-4.64569500	-2.20956600
H	-5.31211700	-3.63558700	-1.64113000
Ti	-1.39054400	2.27928400	-0.22290500
O	-3.16568000	2.55583900	0.17209100
O	-0.26523500	3.45098600	0.62073200
O	-1.35684300	3.20435500	-1.80545100
C	-4.07878600	3.51322900	-0.31012700
H	-5.03258300	3.02966700	-0.56508500
H	-4.28159200	4.27496400	0.45587400
H	-3.68971600	4.01519000	-1.20519400
C	-1.25212200	2.98747300	-3.18339800
H	-2.20576700	3.20567400	-3.68609100
H	-0.48695900	3.64421200	-3.62140800
H	-0.98046100	1.94524500	-3.39857400
C	0.22764600	4.71953900	0.27233500
H	-0.04383300	4.98028800	-0.75944800
H	-0.17761000	5.48657400	0.94733100
H	1.32316100	4.73997000	0.36519700

15

E(RB+HF-LYP) = -2576.34350996 A.U.

C	0.12092400	-0.29949300	1.57703600
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C	-1.16183200	-0.21451300	1.13969000
C	-1.59718700	0.60792200	-0.03991600
C	-1.81798500	-0.24830500	-1.37387800
C	-0.59089100	-1.06135500	-1.71600500
C	0.66700200	-0.55686800	-1.80107100
C	1.78389100	-1.48626100	-2.10633900
O	1.03052300	0.69758900	-1.67726300
N	2.80265400	-1.20832500	-2.94885300
N	2.04110100	-2.70113000	-1.56065900
C	3.70261300	-2.25346500	-2.94065200
C	2.97288000	0.04276700	-3.70000300
C	3.22791100	-3.19049900	-2.07801500
C	1.25978400	-3.37126200	-0.51888300
H	-0.73454800	-2.11605900	-1.92752700
H	-1.95437500	0.51330800	-2.15442800
H	-0.77202900	1.26460200	-0.30882100
H	-1.91229200	-0.80018200	1.65758200
O	1.15589900	0.32826700	1.00440600
H	4.59632900	-2.23881200	-3.54275100
H	3.71922700	-0.13719000	-4.47521500
H	3.29205500	0.81876500	-3.00174400
H	2.02483000	0.32541000	-4.15496100
H	3.62726500	-4.14690900	-1.78282900
H	0.57937000	-4.10312200	-0.96135400
H	0.68551400	-2.62379200	0.02676600
H	1.94894200	-3.87426600	0.16093600
C	-3.06928800	-1.11035300	-1.35504800
C	-4.21559500	-0.71129200	-2.05500300
C	-3.12447200	-2.31472600	-0.63551200
C	-5.37739100	-1.48398500	-2.04106500
H	-4.19656300	0.22083200	-2.61310200
C	-4.28530100	-3.08896700	-0.61427200
H	-2.25209200	-2.64314500	-0.07805400
C	-5.41743700	-2.67732300	-1.31941200
H	-6.25147800	-1.15161300	-2.59408100
H	-4.30488600	-4.01554000	-0.04664300
H	-6.32052400	-3.28082300	-1.30658100
C	-2.78456000	1.51956300	0.24607200
C	-3.93971900	1.08950400	0.91495700
C	-2.72829600	2.85368500	-0.18464000
C	-5.00112700	1.96468600	1.14732300
H	-4.01732800	0.06156200	1.25444100
C	-3.78958700	3.73091900	0.04322600
H	-1.83372600	3.20297700	-0.69485000
C	-4.93156200	3.28914200	0.71214600
H	-5.88574000	1.60934800	1.66898100
H	-3.71988800	4.76105500	-0.29582000
H	-5.75792600	3.97010400	0.89593700
C	0.50399700	-1.17145200	2.73129000

C	1.83507100	-1.60485500	2.85843200
C	-0.41922000	-1.58489400	3.70819900
C	2.22180800	-2.44542000	3.90254600
H	2.56125000	-1.26207600	2.12961800
C	-0.03228700	-2.42304600	4.75117700
H	-1.44215000	-1.22573800	3.66700400
C	1.28969600	-2.86399300	4.85237300
H	3.25735100	-2.76711800	3.97812800
H	-0.76354100	-2.72148600	5.49739300
H	1.59046900	-3.51262700	5.67009700
Ti	1.92982200	1.68244900	-0.09509400
O	3.58453600	1.27227100	-0.84192200
O	1.12912100	3.19193800	-0.73069100
O	2.60983200	2.51694300	1.38384900
C	4.86917400	1.72736600	-0.49457100
H	5.58481200	0.89127200	-0.50107500
H	5.22772200	2.47815100	-1.21529000
H	4.87596300	2.18400300	0.50311200
C	2.72710800	2.31660900	2.76397600
H	3.78479200	2.25191500	3.05936400
H	2.27865400	3.15435400	3.31655100
H	2.22414000	1.38942500	3.06785600
C	1.15794100	4.53709400	-0.32334800
H	1.73074100	4.65246800	0.60614400
H	1.61629500	5.16261900	-1.10214200
H	0.13530700	4.90300100	-0.15588500

16

E(RB+HF-LYP) = -1614.99969548 A.U.

C	-1.49582600	0.06887900	0.00479500
N	-2.44194100	1.04512100	-0.09774300
N	-2.22851900	-1.08255200	-0.02044000
C	-3.72225300	0.51915400	-0.19220100
C	-2.16554600	2.47846500	-0.09175400
C	-3.58552500	-0.82952900	-0.14812300
C	-1.65433400	-2.42594400	-0.00758200
Ti	0.92865200	0.03591700	-0.03865200
O	2.75533500	-0.10067000	-0.06339700
O	0.64351900	-0.91808000	-1.58305000
O	0.87666500	1.87628900	-0.11335600
O	0.74615300	-0.86545300	1.56480200
C	0.19029700	-0.60480100	2.82485900
C	3.73167600	-0.63342500	0.78816400
C	1.51393400	-1.49315000	-2.52369500
C	1.86495600	2.82614400	-0.43744800
H	-4.60054900	1.14011900	-0.27314000
H	-2.60826400	2.94406400	0.79441100

H	-2.59196900	2.94134300	-0.98658000
H	-1.08401800	2.60891100	-0.08414800
H	-4.32145200	-1.61700700	-0.19177800
H	-0.75280700	-2.41340400	0.60311800
H	-1.39439900	-2.73765000	-1.02154300
H	-2.38302800	-3.11881200	0.41954400
H	4.33247900	-1.39108900	0.26492400
H	4.41768000	0.15297600	1.13489200
H	3.26385800	-1.10296100	1.66537000
H	1.31889600	-1.08784800	-3.52684000
H	2.56275600	-1.29435600	-2.26470400
H	1.36723600	-2.58282000	-2.57010000
H	1.86259600	3.64049000	0.30069400
H	2.86080900	2.36541600	-0.45023000
H	1.67172200	3.26671800	-1.42631100
H	-0.83732500	-0.21936500	2.74030500
H	0.15822100	-1.52723500	3.42175700
H	0.78278300	0.13292200	3.38590100

17

E(RB+HF-LYP) = -1733.16666094 A.U.

O	0.00000000	0.00000000	0.00000000
C	1.23133605	0.00000000	0.00000000
C	2.02781735	1.21338638	0.00000000
Ti	-1.28565643	-2.00365257	0.24605944
O	-1.24679932	-1.38413163	1.95895707
O	-2.31944112	-1.18291034	-0.98557291
O	-2.21143458	-3.54531995	0.49397444
O	0.30226736	-2.76453980	-0.31713590
C	0.56097059	-3.60733102	-1.41340630
C	-1.95814452	-1.70514642	3.12764780
C	-2.83418600	0.06207050	-1.37359861
C	-1.87739529	-4.77862510	1.07748937
C	3.37790569	1.13468188	0.01069528
H	1.48767565	2.15559254	-0.00068216
H	3.81297399	0.13452556	0.01258517
H	1.76693003	-0.96529344	-0.00179304
H	-2.42101617	-0.80265384	3.54989338
H	-2.75240216	-2.43864107	2.93145436
H	-1.28167594	-2.12158303	3.88742218
H	-2.12683338	0.87032893	-1.14732551
H	-3.03149731	0.06426303	-2.45387340
H	-3.78105540	0.27104587	-0.85655583
H	-2.10153180	-4.78069799	2.15363323
H	-2.46042796	-5.58417963	0.61207872
H	-0.80865575	-5.00359267	0.95151671
H	0.68919891	-3.03161461	-2.34240278

H	1.48499852	-4.17649682	-1.24039273
H	-0.25461748	-4.32721647	-1.57330571
C	4.34581435	2.22641973	0.02395005
C	5.71780683	1.91246690	0.03220070
C	3.96909393	3.58432809	0.03153762
C	6.68264887	2.91623601	0.04758290
H	6.02248138	0.86932741	0.02730171
C	4.93283137	4.58546409	0.04709116
H	2.91825276	3.85472576	0.02665787
C	6.29243383	4.25597667	0.05520289
H	7.73617185	2.65422676	0.05412767
H	4.62686831	5.62715912	0.05345655
H	7.04177088	5.04166688	0.06776391

18

E (RB+HF-LYP) = -4006.93626039 A.U.

C	0.96819200	1.95115800	-0.04035000
N	1.70733400	2.51931900	-1.02246200
N	1.07631900	2.79163900	1.01612600
C	2.27142900	3.70490600	-0.58817700
C	1.83838900	1.99406100	-2.38416200
C	1.87700700	3.87426300	0.70148700
C	0.47430400	2.56090300	2.33266700
H	2.89012700	4.31717600	-1.22441200
H	2.82000000	2.26813000	-2.77376000
H	1.06086600	2.41373500	-3.02741100
H	1.75358900	0.90841000	-2.35965800
H	2.09545600	4.65614100	1.41090700
H	1.12092100	1.92005300	2.93741600
H	-0.50080800	2.09076500	2.20570800
H	0.34809900	3.52209800	2.83257600
Zn	-0.07480200	0.24573300	-0.12604100
O	-1.77034500	0.15289500	-1.25687800
O	0.51167200	-1.42964100	0.86509100
S	-2.75455400	0.55526500	-0.16575700
O	-1.91888600	0.71183800	1.07782700
O	-3.69848400	1.61373000	-0.49531800
S	1.37821000	-2.03621800	-0.23123000
O	1.23735900	-3.46258300	-0.47016600
O	1.26870200	-1.08981000	-1.39333000
C	-3.75453100	-0.99218300	0.11661000
C	3.10814400	-1.77944000	0.41060200
F	-4.42899100	-1.29310200	-0.99305800
F	-4.61322500	-0.78590300	1.11668200
F	-2.94335500	-2.00266600	0.43072200
F	3.29305300	-2.47669500	1.53015000
F	3.99497800	-2.16658700	-0.50717500

F 3.30353800 -0.47542300 0.67447200

19

E (RB+HF-LYP) = -4125.07461526 A.U.

Zn	1.12400200	0.05343700	-0.36859000
O	1.71225100	-1.61439500	-1.35201800
O	2.24188300	1.08181400	0.99026200
S	1.21430900	-2.62478600	-0.32473600
O	0.63194000	-1.78442400	0.78655000
O	0.41713800	-3.73510100	-0.82591100
S	2.83788400	2.03506300	-0.04085700
O	4.27519600	2.24283300	-0.01002300
O	2.19298800	1.61318000	-1.34128200
C	2.77859400	-3.34661700	0.38556100
C	2.05199600	3.67649000	0.36179400
F	3.43365100	-4.00734800	-0.56712400
F	2.46588700	-4.18337000	1.37532600
F	3.54780500	-2.36575100	0.85833700
F	2.47470900	4.09810500	1.55291200
F	2.38304000	4.56880700	-0.57033000
F	0.72007200	3.54352300	0.39018200
O	-0.76222000	0.58396500	-0.60303700
C	-1.73839100	-0.03849800	-0.12703100
H	-1.55752400	-0.95406500	0.45449800
C	-3.08866000	0.39045000	-0.31420400
H	-3.25073700	1.29511800	-0.89121500
C	-4.09897800	-0.34318300	0.22750400
H	-3.81377600	-1.23453000	0.78696200
C	-5.52540200	-0.09222100	0.15662500
C	-6.39823200	-0.98939400	0.80525000
C	-6.07622500	1.00970200	-0.53199100
C	-7.77502800	-0.79436400	0.77030700
H	-5.98428100	-1.84177900	1.33684100
C	-7.45078800	1.20137300	-0.56550600
H	-5.42625100	1.71345800	-1.04121700
C	-8.30325500	0.30138000	0.08499500
H	-8.43469800	-1.49321200	1.27438300
H	-7.86413200	2.05175800	-1.09831800
H	-9.37741300	0.45633000	0.05540300

20

E (RB+HF-LYP) = -2038.00529556 A.U.

O	-0.17097700	-0.51921500	-0.16023400
C	0.34205200	0.64167100	-0.68055000
C	-0.17037900	1.85914300	0.08358200

N	-0.24239300	1.98330300	1.42055500
N	-0.56629500	3.03132500	-0.45171400
C	-0.73282400	3.23884700	1.73504800
C	0.01468400	0.92393100	2.40655600
C	-0.93459900	3.89658900	0.56447500
C	-0.78333000	3.25851800	-1.88067700
C	1.86700100	0.66977000	-0.65406100
Ti	-2.03587600	-1.06824500	-0.04944800
O	-2.97197300	-1.93640300	-1.37998900
O	-1.52689300	-2.69752000	0.67854900
O	-2.94720100	-0.53401800	1.47537800
O	-2.39319800	0.68499100	-0.89261300
C	-3.65539700	1.29040800	-0.84622300
C	-3.30987700	-1.59266000	-2.69543400
C	-1.39964000	-3.99806100	0.19030600
C	-3.58961000	-1.33625300	2.43648300
C	2.59878800	-0.36558600	-0.22103300
H	2.33043900	1.57715300	-1.04129200
H	2.04230500	-1.23709400	0.11766600
H	-0.89205100	3.54605800	2.75550900
H	0.26685000	1.40438400	3.35316200
H	0.84238000	0.30732300	2.06551200
H	-0.88362200	0.31026500	2.50494700
H	-1.30563200	4.88823700	0.36427800
H	-1.42502000	2.45570300	-2.25000200
H	0.16595000	3.27425500	-2.42021600
H	-1.27809600	4.22200300	-2.00232900
H	0.02173600	0.80546700	-1.72349500
H	-2.82549500	-2.27593500	-3.40974600
H	-4.39622000	-1.67257100	-2.85038300
H	-2.99991000	-0.56593100	-2.93537400
H	-1.74094700	-4.73331000	0.93536200
H	-1.99475600	-4.12897700	-0.72641000
H	-0.34922200	-4.23542200	-0.04380000
H	-3.56090600	-0.84180000	3.41924100
H	-4.64743300	-1.49427200	2.17830700
H	-3.10280500	-2.31710400	2.51865000
H	-3.59088900	2.36537300	-1.09776100
H	-4.36193800	0.84261800	-1.56540800
H	-4.10652200	1.20994200	0.15447900
C	4.06449400	-0.47058900	-0.17441800
C	4.63792200	-1.69546400	0.20969200
C	4.93150900	0.59253300	-0.48959300
C	6.02085800	-1.85833100	0.27088200
H	3.98397100	-2.52710900	0.45828600
C	6.31223800	0.43176800	-0.42845500
H	4.52259800	1.55562400	-0.78058300
C	6.86507200	-0.79487800	-0.04868500
H	6.43820700	-2.81598700	0.56836600

H	6.96220900	1.26644700	-0.67578300
H	7.94310100	-0.91717100	-0.00130600

21

E (RB+HF-LYP) = -2038.00170768 A.U.

O	0.86551100	0.10090500	-0.63103900
C	0.13246600	1.21812700	-0.35785100
C	0.84261300	2.42823400	-0.30294100
N	2.11115300	2.64649200	-0.82745300
N	0.46941600	3.63100600	0.28746100
C	2.48041100	3.96846300	-0.58452000
C	2.73582900	1.84731600	-1.88144100
C	1.48717200	4.56880300	0.09982900
C	-0.63447000	3.82517500	1.20577900
C	-1.28344800	1.10811600	-0.27909600
Ti	1.57311100	-1.47511200	0.02315100
O	0.61829200	-2.96561000	-0.33944800
O	2.93856000	-1.68922800	-1.16306900
O	2.57090600	-1.42249800	1.54940700
O	-0.13868600	-1.21628900	1.65999400
C	0.05889800	-0.53686100	2.90119200
C	-0.11082100	-4.01364300	0.24463800
C	3.32176600	-2.72565200	-2.03302000
C	3.95347400	-1.50473900	1.80166300
C	-2.01028800	-0.04347600	-0.47368900
H	-1.82974500	2.02701500	-0.09316500
H	-1.47743700	-0.93081200	-0.80986000
H	3.42662700	4.35603600	-0.92597300
H	2.11377300	1.85169000	-2.78406200
H	2.88152500	0.81601100	-1.56904000
H	3.70033500	2.30295600	-2.11425400
H	1.40812300	5.56848700	0.49488300
H	-0.77873100	2.92048600	1.80401100
H	-1.57294500	4.05219600	0.68724900
H	-0.39640800	4.65812200	1.87075600
H	-0.89643900	-0.81052700	1.19147300
H	-0.90618900	-4.34146500	-0.43755400
H	0.53978100	-4.87561400	0.44734200
H	-0.56859300	-3.68841400	1.18653900
H	4.26032900	-3.18827800	-1.69678800
H	2.54573700	-3.50123100	-2.08156500
H	3.48488300	-2.33030500	-3.04476400
H	4.28612300	-0.63190000	2.38031500
H	4.18043900	-2.40476800	2.38937600
H	4.52581300	-1.54303900	0.86553900
H	-0.80175800	-0.68658400	3.56308800
H	0.95323400	-0.96304800	3.35283700

H	0.21777400	0.53692300	2.74502500
C	-3.46162200	-0.16216300	-0.40727800
C	-4.31165900	0.84243500	0.10867000
C	-4.07985200	-1.34597900	-0.86833600
C	-5.69270400	0.67697900	0.14170500
H	-3.88405500	1.76058600	0.50198200
C	-5.46074700	-1.51236600	-0.82913500
H	-3.45383800	-2.13902400	-1.27041800
C	-6.28239600	-0.50053000	-0.32657700
H	-6.31570100	1.47163500	0.54464500
H	-5.89921500	-2.43670500	-1.19633500
H	-7.36025600	-0.62814400	-0.29498400

22

E (RB+HF-LYP) = -727.790916399 A.U.

O	1.17125800	-1.30510800	1.79232100
C	1.17125200	-0.08929100	1.29113600
C	2.26326400	0.02301100	0.16420400
N	2.50460800	-0.94605500	-0.74440200
N	3.25078700	0.94092100	0.01151600
C	3.63889100	-0.63989700	-1.47301600
C	1.69472100	-2.16264200	-0.87405800
C	4.11088900	0.54369500	-1.00493900
C	3.37197100	2.19634900	0.74600000
C	-0.14267600	0.42441400	0.66488900
C	-1.24406000	-0.33498800	0.71309700
H	-0.14160000	1.42865000	0.23485100
H	-1.10789100	-1.29781500	1.20606300
H	4.01327600	-1.29342600	-2.24439300
H	2.33775200	-2.97098100	-1.22681100
H	0.88080800	-1.99545500	-1.58350700
H	1.29771300	-2.34628600	0.13606600
H	4.97297100	1.12558000	-1.28847400
H	2.98507100	2.06191200	1.75613700
H	2.81076100	2.99389200	0.25117900
H	4.42617800	2.47414900	0.79586100
H	1.47188100	0.72974700	2.01081500
C	-2.59083200	-0.02228000	0.21766000
C	-3.63517200	-0.92988300	0.47178400
C	-2.90190600	1.14290700	-0.50966100
C	-4.93374800	-0.68588500	0.02779600
H	-3.41621700	-1.83597300	1.03074100
C	-4.19751200	1.38850900	-0.95438400
H	-2.11814300	1.86136500	-0.73160200
C	-5.22278800	0.47605200	-0.68818600
H	-5.72041900	-1.40429200	0.24163000

H	-4.41073500	2.29555600	-1.51381500
H	-6.23300100	0.66975200	-1.03704300

23

E(RB+HF-LYP) = -727.811325973 A.U.

O	1.19103900	-2.04157800	0.46102000
C	1.08558700	-0.66607100	0.18953900
C	2.29360400	0.00983500	0.04895300
N	3.55047000	-0.57793600	-0.08636800
N	2.52369200	1.38488400	-0.00348600
C	4.51006500	0.42257700	-0.24147200
C	3.81063900	-1.97502300	-0.40987100
C	3.89100400	1.61608700	-0.18437400
C	1.59707400	2.41997700	0.41055300
C	-0.22638700	-0.12955400	0.04250100
C	-1.37953500	-0.85567800	0.13502400
H	-0.30622600	0.92894400	-0.17530700
H	-1.29711700	-1.93194400	0.26712300
H	5.55127000	0.18113700	-0.38119000
H	3.22460400	-2.28610800	-1.28001500
H	3.55489000	-2.62976100	0.42175000
H	4.87334600	-2.07147000	-0.64149300
H	4.28602600	2.61714900	-0.24237600
H	1.01666800	2.08061500	1.27408300
H	0.90330900	2.70114300	-0.38963800
H	2.16876100	3.30522000	0.69668600
C	-2.73771300	-0.34395200	0.02049800
C	-3.06045300	1.03013700	-0.05496600
C	-3.81684800	-1.25480800	-0.01028900
C	-4.37852700	1.45964600	-0.16839700
H	-2.26876900	1.77297600	-0.01399500
C	-5.13561600	-0.82394900	-0.11995400
H	-3.60299700	-2.31944600	0.04826000
C	-5.42992300	0.53872200	-0.20251500
H	-4.58969700	2.52464600	-0.22435800
H	-5.93853600	-1.55630700	-0.14236600
H	-6.45789800	0.87822400	-0.28723400
H	0.69708200	-2.19869900	1.27950700

24

E(RB+HF-LYP) = -2692.09277127 A.U.

C	0.00000000	0.00000000	0.00000000
C	1.52193213	0.00000000	0.00000000
C	2.18947043	1.38595260	0.00000000
C	2.39300602	2.02071577	1.44472473

C	1.11644267	2.51713988	2.07480565
C	0.77116306	3.83041535	2.01813146
C	-0.42419086	4.28412128	2.77888265
O	1.44304913	4.79765553	1.44491280
N	-0.40157665	5.30329513	3.66478028
N	-1.69508823	3.83154678	2.72301582
C	-1.67184784	5.49708326	4.16910298
C	0.79251216	6.07479057	4.03475207
C	-2.48259640	4.57719493	3.58223237
C	-2.20106455	2.80860311	1.80909228
H	0.48246750	1.83797461	2.63586359
H	2.98152928	2.92211245	1.25098286
H	1.50942355	2.07348580	-0.51103798
H	1.89884824	-0.61761137	0.81971064
O	-0.74930115	5.23462000	-0.04108443
H	-1.88474925	6.26557615	4.89396922
H	0.53202179	6.69393618	4.89414769
H	1.10030223	6.68494719	3.18045132
H	1.59211179	5.38523063	4.30996437
H	-3.53975823	4.39665006	3.68759521
H	-2.41308795	1.88551647	2.35504377
H	-1.45496001	2.61358048	1.04318453
H	-3.11629224	3.17871309	1.34370727
C	3.21152045	1.13894641	2.38269942
C	4.60200806	1.31270170	2.45833106
C	2.63507215	0.14212625	3.18671400
C	5.38701361	0.52293599	3.29861983
H	5.07099263	2.07913276	1.84864735
C	3.41638529	-0.65278596	4.02770586
H	1.56012557	-0.01484634	3.17116959
C	4.79746635	-0.46571398	4.08746341
H	6.46073507	0.68390092	3.33848951
H	2.94233075	-1.41429215	4.64127488
H	5.40622130	-1.07988277	4.74484934
C	3.50966646	1.40324863	-0.76378441
C	4.34418457	0.28360829	-0.88249147
C	3.93027480	2.60994514	-1.34684723
C	5.55378100	0.35849668	-1.57761373
H	4.06100959	-0.65919514	-0.42450146
C	5.13910797	2.68666827	-2.03750756
H	3.30810972	3.49668637	-1.24409164
C	5.95494183	1.55942867	-2.16064110
H	6.18257755	-0.52411104	-1.65810489
H	5.44161436	3.62977403	-2.48418681
H	6.89421709	1.61818021	-2.70339474
C	-0.72427951	-1.27936266	0.32231720
C	-2.12400559	-1.28696499	0.20140848
C	-0.07320609	-2.45675581	0.72251489
C	-2.85506121	-2.43697293	0.47911981

H	-2.61277476	-0.37451341	-0.12244003
C	-0.80657053	-3.61028453	1.00052599
H	1.00632362	-2.48442096	0.81784562
C	-2.19668403	-3.60284198	0.88122165
H	-3.93652585	-2.43009084	0.37902949
H	-0.29118364	-4.51473389	1.30938287
H	-2.76560757	-4.50242302	1.09765532
Ti	0.88192403	6.15534641	-0.02379006
O	1.07981128	7.50177073	1.25660993
O	2.30219170	5.68807310	-1.07230391
O	0.28815791	7.34799909	-1.32789441
C	1.61431100	8.79056259	1.08232159
H	1.08576853	9.51370576	1.72173669
H	2.67934919	8.81884978	1.35941913
H	1.52601804	9.12662069	0.04021192
C	-0.86118499	8.14746213	-1.32714954
H	-0.78229807	8.96994375	-0.59872634
H	-1.01890616	8.59484852	-2.31912277
H	-1.75908370	7.56520650	-1.06932183
C	2.79987443	6.14710936	-2.30455468
H	2.10220192	6.86120344	-2.76026633
H	3.77236618	6.64074013	-2.16577119
H	2.94572885	5.30214892	-2.99233563
H	1.79940790	-0.53869495	-0.91799205
O	-0.64453824	0.99340769	-0.31370769
C	-1.43348088	4.75645529	-1.17400792
H	-1.19693426	3.69885483	-1.36297217
H	-2.52208262	4.83308744	-1.02517391
H	-1.17848573	5.33228199	-2.07524728

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E(RB+HF-LYP) = -2576.31838633 A.U.

C	1.76176600	-0.81707200	-1.16412200
C	0.69117400	-1.71198800	-1.31894700
C	-0.62700900	-1.28615600	-1.43686400
C	-1.15943300	-0.50387500	1.13643900
C	-2.03591700	0.52548900	0.82654600
C	-1.60910100	1.73775700	0.24303000
C	3.11526200	-1.28545500	-1.04213700
O	1.58609800	0.49990700	-1.17832500
N	4.22208500	-0.60494900	-1.47934000
N	3.58144200	-2.45826900	-0.49599900
C	5.35507300	-1.34917100	-1.21000800
C	4.21647400	0.62090700	-2.28309200
C	4.96433800	-2.49737800	-0.60573800
C	2.80575800	-3.42581900	0.26523700
H	0.91708800	-2.77156600	-1.38093500

H	-0.77361500	-0.21673000	-1.51962500
H	6.33815000	-0.99912700	-1.47963700
H	3.84077000	1.46720500	-1.70718500
H	3.57844500	0.48040200	-3.15852900
H	5.24233100	0.80044700	-2.60985800
H	5.53955800	-3.32910700	-0.23335700
H	3.45719200	-3.88063800	1.01429000
H	2.40000500	-4.21343600	-0.37700800
H	1.97845200	-2.91478800	0.76055900
H	-0.09573400	-0.29813900	1.10397800
H	-3.09983200	0.37738500	0.96556700
O	-0.36566200	1.94823500	-0.05354300
C	-1.51536100	-1.77447500	1.74037500
C	-2.81166100	-2.32977000	1.67275400
C	-0.52305900	-2.50024200	2.43742400
C	-3.09932900	-3.54374900	2.28831200
H	-3.58507000	-1.82049900	1.10777000
C	-0.81559600	-3.71225000	3.05476100
H	0.47518100	-2.07613500	2.51214100
C	-2.10853800	-4.24024200	2.98637900
H	-4.10203600	-3.95526500	2.21630600
H	-0.03893100	-4.24296000	3.59900300
H	-2.34069200	-5.18539700	3.46833400
C	-1.77783000	-2.12142400	-1.71000700
C	-1.77057100	-3.53178700	-1.60240100
C	-2.99544400	-1.51062700	-2.09360000
C	-2.90581900	-4.28336700	-1.88594200
H	-0.86639500	-4.04176300	-1.28367100
C	-4.13181200	-2.26519700	-2.36827900
H	-3.02918500	-0.42842000	-2.18489300
C	-4.09554100	-3.65942700	-2.27378600
H	-2.86591200	-5.36599500	-1.79771300
H	-5.04856000	-1.76417100	-2.66823300
H	-4.97941200	-4.25010900	-2.49581400
C	-2.57080300	2.79979900	-0.13671100
C	-3.87969500	2.86088500	0.38015400
C	-2.16296300	3.80118500	-1.03886100
C	-4.74926600	3.87805700	-0.00284500
H	-4.21380300	2.12676000	1.10540900
C	-3.03738200	4.81302500	-1.42393300
H	-1.15522400	3.76002700	-1.43602600
C	-4.33529600	4.85721500	-0.90946300
H	-5.75206200	3.91100500	0.41342700
H	-2.70573800	5.57022900	-2.12875200
H	-5.01642700	5.64898100	-1.20729100
Ti	1.56389200	1.78967800	0.35620300
O	2.38835200	0.48358000	1.36499100
O	2.72823700	2.92649000	-0.48666300
O	1.24775500	2.86903100	1.80074500

C	2.83761800	0.48619200	2.69688300
H	2.41013300	-0.36601200	3.24610100
H	3.93267100	0.39173400	2.73506900
H	2.55038500	1.41195900	3.21138700
C	3.22385800	4.20011600	-0.15092000
H	2.94384200	4.93243600	-0.92079000
H	2.82575900	4.53486800	0.81511800
H	4.32140600	4.17834100	-0.08944200
C	0.27696200	3.43423500	2.63193200
H	0.63783800	4.38539500	3.04751800
H	-0.65152100	3.63341700	2.08010600
H	0.03725200	2.76899700	3.47451200

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E (RB+HF-LYP) = -2576.34138094 A.U.

C	0.00000000	0.00000000	0.00000000
C	1.36038791	0.00000000	0.00000000
C	2.07280476	1.32598655	0.00000000
C	1.89652462	2.04388502	-1.43457903
C	1.76076641	3.53208118	-1.27897671
C	0.56047087	4.15676967	-1.19122110
C	-0.76083693	-1.26566188	-0.02671838
O	-0.74669171	1.07822069	0.05918620
N	-1.90675910	-1.47957016	0.65899740
N	-0.52107403	-2.38269153	-0.75671234
C	-2.38750742	-2.73908701	0.36261616
C	-2.55006115	-0.52957502	1.58057112
C	-1.52415716	-3.30663651	-0.51973139
C	0.54707742	-2.56047345	-1.73859535
H	1.91341160	-0.93172118	0.03835937
H	1.49037974	1.97728914	0.65939561
H	-3.29513334	-3.11845329	0.80269235
H	-2.90924140	0.34017736	1.02432944
H	-1.82593560	-0.20371167	2.32790896
H	-3.36869248	-1.05811784	2.07117860
H	-1.53800630	-4.26980813	-1.00280978
H	0.16156620	-3.16350113	-2.56232183
H	1.40706777	-3.06395044	-1.28980239
H	0.85100081	-1.58035403	-2.10311646
H	0.93090308	1.67771838	-1.78118774
H	2.65922284	4.13037789	-1.17750284
O	-0.61459497	3.50966969	-1.24303164
C	2.90478397	1.62670048	-2.49157169
C	4.22604705	2.09967264	-2.51634200
C	2.50428198	0.74542571	-3.50787098
C	5.11318028	1.69935952	-3.51542233
H	4.56765034	2.78351687	-1.74596800

C	3.39005194	0.33914293	-4.50787834
H	1.47321042	0.39985473	-3.52279768
C	4.70131920	0.81451302	-4.51408064
H	6.13076055	2.08041881	-3.51335397
H	3.05114160	-0.33746289	-5.28814311
H	5.39342660	0.50663621	-5.29280587
C	3.49009560	1.28295727	0.53394180
C	4.39830707	0.27101096	0.18799483
C	3.93221724	2.29316346	1.40108708
C	5.69712008	0.26347592	0.69695293
H	4.09398400	-0.51239243	-0.49974728
C	5.23310587	2.29521135	1.90623726
H	3.24353113	3.08561982	1.68177001
C	6.12105413	1.27640867	1.55852525
H	6.38118473	-0.53203401	0.41410756
H	5.54911487	3.08887913	2.57764527
H	7.13249172	1.27106046	1.95473719
C	0.43801446	5.63108123	-1.00043040
C	1.44175782	6.52347131	-1.41418923
C	-0.71278208	6.16072634	-0.39404904
C	1.31017042	7.89420443	-1.20337321
H	2.31880406	6.14279457	-1.92769130
C	-0.84327937	7.53261949	-0.18290525
H	-1.49858815	5.47980393	-0.08659998
C	0.16840082	8.40661528	-0.58308937
H	2.09594241	8.56627775	-1.53752650
H	-1.73903236	7.91968677	0.29532371
H	0.06522810	9.47618657	-0.42353218
Ti	-1.78419563	2.05978789	-1.44097415
O	-1.41083137	0.52257538	-2.43558010
O	-3.27839302	1.96896812	-0.35576928
O	-2.65047467	2.87939531	-2.83083381
C	-1.81542303	0.17783925	-3.73759523
H	-0.94271797	0.07713007	-4.40148731
H	-2.34260236	-0.78900496	-3.73398055
H	-2.48603479	0.93473859	-4.16254228
C	-4.56262697	2.52572849	-0.49034422
H	-4.69264581	3.37725519	0.19344324
H	-4.73724483	2.87277430	-1.51688409
H	-5.32877798	1.77700900	-0.23973406
C	-2.49324053	4.03114292	-3.61447445
H	-3.44911176	4.56607131	-3.70494424
H	-1.75375353	4.70807435	-3.16738546
H	-2.16036074	3.77084118	-4.62995398

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E(RB+HF-LYP) = -1381.88290463 A.U.

C	0.000000000000	0.000000000000	0.000000000000
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C	0.000000000000	0.000000000000	1.465459660000
C	1.165046819512	0.000000000000	2.158783886342
C	3.262308887921	2.477309552653	0.509033014149
C	2.100588441602	3.180803968825	0.342652170687
C	1.232521966099	3.038687837309	-0.775510741583
C	0.030825474876	3.734312563495	-0.959261545708
O	1.631658672105	2.218227365855	-1.820338731604
N	-0.634503020486	3.910262558625	-2.164133334506
N	-0.740929282167	4.399720527142	-0.011677024399
C	-1.773277627819	4.679993444916	-1.954398134470
C	-0.123480211186	3.577105901463	-3.488422834636
C	-1.843606248538	4.980347809433	-0.642037202463
C	-0.658061689012	4.216258000349	1.426490556216
H	1.825732668666	3.913645382545	1.093806948749
H	3.533495831999	1.772102450318	-0.271294189873
H	2.077840684337	0.038222377701	1.569698243078
H	-0.954141201992	-0.011152647442	1.981172963396
O	1.055567148965	-0.150141853220	-0.646385745459
H	1.507341749103	1.283248013580	-1.527913329617
H	-2.425147278109	4.949351865159	-2.769441408278
H	0.880283151764	3.985858070396	-3.625467579237
H	-0.798446706357	4.018797089360	-4.224600357755
H	-0.074229151832	2.498735982633	-3.630644571698
H	-2.574720363091	5.545808655797	-0.087831689223
H	0.045994436957	4.911705773870	1.895336744166
H	-0.340824736641	3.192986361699	1.647544178644
H	-1.647500177586	4.385397329747	1.857552150439
C	1.328754082870	-0.012313083620	3.608509525705
C	0.267078937813	-0.265553795848	4.502127772694
C	2.606310027839	0.239879842170	4.146138811884
C	0.476537195285	-0.257127793884	5.876089858703
H	-0.722902010027	-0.488184793454	4.115775343186
C	2.811664273247	0.255924326511	5.523887738727
H	3.434802950266	0.440829419143	3.474053743544
C	1.749457091373	0.007349171242	6.393790629026
H	-0.351394515135	-0.461982939166	6.548867908837
H	3.802791082144	0.465963399689	5.914003054886
H	1.909149069806	0.013882552433	7.468123178128
C	4.199886554403	2.592143759533	1.613903100206
C	4.033175058997	3.468000749947	2.712476165124
C	5.355210194252	1.775711034365	1.620726325423
C	4.962077635219	3.519640654883	3.746280350853
H	3.163951744310	4.117668127786	2.756554771984
C	6.282510842617	1.826797461596	2.657858146075
H	5.516393310784	1.094466360407	0.788834962769
C	6.095406791212	2.700065492962	3.732564333058
H	4.801036809587	4.206573450515	4.573331499262
H	7.158184893177	1.183616942598	2.625401585266
H	6.818906402594	2.744987168918	4.541125587000
C	-1.296163125849	0.138505831635	-0.739758842245
C	-2.485952793198	0.589521074034	-0.144594453629
C	-1.310746983044	-0.195012021803	-2.104989169216
C	-3.655467675449	0.703811426456	-0.894314526228
H	-2.500943224190	0.876003903389	0.901536748899
C	-2.480371555442	-0.087821230033	-2.851404021064
H	-0.388560810705	-0.546958898939	-2.554138146254
C	-3.657817081932	0.362885791462	-2.248070501792
H	-4.565982861701	1.060448386931	-0.421575622993
H	-2.477929138629	-0.360473206463	-3.902909947240
H	-4.571897262950	0.445887587399	-2.828986288183

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E(RB+HF-LYP) = -1381.88855162 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.354339540000
C	1.223974728845	0.000000000000	2.231548211132
C	1.513514424419	1.388907088535	2.964011179075
C	1.702593174002	2.526861229903	1.985017538220
C	2.436589617252	2.455228163799	0.834322152693
C	2.516970953618	3.708610676858	0.017962259992
O	3.083514597405	1.450658436517	0.325800523525
N	3.637204983587	4.158803689113	-0.594675528650
N	1.511064604535	4.540781174404	-0.353874854198
C	3.341427960850	5.288205791771	-1.334344490437
C	4.968086400954	3.556908794647	-0.461500694948
C	2.013460485059	5.529140271237	-1.185990163911
C	0.090968069406	4.377370631362	-0.037395391740
H	1.266649394844	3.482959125204	2.257750188582
H	2.468376845194	1.218814163325	3.484424985571
H	2.098307542449	-0.128137160421	1.592651368660
H	-0.966397024039	-0.026631401960	1.843682628135
O	1.094575743393	0.101391811121	-0.795783134456
H	1.883231302464	0.499467576108	-0.331043233854
H	4.094954731972	5.812646624669	-1.899242198418
H	5.528315291453	4.059383163833	0.331386914135
H	5.495240776140	3.668259501686	-1.410584659421
H	4.817474749803	2.502449863218	-0.222523731463
H	1.383457856533	6.296164313082	-1.606023651784
H	-0.183916771398	4.981507493830	0.830529804249
H	-0.098647418972	3.327157591333	0.183677532857
H	-0.494016158242	4.692663019994	-0.903188555014
C	1.242244132721	-1.161294293444	3.222080860748
C	0.129149426120	-1.532638793608	3.990706596683
C	2.427037017699	-1.893275630384	3.388829574817
C	0.198900989766	-2.597549545511	4.889452957154
H	-0.802274412604	-0.984853623994	3.892500325903
C	2.502960579506	-2.957813107867	4.287843733245
H	3.299476190904	-1.626450599976	2.797090472418
C	1.385833704804	-3.315744361064	5.042820604847
H	-0.678233530618	-2.866120554244	5.472087159751
H	3.432423387973	-3.511313843807	4.391727706459
H	1.437765651164	-4.146937693728	5.740481854316
C	0.488177684597	1.747583311726	4.029022375226
C	-0.775518779877	2.257062506245	3.690093628706
C	0.782144289866	1.576823208083	5.388479111069
C	-1.712483394271	2.576397503226	4.673715432419
H	-1.026491443586	2.394595222834	2.642687627626
C	-0.148926594670	1.899214126748	6.376694266313
H	1.753197586387	1.181498028389	5.673887243047
C	-1.402163726941	2.400159975516	6.023274076668
H	-2.685879531131	2.964521566174	4.385356727067
H	0.106212606912	1.758167075671	7.423390673674
H	-2.128871945838	2.651951775080	6.790484925343
C	-1.254481152547	-0.100255535219	-0.796053872565
C	-2.424486883892	-0.684588824990	-0.281147725648
C	-1.284427173500	0.392452320456	-2.111651600983
C	-3.591137345452	-0.739323795905	-1.040103825226
H	-2.410972920037	-1.123614500469	0.710984178640
C	-2.451400517188	0.333400345008	-2.872263065072
H	-0.375843096348	0.814027592613	-2.526032857447
C	-3.613242998393	-0.226739732374	-2.339394016335
H	-4.481963957097	-1.199883867289	-0.621736490549

H	-2.451837907634	0.722347708132	-3.887251121912
H	-4.521455293350	-0.277600963248	-2.933296780547

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E(RB+HF-LYP) = -1381.88294738 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.422685840000
C	1.129231672503	0.000000000000	2.198048967444
C	0.981463524673	-3.386359549058	1.639127543844
C	2.219484392397	-3.778110757161	1.249389846945
C	2.745577824397	-3.408817396944	-0.064249745354
C	-1.141441922102	0.043890280367	-0.806308523786
O	1.213147650128	-0.039925745854	-0.670708925309
N	-1.219569986109	-0.353333461763	-2.134490496529
N	-2.412235907920	0.513676140412	-0.484993002007
C	-2.514266191537	-0.151511433595	-2.599242285881
C	-0.204464980750	-1.108983412638	-2.857645084267
C	-3.245470860912	0.379614293993	-1.597692034830
C	-2.743793200876	1.333212632337	0.666094383052
H	-0.967668529251	-0.060613299621	1.912295972248
H	2.083123509996	0.080893045461	1.683899533252
H	-2.795205439029	-0.412450199184	-3.606779762794
H	0.100074139708	-1.993922750406	-2.290363057871
H	0.682537146109	-0.500774770952	-3.031854884928
H	-0.636966263145	-1.421732651901	-3.810267016128
H	-4.277849370315	0.687603998339	-1.567829671894
H	-1.872063401385	1.927169332912	0.952869270385
H	-3.056254409690	0.734529002113	1.528789093463
H	-3.562117744243	2.005023299653	0.396266298012
H	0.394553018765	-2.822711031425	0.918396773181
H	2.840569044481	-4.377270236100	1.905043919536
O	2.151335815339	-2.602412931341	-0.807315522562
H	1.615067633985	-0.930935337353	-0.553929601354
C	0.314940626139	-3.702735345962	2.897201639787
C	0.995421430720	-4.200966036476	4.025647831755
C	-1.077484951004	-3.515118559372	2.989956787099
C	0.304659229483	-4.515672162726	5.190326098212
H	2.073753865659	-4.319171772688	3.995482719535
C	-1.770043159067	-3.838984257467	4.153549238140
H	-1.612285260761	-3.121320606598	2.129962690322
C	-1.081127811572	-4.342973581272	5.258015904475
H	0.847425371744	-4.889712232355	6.053319385611
H	-2.845720678958	-3.695983652210	4.200787224540
H	-1.616947250864	-4.590913052315	6.169499643023
C	1.194004283307	-0.034681007198	3.649573101472
C	0.067012367979	-0.173117507661	4.492481774541
C	2.452884654439	0.080717884844	4.282177824719
C	0.195860245105	-0.184347344750	5.877147266154
H	-0.921754522781	-0.283156662224	4.057358949401
C	2.579920010223	0.069798638287	5.667665601277
H	3.339474215870	0.186458941934	3.661592789656
C	1.451232966441	-0.060797936494	6.480301005874
H	-0.692503924477	-0.293715170145	6.494216211361
H	3.565475638371	0.165632963198	6.116335659131
H	1.546648223710	-0.068587217417	7.562108588701
C	4.032628393235	-4.006922519119	-0.537380152322
C	4.623907533605	-5.134979455196	0.055498465981
C	4.664190714912	-3.416605523303	-1.645413766873
C	5.818539164620	-5.652164665017	-0.442862004366
H	4.144253699992	-5.630567020138	0.892456501454

C	5.860894408503	-3.927831414654	-2.136279943931
H	4.192794310965	-2.553029807154	-2.101178017891
C	6.442700095108	-5.047765230488	-1.535398860671
H	6.260768815864	-6.529257779881	0.020309977379
H	6.342696130138	-3.455634312946	-2.987476858765
H	7.376321456597	-5.449094116543	-1.918928740184

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E(RB+HF-LYP) = -1381.88722576 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.373058640000
C	1.322307536189	0.000000000000	2.091405232527
C	2.109099877958	-1.385080166480	1.844848176087
C	3.600837209910	-1.171062303974	1.829749312689
C	4.256918534490	-0.627076351080	0.778479948064
C	-1.322705301500	-0.024640496012	-0.691256330262
O	1.023046894873	-0.026705066245	-0.789227937490
N	-1.587575573772	-0.711605989451	-1.829813612193
N	-2.451669488064	0.671132301663	-0.389806096736
C	-2.887346864555	-0.465805368946	-2.229917260538
C	-0.665613172660	-1.634540146386	-2.502925373669
C	-3.429300033706	0.396745247634	-1.333213196942
C	-2.616051619502	1.640626973080	0.693032791385
H	-0.929056705106	-0.043575755756	1.928319867866
H	1.951698804005	0.730640352151	1.571710527806
H	-3.306303669377	-0.921911085519	-3.112203396656
H	-0.865421906993	-2.659552498553	-2.179038860867
H	0.345703006829	-1.331860729983	-2.226888153228
H	-0.820269906131	-1.553772095682	-3.580247822507
H	-4.406598909757	0.849111099081	-1.289218468291
H	-1.630390815277	1.993518412030	0.995297880964
H	-3.103608064425	1.178464464546	1.555066679980
H	-3.226893472932	2.468947330646	0.328837291526
H	1.812044808089	-1.659942358833	0.828166835099
H	4.179077721101	-1.438055780121	2.704865136298
O	3.674131363206	-0.173697818933	-0.358885428206
H	2.678836035890	-0.170150546366	-0.359951925263
C	1.652039556920	-2.513419232064	2.750896656372
C	2.163529547052	-2.700472015301	4.043963847488
C	0.668997080402	-3.408045543327	2.302058807924
C	1.716875563196	-3.746622968232	4.851575676792
H	2.911688126685	-2.015676855344	4.430045041785
C	0.213647823779	-4.452771919087	3.107576741607
H	0.261454084799	-3.281119350190	1.302563116589
C	0.739683596371	-4.628713588681	4.387763346573
H	2.132264134133	-3.869818624263	5.848067916377
H	-0.544309801104	-5.134861665858	2.731076165205
H	0.394585898026	-5.445140369213	5.015967527010
C	1.250864056577	0.432876421652	3.542044794049
C	0.246974637563	-0.015515493304	4.414156435661
C	2.220619843418	1.308497857798	4.052381123811
C	0.206640152967	0.405934043080	5.743498433449
H	-0.502018541884	-0.715843351767	4.056799400157
C	2.188520940941	1.727568946537	5.383225456818
H	3.009527506279	1.661864367858	3.394141525684
C	1.176853289368	1.281124460966	6.234311347051
H	-0.581083924867	0.043945648368	6.398878438898
H	2.951240517474	2.407994831947	5.752002629772
H	1.145297363070	1.610056486331	7.269243422283
C	5.730230717932	-0.430048762331	0.760497903804

C	6.596759621152	-1.205487391273	1.549407821899
C	6.290580645727	0.553077793371	-0.071871215658
C	7.971665119053	-0.983298116033	1.531085091708
H	6.192720929404	-2.004765952559	2.162220821784
C	7.667099178164	0.772525401160	-0.091273073382
H	5.629284465354	1.139850987575	-0.698580720593
C	8.515119825060	0.009659242032	0.712713256326
H	8.622602899498	-1.597646658183	2.147274488616
H	8.078656854807	1.542785566513	-0.738150567655
H	9.588191464141	0.178350186877	0.694901442320

TS1

E(RB+HF-LYP) = -2037.97616813 A.U.

1 imaginary frequencies -112.1162 cm⁻¹

O	-0.46922100	-0.61285100	0.69677000
C	0.48206300	-0.17990300	0.00234500
C	0.35548400	2.11499700	0.21046200
N	-0.48986300	2.71500400	1.08585400
N	0.58274400	3.07232100	-0.72832800
C	-0.80014300	4.01077600	0.69527900
C	-1.05786400	2.05378800	2.25956000
C	-0.11953900	4.24080400	-0.45619300
C	1.42814100	2.87507500	-1.89629000
C	1.87462400	-0.36950700	0.44839000
Ti	-2.52649500	-0.96799400	-0.10772500
O	-1.88598300	-2.61410600	-0.55027600
O	-3.01609000	-0.62544300	1.63938400
O	-4.23064300	-1.18247200	-0.71875100
O	-2.08253900	0.42354000	-1.24376500
C	-2.78240400	1.03720800	-2.29295600
C	-2.40110000	-3.68559700	-1.29910100
C	-2.60518400	-1.16124700	2.87228600
C	-5.50627400	-1.16211500	-0.13597100
C	2.87820100	-0.54695900	-0.42940500
H	2.02136700	-0.44080900	1.52261100
H	2.62814200	-0.50397400	-1.49069500
H	-1.45500300	4.64961300	1.26716400
H	-0.32680700	1.35228400	2.65771900
H	-1.95952000	1.49719800	1.99413500
H	-1.28422300	2.80859400	3.01605200
H	-0.06325200	5.11805200	-1.08169900
H	2.04748200	1.99563700	-1.72673300
H	2.07666200	3.74329100	-2.04165300
H	0.82352900	2.72544900	-2.79625600
H	0.32856500	-0.01516400	-1.07166500
H	-2.33152500	-4.61785800	-0.72158500
H	-3.45319900	-3.51520700	-1.56589400
H	-1.82466400	-3.82195600	-2.22531500
H	-1.51471300	-1.28420300	2.90758500

H	-2.90483300	-0.49124000	3.69144100
H	-3.07017600	-2.14033400	3.05906200
H	-6.13754000	-0.39910500	-0.61328400
H	-6.00542500	-2.13335500	-0.26259500
H	-5.43673600	-0.93903000	0.93787500
H	-2.86665700	2.12082600	-2.11967300
H	-2.25634400	0.89394100	-3.24977500
H	-3.79460900	0.62232300	-2.39526000
C	4.29061700	-0.81765600	-0.14231700
C	4.81622000	-0.86305300	1.16330500
C	5.17076800	-1.04248600	-1.21606100
C	6.16479400	-1.12594200	1.37981900
H	4.16478000	-0.68975400	2.01401600
C	6.52186300	-1.30556300	-0.99978200
H	4.78322700	-1.01385600	-2.23138200
C	7.02524800	-1.34886000	0.30046900
H	6.54914300	-1.15687300	2.39528500
H	7.18037700	-1.47790100	-1.84614400
H	8.07739800	-1.55389700	0.47399500

TS2

E(RB+HF-LYP) = -2037.98065063 A.U.

1 imaginary frequencies -1163.6045 cm⁻¹

O	0.77755400	-0.17457000	-0.79390800
C	-0.23208400	0.40178200	-0.00726700
C	-0.23773300	1.86458900	-0.05945600
N	0.40135000	2.69062900	-0.93352600
N	-0.79156100	2.67490400	0.89305700
C	0.25045100	4.00727300	-0.52227300
C	1.02434500	2.31817100	-2.20925300
C	-0.49569300	3.99911500	0.60773500
C	-1.47740400	2.21039700	2.09063400
C	-1.53006600	-0.30102900	-0.09891100
Ti	2.42349400	-0.85996800	-0.10825800
O	2.72423300	-2.61277800	0.31057700
O	3.22852800	-0.96262000	-1.75122600
O	3.57396500	0.36461700	0.63499100
O	1.26612000	-0.67976800	1.65308400
C	1.72299700	-0.31887100	2.93797700
C	2.12556000	-3.59033600	1.11784900
C	3.78055400	-1.98959300	-2.52718200
C	4.89017900	0.71522600	0.28972200
C	-2.76021600	0.22519100	-0.28146800
H	-1.41845500	-1.37779300	0.01685900
H	-2.84713300	1.29184800	-0.49186000
H	0.68583600	4.82435400	-1.07410700
H	0.32844400	2.51820600	-3.02899400

H	1.27333400	1.25952900	-2.17816100
H	1.92693900	2.91815200	-2.34220400
H	-0.83208800	4.80485300	1.23943000
H	-0.87573400	1.43764300	2.57624000
H	-2.45108300	1.78324800	1.84108900
H	-1.60078900	3.05597400	2.76772700
H	0.35358900	0.00967100	1.15926400
H	1.65960300	-4.37155200	0.49939800
H	2.88037200	-4.07501600	1.75347400
H	1.35402600	-3.15113600	1.76420000
H	4.82009200	-1.75624400	-2.80087200
H	3.76847600	-2.94052700	-1.97536300
H	3.21350600	-2.11973100	-3.46070700
H	5.05882300	1.78416500	0.48518700
H	5.61939700	0.14904800	0.88796100
H	5.08839600	0.51860700	-0.77296900
H	0.90525500	0.11676000	3.53401800
H	2.07891300	-1.20681700	3.47659800
H	2.54705400	0.40340900	2.87917200
C	-4.03393000	-0.50387900	-0.27668100
C	-5.19181900	0.13453800	-0.76041500
C	-4.16505700	-1.82650100	0.19130800
C	-6.42091200	-0.52033400	-0.79558900
H	-5.11738100	1.15737300	-1.12245800
C	-5.39158800	-2.48271200	0.15113600
H	-3.30064700	-2.33951100	0.60134000
C	-6.52797700	-1.83598900	-0.34277900
H	-7.29612300	-0.00256700	-1.17835700
H	-5.46436500	-3.50313700	0.51719800
H	-7.48450200	-2.34949700	-0.36679900

TS3

E(RB+HF-LYP) = -727.78378544 A.U.

1 imaginary frequencies -205.3737 cm⁻¹

O	1.59432300	-2.07045700	1.46782100
C	1.07559600	-0.94313300	1.24307900
C	2.23290000	0.08644800	0.08266700
N	3.32002400	-0.43804200	-0.52602200
N	2.38345800	1.43043900	-0.03166400
C	4.14749100	0.56269500	-1.01735800
C	3.56263800	-1.87608600	-0.68019300
C	3.55923100	1.74489100	-0.70168300
C	1.45077600	2.40796100	0.51833500
C	-0.22078300	-0.88023000	0.46918800
C	-1.28569900	-0.17170600	0.87793600
H	-0.26473900	-1.53103900	-0.40211000
H	-1.17755400	0.40669700	1.79813800

H	5.06326600	0.34754700	-1.54533300
H	2.88322400	-2.39225000	0.00499200
H	4.60233300	-2.09336200	-0.42344600
H	3.37700200	-2.17464000	-1.71601100
H	3.86578200	2.76136600	-0.89279200
H	0.45403100	1.96871400	0.53852500
H	1.44007800	3.29479900	-0.11877000
H	1.74164100	2.69732600	1.53269900
H	1.08364400	-0.16611200	2.04957400
C	-2.61605900	-0.09134500	0.25669300
C	-2.93649100	-0.71726400	-0.96319000
C	-3.62622900	0.64712900	0.89855000
C	-4.21231300	-0.61179100	-1.50844100
H	-2.17895800	-1.29043900	-1.48867800
C	-4.90435600	0.75466400	0.35304700
H	-3.40083000	1.13771000	1.84241900
C	-5.20464600	0.12463200	-0.85472100
H	-4.43536700	-1.10553800	-2.45025600
H	-5.66579600	1.32963600	0.87263600
H	-6.19904300	0.20526400	-1.28380000

TS4

E(RB+HF-LYP) = -843.511275689 A.U.

1 imaginary frequencies -458.1702 cm⁻¹

N	0.00000000	0.00000000	0.00000000
C	0.00000000	1.35463900	0.00000000
C	1.14297200	2.29984100	0.00000000
C	1.33334000	3.07708400	1.25558800
N	-1.29844700	1.74203300	-0.10327200
C	-1.30236400	-0.46209300	-0.11178700
C	1.17259300	-0.86575600	0.16548800
C	-2.11270600	0.62479900	-0.17019200
C	-1.74010900	3.13111300	-0.22065200
O	2.34696600	1.70868600	-0.46901900
C	0.59757100	3.03200500	2.38360400
C	0.77112800	3.86182100	3.58304100
C	0.08232800	3.51505500	4.76013100
C	1.59942300	5.00057600	3.62072100
C	0.22403500	4.25881800	5.92983100
C	1.74413700	5.74146900	4.78971000
C	1.05921000	5.37624600	5.95222000
H	0.98570900	3.03327700	-0.95929400
H	2.17884700	3.75805000	1.18232800
H	-1.53019200	-1.51515700	-0.14165700
H	2.05467900	-0.27318700	-0.07599500
H	1.07902700	-1.71355400	-0.51622800
H	1.22181000	-1.22786200	1.19585700
N	0.00000000	0.00000000	0.00000000

C	0.00000000	1.35463900	0.00000000
C	1.14297200	2.29984100	0.00000000
C	1.33334000	3.07708400	1.25558800
N	-1.29844700	1.74203300	-0.10327200
C	-1.30236400	-0.46209300	-0.11178700
C	1.17259300	-0.86575600	0.16548800
C	-2.11270600	0.62479900	-0.17019200
C	-1.74010900	3.13111300	-0.22065200
O	2.34696600	1.708686006	-0.46901900
C	0.59757100	3.03200500	2.38360400
C	0.77112800	3.86182100	3.58304100
C	0.08232800	3.51505500	4.76013100
C	1.59942300	5.00057600	3.62072100
C	0.22403500	4.25881800	5.92983100
C	1.74413700	5.74146900	4.78971000
C	1.05921000	5.37624600	5.95222000
H	0.98570900	3.03327700	-0.95929400
H	2.17884700	3.75805000	1.18232800
H	-1.53019200	-1.51515700	-0.14165700
H	2.05467900	-0.27318700	-0.07599500
H	1.07902700	-1.71355400	-0.51622800
H	1.22181000	-1.22786200	1.19585700
H	-3.18333000	0.70383300	-0.26534900
H	-2.79102200	3.13402000	-0.50993200
H	-1.61198100	3.65130400	0.73108300
H	-1.14580700	3.63437600	-0.98591400
H	2.39380500	2.18880700	-1.36492700
H	-0.20207400	2.29337900	2.45896100
H	-0.56723800	2.64270100	4.75346600
H	2.12429400	5.31442800	2.72389500
H	-0.31809300	3.96489000	6.82435300
H	2.38926200	6.61562900	4.79229200
H	1.17123400	5.96031600	6.86080200
O	1.59236800	3.31237400	-2.28446000
C	0.86531600	2.68250500	-3.27644600
H	0.24231200	1.82391200	-2.91720000
H	0.15491600	3.36061700	-3.79571000
H	1.50487900	2.25028200	-4.07299400

TS5

E(RB+HF-LYP) = -2576.32248728 A.U.

1 imaginary frequencies -274.8967 cm⁻¹

C	0.75818800	-0.34840100	1.56567900
C	-0.60749700	-0.57222700	1.51708800
C	-1.54658400	0.30998000	0.91098500
C	-1.70570000	-0.15636200	-1.26264700
C	-0.58721300	-0.98068100	-1.56650400
C	0.70867800	-0.50510700	-1.60973900

C	1.82049800	-1.39488800	-1.94745100
O	1.03844100	0.75582700	-1.46990900
N	2.90664900	-1.02479200	-2.67708000
N	2.02262200	-2.69175200	-1.57697600
C	3.77813000	-2.09184900	-2.77252600
C	3.10104800	0.27150300	-3.34371800
C	3.23094800	-3.13066500	-2.09137300
C	1.18423700	-3.47687000	-0.67478200
H	-0.75038200	-2.03505200	-1.76272500
H	-1.54888300	0.90124300	-1.45689900
H	-1.15252400	1.28882000	0.65708200
H	-0.97239100	-1.50295700	1.93565600
O	1.33420600	0.74585800	1.12445400
H	4.70634100	-2.01777300	-3.31503400
H	4.00449400	0.19014200	-3.95012500
H	3.18977500	1.07147100	-2.60438700
H	2.24651300	0.47793600	-3.99034200
H	3.59478700	-4.12909400	-1.91282600
H	0.44874100	-4.06067600	-1.23506200
H	0.67170400	-2.79589900	0.00525900
H	1.82614900	-4.14805600	-0.10275800
C	-3.06711900	-0.64220100	-1.53752000
C	-4.06274500	0.26347300	-1.95063700
C	-3.43702200	-1.99548000	-1.40373600
C	-5.35754000	-0.16273000	-2.23642700
H	-3.80478900	1.31325400	-2.05770500
C	-4.73000400	-2.42370900	-1.69303400
H	-2.70576100	-2.72123600	-1.05821900
C	-5.69944100	-1.51054500	-2.11368200
H	-6.10172800	0.56016000	-2.55928100
H	-4.98526700	-3.47445400	-1.58281500
H	-6.70824800	-1.84477100	-2.33760200
C	-2.95297400	0.35459500	1.34461200
C	-3.64071100	-0.75776900	1.86638600
C	-3.65636500	1.57073500	1.24986000
C	-4.96386000	-0.65203400	2.28608100
H	-3.13785300	-1.71665000	1.94286100
C	-4.97891600	1.67823800	1.67281000
H	-3.14450400	2.44188700	0.84889000
C	-5.64102000	0.56628100	2.19549000
H	-5.47105300	-1.52606600	2.68550300
H	-5.49251000	2.63276800	1.59714600
H	-6.67224200	0.64623700	2.52678000
C	1.68859700	-1.33326000	2.19745000
C	3.06602000	-1.24252600	1.92697500
C	1.25398700	-2.35837100	3.05918600
C	3.96742900	-2.15894100	2.46602900
H	3.41432500	-0.43772100	1.28963600
C	2.15602300	-3.27212700	3.59943800

H	0.20683000	-2.43008800	3.33323500
C	3.51829900	-3.18365500	3.30093900
H	5.02620900	-2.06747900	2.23853700
H	1.79518600	-4.04840700	4.26865900
H	4.22052100	-3.89408000	3.72757900
Ti	1.43974000	2.20007900	-0.15984300
O	3.02749500	2.53743900	-1.05763100
O	-0.00218600	3.16949300	-0.73420300
O	1.82859600	3.30628800	1.24582400
C	4.00833000	3.52536500	-0.86010100
H	5.00413500	3.06545100	-0.77258400
H	4.03518500	4.22036100	-1.71240800
H	3.81098000	4.10355600	0.05166500
C	2.10608100	3.23056600	2.61515800
H	3.12065400	3.59903100	2.82676700
H	1.40092800	3.84799600	3.18957200
H	2.03059000	2.19382300	2.96932100
C	-0.44283900	4.46703900	-0.41792100
H	0.07677100	4.85624500	0.46750600
H	-0.26378500	5.15078800	-1.25966700
H	-1.52415400	4.45984500	-0.21875400

TS6

E(RB+HF-LYP) = -2576.31816613 A.U.

1 imaginary frequencies -117.2709 cm⁻¹

C	1.68800500	-0.96605200	-1.10440800
C	0.57407000	-1.79725200	-1.19819300
C	-0.72661000	-1.27396000	-1.31165700
C	-1.18826900	-0.48974800	0.97279300
C	-1.99556500	0.62858300	0.70415500
C	-1.48729200	1.82820000	0.20221200
C	3.02361900	-1.51380700	-0.98601500
O	1.60510100	0.35225600	-1.17568900
N	4.14726400	-0.92930900	-1.49710100
N	3.43673300	-2.66564100	-0.37003600
C	5.24637900	-1.71233400	-1.20316700
C	4.18948100	0.26359800	-2.35164800
C	4.81060700	-2.79161500	-0.50734200
C	2.62173600	-3.54858500	0.45367100
H	0.72544700	-2.87138100	-1.21141800
H	-0.77485500	-0.21217700	-1.51764900
H	6.23874600	-1.43615900	-1.52009700
H	3.88506200	1.15123600	-1.79533400
H	3.51332000	0.12872600	-3.19794600
H	5.21272300	0.36329900	-2.71794000
H	5.34910800	-3.62638600	-0.08968000
H	3.25235000	-3.97042500	1.23869300

H	2.19324900	-4.36330100	-0.13736100
H	1.81136600	-2.97265100	0.90143200
H	-0.11833600	-0.32928200	1.03413200
H	-3.06874900	0.54273300	0.82291300
O	-0.21586800	1.98398900	-0.06020900
C	-1.65420200	-1.69825600	1.64002900
C	-2.98612400	-2.15732600	1.56758700
C	-0.74048700	-2.45429400	2.40688700
C	-3.38305000	-3.30778000	2.24350200
H	-3.70546000	-1.62035500	0.95857400
C	-1.14043600	-3.60376000	3.08218900
H	0.28329700	-2.09922200	2.49528100
C	-2.46710300	-4.03662400	3.00636000
H	-4.41383900	-3.64248800	2.16869700
H	-0.42106100	-4.15689700	3.68043000
H	-2.78330400	-4.93088800	3.53541800
C	-1.91040000	-2.04583100	-1.65102100
C	-2.00638100	-3.44543900	-1.48721000
C	-3.04796300	-1.37334600	-2.15295500
C	-3.16464100	-4.13466600	-1.83467900
H	-1.16800500	-3.99765400	-1.07331900
C	-4.20820100	-2.06360200	-2.49049300
H	-3.00096700	-0.29589700	-2.28471800
C	-4.27357400	-3.45192300	-2.34111300
H	-3.20576300	-5.21259400	-1.70193000
H	-5.06258700	-1.51785600	-2.88212400
H	-5.17533500	-3.99288900	-2.61258200
C	-2.36638900	2.97715700	-0.13044900
C	-3.67531700	3.10326600	0.37308800
C	-1.87750100	3.99362900	-0.97226600
C	-4.46802300	4.19580400	0.03276200
H	-4.06903200	2.35773800	1.05570900
C	-2.67473800	5.08269800	-1.31458300
H	-0.86801200	3.90560700	-1.35719800
C	-3.97454400	5.18997500	-0.81588400
H	-5.47258200	4.27603000	0.43851400
H	-2.27999900	5.85097300	-1.97362800
H	-4.59506900	6.04145800	-1.07971100
Ti	1.66881600	1.70022600	0.34123800
O	2.37383600	0.34960800	1.38615100
O	2.92137500	2.69363800	-0.56220400
O	1.49288100	2.85650700	1.74591200
C	2.78467600	0.33886300	2.73052500
H	2.22266000	-0.41877000	3.29697700
H	3.85289400	0.08739600	2.80467100
H	2.62429000	1.31606000	3.20311200
C	3.52632400	3.93412000	-0.28899800
H	3.28230500	4.66051100	-1.07681900
H	3.18777200	4.33365100	0.67524500

H	4.62030400	3.82633300	-0.25802800
C	0.57517000	3.56420100	2.52919000
H	1.00060600	4.52982400	2.83605000
H	-0.35178600	3.75801100	1.97384200
H	0.31917200	3.00601600	3.44160500

TS7

E(RB+HF-LYP) = -1381.86319369 A.U.

1 imaginary frequencies -232.647 cm⁻¹

C	1.11093000	1.54962100	-0.87286700
C	-0.18874600	1.48943900	-0.41071600
C	-1.24927100	0.83041600	-1.08806900
C	-1.32968900	-1.35684200	-0.33843900
C	-0.03682100	-1.63705800	0.16652700
C	1.07903600	-1.66664000	-0.66060700
C	2.39653200	-1.98455000	-0.08419500
O	1.04844600	-1.45446600	-1.94571400
N	3.38362700	-2.66566500	-0.73005200
N	2.91688500	-1.61192000	1.12258200
C	4.50345000	-2.73799100	0.07743500
C	3.25537000	-3.32999700	-2.02996900
C	4.21584700	-2.08243700	1.22930700
C	2.29440100	-0.71484900	2.09307200
H	0.08611300	-1.82240200	1.22831700
H	-1.47196900	-1.59375400	-1.38826900
H	-0.99335900	0.47901000	-2.08285900
H	-0.40040700	1.96774300	0.53973100
O	1.50205300	1.00561400	-2.03750900
H	1.23440300	0.01274100	-2.10970800
H	5.40075600	-3.24344600	-0.24076300
H	2.97863900	-4.37882800	-1.88826400
H	4.21639200	-3.27261500	-2.54464600
H	2.48062200	-2.80470100	-2.58880400
H	4.81930800	-1.88951300	2.10109100
H	1.70817200	-1.27591900	2.82565800
H	1.64410200	-0.02122800	1.55803600
H	3.08209300	-0.15952400	2.60400300
C	-2.65155400	1.22778200	-0.93662500
C	-3.16747800	1.83818500	0.22467100
C	-3.54460800	1.00427500	-2.00416200
C	-4.50474100	2.21472700	0.30516900
H	-2.51696300	2.01510100	1.07504300
C	-4.88185100	1.38430700	-1.92475400
H	-3.16955300	0.53981900	-2.91287300
C	-5.37134200	1.99431300	-0.76845300
H	-4.87501000	2.68304000	1.21312300
H	-5.54207400	1.20858200	-2.76984100

H	-6.41339800	2.29318900	-0.70299300
C	-2.51614900	-1.49752800	0.51105700
C	-2.49096200	-1.23986500	1.89732600
C	-3.74465100	-1.89638100	-0.05108600
C	-3.62851700	-1.40105300	2.68361800
H	-1.57029800	-0.89614800	2.36073100
C	-4.88427000	-2.05272200	0.73357600
H	-3.79436800	-2.09300800	-1.11802600
C	-4.83326200	-1.81144800	2.10773900
H	-3.57804000	-1.19760100	3.75016400
H	-5.81603400	-2.36571900	0.27055700
H	-5.72115800	-1.93453300	2.72099400
C	2.18095800	2.28780100	-0.15692900
C	1.92125300	3.22561500	0.86237800
C	3.52469800	2.05326000	-0.50637200
C	2.96164100	3.87145500	1.52472900
H	0.89749700	3.47250700	1.12329400
C	4.56404600	2.70134300	0.15750500
H	3.72770900	1.35739900	-1.31209700
C	4.29120100	3.60987000	1.18216900
H	2.73311800	4.59425500	2.30325600
H	5.59269200	2.50104300	-0.13107500
H	5.10073200	4.12013700	1.69608800

TS8

E(RB+HF-LYP) = -1381.86568466 A.U.

1 imaginary frequencies -365.7579 cm⁻¹

C	0.86967500	2.07175500	-0.67735400
C	1.50508900	0.84582100	-0.63346500
C	0.84179900	-0.37076900	-0.98503600
C	-0.20565100	-0.81678900	0.76789300
C	-1.57630700	-1.01798000	0.42334700
C	-2.44185800	0.06447100	0.26980700
C	1.46434300	3.26938500	-0.13227800
O	-0.37067800	2.25081200	-1.17074800
N	0.76290200	4.27991400	0.45973400
N	2.77540300	3.66183200	-0.13892200
C	1.63533500	5.28740100	0.82959100
C	-0.67382900	4.27020200	0.75913700
C	2.88464000	4.90658400	0.46530500
C	3.87742800	2.96376500	-0.78901400
H	2.48816400	0.79313000	-0.17452700
H	-0.05420800	-0.20449700	-1.57450500
H	1.29072700	6.18170300	1.32262000
H	-0.96762300	3.30925800	1.18650900
H	-1.24873000	4.42126200	-0.15355000
H	-0.86569300	5.07324200	1.47238600

H	3.83368100	5.40636000	0.56963100
H	3.48528000	2.39221100	-1.63163500
H	4.37847900	2.27906500	-0.09881900
H	4.59702800	3.70278700	-1.14612900
H	-0.03014500	0.16786200	1.19194100
H	-1.95038400	-2.02293800	0.26755900
O	-2.04099800	1.29925500	0.32540500
H	-1.10124100	1.75194700	-0.56438300
C	0.57449900	-1.88119300	1.44073600
C	0.39535600	-3.24874600	1.16817300
C	1.53793300	-1.52498600	2.40036700
C	1.14056000	-4.21687300	1.83714100
H	-0.32511600	-3.55601400	0.41753800
C	2.28379700	-2.49192900	3.07283200
H	1.68776200	-0.47243800	2.62916600
C	2.08691500	-3.84531800	2.79469900
H	0.98395900	-5.26718900	1.60777900
H	3.01332900	-2.18916800	3.81936500
H	2.66416000	-4.60253700	3.31748000
C	1.60148100	-1.56261300	-1.41660900
C	2.89773800	-1.86825100	-0.96113500
C	1.00168900	-2.46068600	-2.31948100
C	3.56512800	-3.00968000	-1.39882000
H	3.38697000	-1.21702300	-0.24321600
C	1.66769800	-3.60394100	-2.75694200
H	0.00061900	-2.24630800	-2.68492800
C	2.95703200	-3.88469600	-2.30171700
H	4.56499900	-3.22027000	-1.02871000
H	1.17991000	-4.27380900	-3.46004900
H	3.48024000	-4.77310300	-2.64316000
C	-3.90304300	-0.15281900	0.02957300
C	-4.55878300	-1.36144400	0.31991100
C	-4.66348200	0.90652800	-0.49162100
C	-5.92235800	-1.51120800	0.07475500
H	-4.00572000	-2.18195000	0.76543200
C	-6.02598400	0.75681600	-0.73969300
H	-4.15665400	1.84342900	-0.69375600
C	-6.66239800	-0.45448300	-0.46062900
H	-6.41121700	-2.45233900	0.31180600
H	-6.59428000	1.58680300	-1.15138600
H	-7.72569100	-0.57218500	-0.65024400