

Supplementary Data 1

Asymmetric Formation of γ -Lactams via C–H Amidation Enabled by Chiral Hydrogen-Bond-Donor Catalysts

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Cartesian Coordinates of DFT-Optimized Structures

I				C	-6.37662	2.35672	-0.87861
E(B3LYP) = -1965.65888732				C	-5.13338	2.95991	-1.56435
# of imaginary frequency = 0				C	-7.12597	1.50006	-1.89371
Ir	8.19667	18.34140	6.18075	H	-6.03278	1.70264	-0.06440
C	5.99360	18.52757	5.88774	N	-4.48723	3.88595	-0.57395
C	6.67473	19.66469	5.28586	H	-5.48177	3.59357	-2.38440
C	7.34195	20.41006	6.32839	C	-4.12935	1.95507	-2.09450
C	7.13853	19.71194	7.56547	S	-8.32222	3.01740	0.79011
C	6.29311	18.55190	7.29227	C	-7.84974	2.08746	-2.93913
C	5.01112	17.63469	5.19544	C	-8.46215	1.29488	-3.90895
H	4.03412	18.13310	5.16499	C	-8.35473	-0.09682	-3.84791
H	4.90044	16.68415	5.71636	C	-7.63635	-0.68992	-2.80925
H	5.31725	17.41228	4.17235	C	-7.02641	0.10568	-1.83800
C	6.59416	20.03758	3.84004	C	-3.47906	1.05603	-1.23450
H	5.68046	20.61885	3.66121	C	-2.53716	0.15592	-1.73131
H	6.55141	19.14933	3.20608	C	-2.23540	0.13983	-3.09519
H	7.44254	20.64945	3.52682	C	-2.87815	1.02787	-3.95821
C	8.08364	21.70054	6.14237	C	-3.81707	1.93195	-3.45889
H	7.39068	22.54636	6.22266	H	-7.95259	3.16814	-2.97475
H	8.55698	21.75864	5.15920	H	-9.02568	1.76162	-4.71166
H	8.85579	21.84209	6.90244	H	-8.83076	-0.71380	-4.60413
C	7.60380	20.14050	8.92426	H	-7.55046	-1.77096	-2.75274
H	6.80369	20.68197	9.44349	H	-6.46611	-0.36162	-1.03270
H	8.46538	20.80957	8.86593	H	-3.70990	1.04212	-0.17128
H	7.88147	19.28353	9.54214	H	-2.04260	-0.53461	-1.05514
C	5.78171	17.58472	8.31056	H	-1.50381	-0.56283	-3.48188
H	4.76900	17.87823	8.61492	H	-2.65069	1.01794	-5.01972
H	6.40792	17.57549	9.20485	H	-4.32108	2.61551	-4.13740
H	5.74359	16.57407	7.90132	Ir	-5.93489	5.13893	0.38468
C	10.36778	16.36095	5.58671	H	-3.77287	4.43652	-1.04887
H	10.59863	15.35036	5.93900	H	-3.98865	3.33441	0.12478
C	11.03158	17.35476	6.56677	O	-8.85982	4.26454	1.38092
H	12.07381	17.48512	6.25999	O	-7.76644	2.00034	1.71552
C	10.95330	16.52285	4.17859	H	-2.89173	7.11623	0.21950
C	10.28083	17.18925	3.14787	H	-3.72413	7.38162	2.30153
H	9.26705	17.54035	3.30545	C	-3.59984	7.33804	-0.58197
C	10.88938	17.35341	1.89859	H	-3.46804	8.39095	-0.85910
H	10.35218	17.86256	1.10387	H	-3.32327	6.74648	-1.45941
C	12.17026	16.85456	1.66709	H	-4.86974	8.70581	2.54147
H	12.63873	16.98019	0.69584	C	-4.78573	7.62385	2.38300
C	12.84361	16.17831	2.68884	H	-5.17957	7.13350	3.27603
H	13.83659	15.77524	2.51390	C	-5.01906	7.09761	-0.16290
C	12.23754	16.01141	3.93215	C	-5.54766	7.22878	1.15487
H	12.76411	15.47250	4.71710	H	-5.08281	6.31909	-2.90437
C	11.02686	17.00805	8.04562	C	-6.12473	6.74823	-1.05908
C	12.10276	17.47080	8.81962	C	-6.05584	6.67487	-2.55622
H	12.91149	18.02187	8.34366	C	-6.99406	7.01474	1.09436
C	12.16264	17.21683	10.19022	H	-6.21345	7.66848	-2.99297
H	13.00590	17.57857	10.77040	H	-7.49783	7.17219	3.18638
C	11.14752	16.48331	10.80575	C	-7.34161	6.77182	-0.27357
H	11.19394	16.27503	11.87024	C	-7.96842	7.26236	2.20564
C	10.07840	16.00802	10.04365	H	-6.82289	6.00949	-2.95804
H	9.29198	15.42639	10.51560	H	-8.80457	6.56417	2.15796
C	10.01182	16.26983	8.67371	H	-8.36327	8.28282	2.12738
H	9.16913	15.90264	8.10004	C	-8.72018	6.59242	-0.81838
C	8.76197	13.83576	5.03735	H	-8.72559	5.87259	-1.63921
C	9.30757	13.47567	3.80192	H	-9.08338	7.55267	-1.20564
H	9.17979	14.12093	2.94038	H	-9.40436	6.23788	-0.04864
C	9.99783	12.27025	3.69864	H	-12.08788	0.06589	5.90238
H	10.42098	11.98213	2.74059	C	-11.41933	0.76529	6.39619
C	10.14718	11.41844	4.80372	C	-10.77380	1.75221	5.65059
C	9.58162	11.80565	6.02934	H	-10.94280	1.81604	4.57795
H	9.67795	11.15311	6.89252	C	-11.21291	0.68092	7.77464
C	8.88409	13.00380	6.15529	H	-9.82568	4.05917	4.62856
H	8.42114	13.28185	7.09553	H	-11.71808	-0.08409	8.35667
C	10.86505	10.09896	4.66992	C	-9.91318	2.66950	6.26876
H	11.34847	9.80819	5.60658	C	-10.35888	1.58969	8.40166
H	11.62535	10.13332	3.88511	C	-9.18638	3.71646	5.45138
H	10.15913	9.30200	4.40631	H	-8.97579	4.59292	6.07803
N	8.90692	16.59210	5.67917	C	-9.71487	2.57544	7.65244
N	10.31988	18.66853	6.33479	H	-10.19785	1.53519	9.47444
H	10.64183	19.06956	5.45105	H	-9.05652	3.28464	8.14939
H	10.56050	19.32527	7.07505	H	-7.79374	4.66901	3.27092
O	6.86478	15.18960	6.28372	C	-7.86754	3.18044	4.86151
O	7.31980	15.71207	3.84001	C	-6.86358	5.10621	4.72677
S	7.81685	15.34480	5.17229	C	-7.14224	4.28137	4.05487
				H	-8.07519	2.33724	4.19740
				H	-7.22115	2.81726	5.66693
				C	-5.89754	3.80111	3.41045
				N	-5.44947	4.01958	2.21105
				O	-5.05350	3.03518	4.14131
				O	-4.19685	3.32741	2.14568
				C	-3.97736	2.70498	3.34674
II-1							
E(B3LYP) = -2671.85796752							
# of imaginary frequency = 0							
N	-7.16633	3.49755	-0.33002				

O	-3.04518	2.03169	3.63417
C	-9.69955	2.25103	-0.06487
C	-9.91689	0.88146	0.08176
C	-10.59393	3.04630	-0.78566
C	-11.03721	0.30525	-0.51511
H	-9.22294	0.28446	0.66155
C	-11.70538	2.45364	-1.37586
H	-10.43078	4.11403	-0.87279
C	-11.94741	1.07605	-1.25043
H	-11.20794	-0.76180	-0.40292
H	-12.40337	3.06958	-1.93656
C	-13.17572	0.45054	-1.86381
H	-14.03167	0.52491	-1.18185
H	-13.45843	0.95112	-2.79428
H	-13.02077	-0.61024	-2.07818

II-2

E(B3LYP) = -2671.84151151
of imaginary frequency = 0

N	-6.79803	4.04124	-0.17669
C	-5.85403	3.14130	-0.89347
C	-4.77544	4.02390	-1.55594
C	-6.51899	2.29759	-1.98043
H	-5.34352	2.46826	-0.18814
N	-4.31064	5.00331	-0.50959
H	-5.26440	4.62870	-2.32264
C	-3.60934	3.28264	-2.17978
S	-7.52352	3.31882	1.16018
C	-7.43001	2.87488	-2.87385
C	-7.97572	2.12760	-3.91680
C	-7.61807	0.78704	-4.07890
C	-6.71703	0.20130	-3.18920
C	-6.17063	0.95354	-2.14779
C	-2.83608	2.37178	-1.44322
C	-1.75466	1.71826	-2.03341
C	-1.42952	1.96698	-3.36915
C	-2.19020	2.87155	-4.11049
C	-3.27156	3.52503	-3.51736
H	-7.73071	3.90759	-2.72727
H	-8.68385	2.58782	-4.60007
H	-8.04336	0.20276	-4.88933
H	-6.43937	-0.84239	-3.30260
H	-5.46926	0.48902	-1.46027
H	-3.08299	2.14613	-0.40846
H	-1.17460	1.01066	-1.44951
H	-0.59135	1.45357	-3.83013
H	-1.94762	3.06483	-5.15086
H	-3.86966	4.21674	-4.10545
Ir	-6.03017	6.02902	0.29658
H	-3.62911	5.63853	-0.92429
H	-3.80638	4.47681	0.20299
O	-8.54910	4.27180	1.62121
O	-6.49086	2.85960	2.12379
H	-3.77585	8.87885	-0.25580
H	-4.63367	9.11119	1.80503
C	-4.49627	8.69916	-1.05671
H	-4.71407	9.66548	-1.52765
H	-4.01750	8.07666	-1.81819
H	-6.15783	9.99394	1.94293
C	-5.71445	8.99157	1.90665
H	-5.92165	8.51084	2.86508
C	-5.76343	8.08358	-0.54412
C	-6.30624	8.21999	0.76741
H	-5.58688	6.99019	-3.16804
C	-6.70772	7.30021	-1.34693
C	-6.62143	7.09608	-2.83053
C	-7.60144	7.53776	0.80150
H	-7.04764	7.95921	-3.35621
H	-8.10347	7.78798	2.88299
C	-7.86544	7.03746	-0.51652
C	-8.58167	7.53544	1.93582
H	-7.17346	6.20988	-3.14889
H	-9.04153	6.55207	2.04527
H	-9.36650	8.27822	1.74778
C	-9.12597	6.35252	-0.92974
H	-9.00584	5.80962	-1.86769
H	-9.91157	7.10534	-1.07102
H	-9.44797	5.65215	-0.15699
H	0.15504	-0.56947	4.39639
C	0.17265	0.05692	3.50953
C	-0.33617	1.35423	3.56783
H	-0.74040	1.72807	4.50584
C	0.71296	-0.43192	2.31783
H	-0.43382	4.13598	3.33705
H	1.11554	-1.43930	2.27435

C	-0.31867	2.18285	2.43669
C	0.74373	0.38607	1.18787
C	-0.88323	3.58738	2.49853
H	-0.60435	4.13207	1.58771
C	0.22911	1.68323	1.24846
H	1.17880	0.01935	0.26237
H	0.26598	2.31883	0.36688
H	-2.41190	5.64961	3.40337
C	-2.41476	3.61257	2.66403
H	-2.80097	5.55286	1.69542
C	-2.96034	5.05949	2.65806
H	-2.69704	3.12917	3.60437
H	-2.89125	3.02765	1.86832
C	-4.39555	5.15759	3.03239
N	-5.42284	5.50898	2.32545
O	-4.71352	4.89343	4.31299
O	-6.51372	5.53982	3.22875
C	-6.08406	5.10973	4.45003
O	-6.72121	4.98622	5.43936
C	-8.37980	1.84677	0.60424
C	-7.93451	0.59866	1.03828
C	-9.53985	1.96778	-0.16608
C	-8.65338	-0.54110	0.67833
H	-7.05116	0.53065	1.66273
C	-10.24083	0.82043	-0.51880
H	-9.88982	2.94462	-0.47991
C	-9.81224	-0.45148	-0.10280
H	-8.31216	-1.51476	1.01896
H	-11.14139	0.91002	-1.12027
C	-10.60446	-1.68288	-0.46650
H	-11.51456	-1.75377	0.14113
H	-10.91813	-1.66020	-1.51488
H	-10.02652	-2.59584	-0.30223

II-3

E(B3LYP) = -2671.84977243
of imaginary frequency = 0

N	1.23861	0.21990	-1.01155
C	2.61279	0.25375	-0.41386
C	2.52994	-0.16667	1.06811
C	3.46285	1.49862	-0.62945
H	3.13199	-0.55766	-0.94227
N	1.77799	-1.47659	1.06826
H	1.88733	0.54368	1.59245
C	3.83764	-0.32930	1.81548
S	0.32061	1.59881	-1.10310
C	3.43639	2.59436	0.24504
C	4.28760	3.68079	0.04401
C	5.17528	3.69167	-1.03317
C	5.20886	2.60733	-1.91098
C	4.36248	1.51896	-1.70341
C	4.90533	-1.06121	1.27194
C	6.08129	-1.24539	1.99838
C	6.20664	-0.70132	3.27867
C	5.15156	0.02801	3.82824
C	3.97470	0.21049	3.10085
H	2.73800	2.61523	1.07381
H	4.25810	4.51946	0.73325
H	5.83964	4.53714	-1.18438
H	5.89917	2.60349	-2.74916
H	4.40263	0.67134	-2.38352
H	4.83574	-1.47520	0.26858
H	6.90241	-1.80648	1.56267
H	7.12341	-0.84295	3.84253
H	5.24310	0.45599	4.82173
H	3.15759	0.78231	3.53380
Ir	0.13448	-1.50433	-0.32215
H	1.45503	-1.67233	2.01496
H	2.43599	-2.21931	0.83303
O	0.23551	2.32766	0.18744
O	-0.96295	1.15745	-1.70543
H	1.71196	-4.64477	0.32592
H	2.69892	-3.73365	-1.55011
C	0.63393	-4.78422	0.20962
H	0.48897	-5.76107	-0.26756
H	0.18509	-4.83273	1.20388
H	1.94181	-4.12024	-3.09420
C	2.02123	-3.35035	-2.31735
H	2.48373	-2.46844	-2.76608
C	0.01364	-3.71453	-0.63710
C	0.66705	-3.02933	-1.75601
H	-1.93070	-4.06522	1.35741
C	-1.32039	-3.22248	-0.53497
C	-2.36784	-3.68187	0.43322
C	-0.33678	-2.19579	-2.39592

H	-2.96131	-4.48844	-0.01425	H	2.00049	-0.01941	-0.94472
H	0.89814	-1.21696	-3.85310	H	1.10383	0.16809	-2.27526
C	-1.53628	-2.26119	-1.61991	O	-1.22405	0.35256	2.10769
C	-0.15638	-1.41393	-3.65546	O	-2.40531	-1.77083	1.35795
H	-3.05933	-2.87688	0.69205	H	-2.18355	-0.99946	-3.71072
H	-0.68354	-0.46024	-3.60290	H	-3.54386	-2.00879	-2.18785
H	-0.55593	-1.99232	-4.49792	C	-1.35907	-1.65690	-3.99441
C	-2.84156	-1.62651	-1.99091	H	-1.71889	-2.32037	-4.79014
H	-3.50614	-1.53174	-1.13000	H	-0.56535	-1.03829	-4.42208
H	-3.35695	-2.24662	-2.73469	H	-3.69690	-3.76521	-2.02887
H	-2.68629	-0.63478	-2.41803	C	-3.18362	-2.87824	-1.63696
H	-2.81305	7.54434	-0.84099	H	-3.44168	-2.75861	-0.58342
C	-3.49824	6.85273	-0.35895	C	-0.87233	-2.45825	-2.82273
H	-2.57287	5.10930	-1.22046	C	-1.71077	-3.05852	-1.79797
C	-3.36406	5.48047	-0.57281	H	1.61346	-1.79787	-4.03459
H	-4.62340	8.40550	0.62958	C	0.46833	-3.02970	-2.67553
C	-4.51524	7.33744	0.46587	C	1.60698	-2.81175	-3.62542
C	-4.24241	4.57120	0.03232	C	-0.88097	-3.86109	-0.95229
C	-5.39693	6.44167	1.07323	H	1.51218	-3.49725	-4.47635
H	-3.68083	2.88536	-1.17878	H	-2.06882	-4.10536	0.81264
C	-5.25970	5.06979	0.85673	C	0.47020	-3.86986	-1.52434
H	-5.04494	2.58136	-0.10309	C	-1.36028	-4.67634	0.21051
C	-4.06991	3.08083	-0.17241	H	2.57557	-3.00150	-3.15825
H	-6.19500	6.81063	1.71096	H	-0.53555	-4.97773	0.85935
H	-5.95546	4.37872	1.32753	H	-1.85074	-5.58915	-0.14868
C	-3.10354	2.46479	0.85754	C	1.60754	-4.70785	-1.02494
H	-2.59063	0.76585	-0.40221	H	2.57470	-4.33240	-1.36654
C	-2.93555	0.94503	0.61521	H	1.50363	-5.73585	-1.39239
H	-3.89642	0.43537	0.77376	H	1.62260	-4.75758	0.06659
H	-2.12364	2.94295	0.77401	H	8.12990	2.54051	3.21387
H	-3.47567	2.64437	1.87148	C	7.50006	2.52607	2.32944
C	-1.95763	0.33244	1.54229	H	7.06734	0.42557	2.50013
N	-0.92205	-0.41363	1.29657	C	6.89812	1.33387	1.92612
O	-2.13402	0.54466	2.86931	H	7.77455	4.62173	1.90090
C	-1.12295	-0.10224	3.54487	C	7.30091	3.69486	1.59200
O	-0.36683	-0.71698	2.58324	C	6.08798	1.29107	0.78327
O	-0.94030	-0.13344	4.71606	C	6.49811	3.66337	0.45048
C	1.06265	2.69931	-2.30988	H	6.05840	-0.85215	0.60391
C	1.21094	4.04671	-1.98429	C	5.89530	2.46950	0.05057
C	1.34616	2.23929	-3.59839	H	5.25284	-0.00872	-0.71385
C	1.65849	4.93614	-2.96119	C	5.40852	0.00109	0.37288
H	0.98290	4.38565	-0.98056	H	6.34917	4.56608	-0.13509
C	1.79554	3.13968	-4.55844	H	5.27503	2.45436	-0.84267
H	1.22722	1.19037	-3.84262	C	4.05629	-0.19612	1.08586
C	1.95520	4.50275	-4.25951	H	4.07338	-2.35568	0.90375
H	1.77923	5.98552	-2.70690	C	3.38259	-1.53108	0.68753
H	2.02455	2.78202	-5.55884	H	3.16379	-1.57835	-0.38304
C	2.41091	5.47451	-5.32001	H	4.20755	-0.18211	2.16997
H	3.15633	5.02409	-5.98216	H	3.39287	0.64678	0.85528
H	1.56841	5.78940	-5.94785	C	2.13762	-1.81737	1.44975
H	2.84510	6.37561	-4.87918	N	0.90644	-1.87650	1.04227

II-4

E(B3LYP) = -2671.83102688

of imaginary frequency = 0

N	-1.56115	-0.23190	-0.41972
C	-1.11256	1.08936	-0.95641
C	0.39395	1.26303	-0.67218
C	-1.93247	2.32559	-0.61238
H	-1.21126	0.96161	-2.04387
N	1.03619	0.02891	-1.26679
H	0.54283	1.19108	0.40790
C	1.07292	2.50355	-1.21351
S	-2.12706	-0.33516	1.15393
C	-1.68683	3.10488	0.52701
C	-2.41969	4.26832	0.75975
C	-3.41078	4.66953	-0.13736
C	-3.66628	3.89968	-1.27290
C	-2.92649	2.74128	-1.50798
C	0.93350	2.88746	-2.55688
C	1.60266	4.00790	-3.04806
C	2.42225	4.76130	-2.20390
C	2.56664	4.39041	-0.86649
C	1.89637	3.26787	-0.37661
H	-0.94270	2.79233	1.25052
H	-2.21593	4.86177	1.64609
H	-3.97831	5.57694	0.04592
H	-4.43304	4.20431	-1.97890
H	-3.12223	2.15208	-2.40098
H	0.28169	2.32817	-3.22460
H	1.47772	4.29887	-4.08661
H	2.93883	5.63612	-2.58652
H	3.19695	4.97259	-0.20150
H	2.00231	2.99395	0.67026
Ir	-0.11439	-1.77218	-0.90453

TS-1

E(B3LYP) = -2671.82769055

of imaginary frequency = 1(-128.60)

N	-0.66896	0.93091	-0.31440
C	-0.30342	1.26226	1.09991
C	-1.43068	0.73137	2.00513
C	-0.12121	2.75336	1.35193
H	0.62597	0.74622	1.37315
N	-1.69499	-0.68392	1.59739
H	-2.34249	1.28476	1.76394
C	-1.16493	0.81617	3.49447
S	0.67854	1.01336	-1.36846
C	-1.05828	3.68546	0.88788
C	-0.92073	5.03867	1.19376
C	0.15356	5.47520	1.97328

C	1.09065	4.55266	2.44014
C	0.95445	3.19900	2.12839
C	-0.08563	0.13154	4.07541
C	0.13175	0.19362	5.45097
C	-0.72385	0.94354	6.26167
C	-1.79694	1.62994	5.69203
C	-2.01788	1.56287	4.31571
H	-1.88287	3.35026	0.26539
H	-1.64966	5.75365	0.82371
H	0.25930	6.52881	2.21352
H	1.92857	4.88484	3.04562
H	1.68613	2.48407	2.49473
H	0.59858	-0.44866	3.45957
H	0.96863	-0.34123	5.88902
H	-0.55332	0.99193	7.33261
H	-2.46286	2.21668	6.31707
H	-2.85122	2.10488	3.87605
Ir	-1.68473	-0.93344	-0.49804
H	-2.57288	-1.00985	2.00161
H	-0.99211	-1.33919	1.95399
O	0.23816	0.37014	-2.62118
O	1.87923	0.48854	-0.68690
H	-3.90523	-3.15312	0.96085
H	-1.86508	-4.16088	-2.21810
C	-4.51883	-2.39000	0.47526
H	-5.42469	-2.87619	0.09450
H	-4.83986	-1.66495	1.22726
H	-2.78115	-4.34854	-0.71581
C	-2.79763	-3.90455	-1.71200
H	-3.61622	-4.36621	-2.27753
C	-3.78191	-1.73428	-0.65426
C	-3.00905	-2.42420	-1.64921
H	-4.78294	0.55193	0.72277
C	-3.79173	-0.31290	-0.99403
C	-4.62560	0.74995	-0.34032
C	-2.52784	-1.44760	-2.60730
H	-5.61495	0.79739	-0.81074
H	-1.29270	-2.72074	-3.82436
C	-3.04707	-0.16143	-2.21749
C	-1.77023	-1.74028	-3.86431
H	-4.16479	1.73515	-0.43802
H	-0.99830	-0.98990	-4.03680
H	-2.45837	-1.74214	-4.71844
C	-2.88854	1.10950	-2.98238
H	-2.78443	1.96428	-2.31121
H	-3.78074	1.27148	-3.60030
H	-2.01554	1.06869	-3.63257
H	7.38014	0.30748	1.15968
C	7.13245	-0.66830	0.75123
H	8.89128	-1.62722	1.55277
C	7.98289	-1.75420	0.97141
C	5.96865	-0.83203	-0.00023
H	5.31020	0.01622	-0.17441
C	7.66239	-3.00238	0.43452
C	5.63730	-2.08018	-0.54611
H	8.32140	-3.85048	0.59601
C	6.49755	-3.16233	-0.31724
H	4.13975	-1.34383	-1.90106
C	4.35783	-2.25631	-1.33431
H	4.47593	-3.06819	-2.06229
H	6.25763	-4.13607	-0.73814
C	3.15543	-2.56462	-0.41586
H	1.66145	-1.76850	-1.78281
H	3.04332	-1.74990	0.30627
C	1.85944	-2.68872	-1.23393
H	1.92509	-3.52034	-1.94725
H	3.33460	-3.48787	0.14361
C	0.66957	-3.02480	-0.34401
N	-0.25715	-2.14095	-0.22053
O	0.70401	-4.18377	0.24460
C	-0.45894	-4.47058	1.24964
O	-1.16955	-3.43753	1.35198
O	-0.43393	-5.58007	1.69067
C	0.99431	2.73671	-1.74281
C	2.11369	3.35541	-1.18348
C	0.18257	3.41193	-2.65703
C	2.40615	4.67059	-1.53535
H	2.74480	2.80867	-0.49369
C	0.48989	4.72663	-2.99449
H	-0.66493	2.91545	-3.11253
C	1.60368	5.37792	-2.44213
H	3.27717	5.15393	-1.10194
H	-0.13799	5.25390	-3.70736
C	1.95132	6.79029	-2.84107
H	2.69089	6.79260	-3.65102
H	1.07355	7.33519	-3.19836

H	2.38509	7.34671	-2.00536
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TS-2

E(B3LYP) = -2671.80435087			
# of imaginary frequency = 1(-364.63)			
N	1.53560	-0.01946	-0.03800
C	1.06565	1.39777	-0.04136
C	-0.07048	1.52000	-1.07221
C	2.15169	2.41326	-0.38649
H	0.65408	1.64937	0.94530
N	-0.98888	0.35463	-0.83001
H	0.35029	1.36719	-2.06930
C	-0.85100	2.81867	-1.04778
S	2.29662	-0.44582	1.44770
C	3.06530	2.17862	-1.42076
C	3.99950	3.15063	-1.77723
C	4.02733	4.37494	-1.10550
C	3.11992	4.61767	-0.07358
C	2.18953	3.64106	0.28465
C	-1.52570	3.23840	0.11047
C	-2.27531	4.41412	0.10475
C	-2.35457	5.18806	-1.05581
C	-1.68318	4.78167	-2.20951
C	-0.93960	3.60048	-2.20576
H	3.05892	1.21930	-1.92880
H	4.70785	2.95261	-2.57641
H	4.75436	5.13234	-1.38238
H	3.13771	5.56494	0.45694
H	1.48700	3.83649	1.09020
H	-1.45795	2.66287	1.03158
H	-2.79114	4.72848	1.00662
H	-2.93422	6.10590	-1.05788
H	-1.73628	5.38273	-3.11194
H	-0.41223	3.29244	-3.10504
Ir	0.09306	-1.45477	-0.65608
H	-1.69833	0.32187	-1.56204
H	-1.49456	0.50816	0.04543
O	2.51970	-1.89526	1.34635
O	1.53033	0.14105	2.55787
H	-2.60429	-2.42629	-2.96738
H	-2.46723	-4.08994	-1.46361
C	-1.65952	-2.18616	-3.45941
H	-1.60776	-2.78348	-4.37791
H	-1.68339	-1.13711	-3.76621
H	-1.31988	-5.42296	-1.62282
C	-1.48002	-4.44209	-1.15985
H	-1.48024	-4.58685	-0.07730
C	-0.47383	-2.49219	-2.59478
C	-0.39190	-3.50732	-1.58744
H	0.44805	-0.27340	-4.11587
C	0.84710	-1.88588	-2.73324
C	1.26727	-0.92832	-3.80895
C	0.97401	-3.54719	-1.08941
H	1.59429	-1.47825	-4.69998
H	0.71880	-4.86902	0.58430
C	1.73756	-2.59409	-1.84479
C	1.50756	-4.51728	-0.08259
H	2.09982	-0.30135	-3.48376
H	2.27601	-4.05189	0.53388
H	1.93307	-5.38919	-0.59472
C	3.21007	-2.37878	-1.76335
H	3.44628	-1.31461	-1.69739
H	3.68041	-2.77736	-2.67083
H	3.63686	-2.88206	-0.89731
H	-5.36714	-0.41480	-1.06310
H	-5.80579	1.98493	-1.16064
H	-6.16047	-1.43693	0.13033
C	-5.62475	-0.48815	0.00183
C	-6.47031	1.88323	-0.30494
H	-3.08981	-1.62274	-0.58923
C	-6.52204	0.66840	0.39048
C	-7.27141	2.96050	0.07744
H	-7.22575	3.89239	-0.47878
H	-3.96749	-2.64585	0.55307
C	-3.41852	-1.70218	0.45049
C	-7.39663	0.55531	1.48010
C	-8.13654	2.83666	1.16567
C	-4.33414	-0.52930	0.84524
C	-8.19779	1.63001	1.86604
H	-7.45643	-0.38320	2.02651
H	-8.76407	3.67167	1.46219
H	-3.80224	0.42565	0.73377
N	-1.00526	-1.83376	0.88230
C	-2.21691	-1.81906	1.39050
H	-8.87370	1.52335	2.70926

H	-4.58491	-0.62016	1.90547
O	-2.48535	-1.94178	2.62606
O	-0.13445	-2.27826	2.67577
C	-0.99109	-2.20048	3.55630
O	-1.23701	-2.24183	4.70907
C	3.91648	0.32818	1.47826
C	4.10825	1.46587	2.26364
C	4.98965	-0.26853	0.81227
C	5.38219	2.02259	2.35368
H	3.27474	1.89342	2.80781
C	6.25472	0.30245	0.91143
H	4.84452	-1.18119	0.24832
C	6.47325	1.45644	1.68018
H	5.53217	2.90749	2.96577
H	7.09094	-0.16273	0.39638
C	7.85601	2.04479	1.81162
H	8.40465	1.56550	2.63161
H	8.44248	1.89866	0.90005
H	7.81750	3.11579	2.02779

TS-3

E(B3LYP) = -2671.82407750
of imaginary frequency = 1(-118.81)

N	0.49838	1.18467	-0.35752
C	0.44911	1.71779	1.04860
C	0.54774	0.52860	2.02670
C	-0.65333	2.71359	1.37205
H	1.39207	2.27483	1.12925
N	1.79300	-0.20059	1.59918
H	-0.28206	-0.15217	1.82421
C	0.62470	0.83685	3.50754
S	-0.94273	0.76540	-1.13487
C	-1.87429	2.33266	1.94611
C	-2.82442	3.29509	2.28760
C	-2.57270	4.64833	2.05640
C	-1.36096	5.03839	1.48319
C	-0.40888	4.07615	1.15129
C	1.43534	1.86899	4.00512
C	1.53061	2.09368	5.37814
C	0.82065	1.28831	6.27149
C	0.01341	0.25828	5.78662
C	-0.08185	0.03388	4.41297
H	-2.09568	1.28595	2.11939
H	-3.76200	2.98556	2.73949
H	-3.31301	5.39487	2.32759
H	-1.15271	6.08925	1.30659
H	0.53981	4.38716	0.71989
H	1.98105	2.51941	3.32585
H	2.15338	2.90130	5.75042
H	0.89471	1.46531	7.33992
H	-0.54261	-0.37009	6.47538
H	-0.71403	-0.76869	4.04086
Ir	1.96646	-0.33877	-0.51834
H	1.80588	-1.17351	1.93024
H	2.60523	0.26137	2.00905
O	-1.83769	-0.00133	-0.24039
O	-0.51087	0.11918	-2.39311
H	5.17022	0.07164	1.19500
H	4.42744	2.13864	0.60267
C	5.16666	-0.70804	0.42991
H	6.18990	-0.78443	0.04298
H	4.91458	-1.65915	0.90412
H	5.05992	2.62305	-0.96928
C	4.17002	2.24243	-0.45415
H	3.38816	3.00000	-0.53993
C	4.22569	-0.38583	-0.69120
C	3.73650	0.93789	-1.05688
C	4.21954	-3.19300	-0.68412
C	3.71190	-1.33227	-1.64300
C	4.02608	-2.79484	-1.68045
C	2.95129	0.78450	-2.26107
H	4.92118	-2.95633	-2.29376
H	2.14376	2.76319	-2.43727
C	2.89206	-0.61146	-2.60082
C	2.34097	1.88781	-3.05713
H	3.21507	-3.37197	-2.12847
H	1.40753	1.56572	-3.52029
H	3.03830	2.18407	-3.35809
C	2.21298	-1.18513	-3.80614
H	2.06867	-2.26255	-3.70831
H	2.82462	-1.01234	-4.69979
H	1.23554	-0.72327	-3.95592
H	-6.91063	-1.72450	1.30661
C	-6.46275	-2.58005	0.80874
H	-4.83280	-1.43650	-0.01703

C	-5.29575	-2.41787	0.06267
H	-7.97134	-3.96577	1.48720
C	-7.06029	-3.83877	0.91002
C	-4.70767	-3.50765	-0.59558
C	-6.48300	-4.93115	0.26098
H	-3.46268	-2.37786	-1.93420
C	-5.31470	-4.76501	-0.48490
H	-3.32480	-4.12511	-2.12240
C	-3.42686	-3.32383	-1.38068
H	-6.94381	-5.91218	0.33076
H	-4.87371	-5.61947	-0.99293
C	-2.18538	-3.31167	-0.46368
H	-0.97015	-2.09563	-1.81058
C	-0.90669	-3.04499	-1.27863
H	-0.74009	-3.84700	-2.00984
H	-2.30239	-2.51913	0.28118
H	-2.10063	-4.26469	0.06752
C	0.32837	-3.04564	-0.39768
N	1.01002	-1.96439	-0.26079
O	0.60952	-4.18238	0.19046
C	1.77627	-4.13573	1.14539
O	2.23179	-2.94886	1.19075
O	2.05931	-5.17767	1.65959
C	-1.79078	2.27717	-1.59550
C	-3.14464	2.39509	-1.28212
C	-1.15072	3.24188	-2.37828
C	-3.85671	3.49706	-1.75453
H	-3.62786	1.63513	-0.68032
C	-1.87588	4.33683	-2.83493
H	-0.10098	3.14393	-2.62282
C	-3.24101	4.48185	-2.53705
H	-4.91123	3.58925	-1.51069
H	-1.37751	5.09112	-3.43791
C	-4.02390	5.65540	-3.07102
H	-3.43513	6.57713	-3.04008
H	-4.30822	5.48821	-4.11698
H	-4.94346	5.81696	-2.50298

TS-4

E(B3LYP) = -2671.79740569
of imaginary frequency = 1(-359.73)

N	-1.64375	-0.12302	-0.32663
C	-1.25452	1.23398	-0.83029
C	0.17087	1.54546	-0.34178
C	-2.25289	2.36297	-0.62477
H	-1.19362	1.08428	-1.91723
N	0.98369	0.36273	-0.82183
H	0.17874	1.48835	0.74906
C	0.83156	2.82378	-0.81156
S	-2.35193	-0.25762	1.22295
C	-2.16364	3.27045	0.43923
C	-3.06244	4.33263	0.53865
C	-4.06664	4.49854	-0.41602
C	-4.16825	3.59647	-1.47671
C	-3.26200	2.54276	-1.58061
C	0.73856	3.25795	-2.14338
C	1.40653	4.40914	-2.55984
C	2.17812	5.13949	-1.65283
C	2.27772	4.71585	-0.32683
C	1.60922	3.56404	0.08984
H	-1.40377	3.14797	1.20225
H	-2.97589	5.03172	1.36495
H	-4.76282	5.32800	-0.33692
H	-4.94328	3.71982	-2.22708
H	-3.33619	1.85210	-2.41761
H	0.12416	2.71638	-2.85858
H	1.31737	4.74170	-3.58953
H	2.69400	6.03763	-1.97790
H	2.87145	5.28155	0.38441
H	1.68219	3.24368	1.12651
Ir	-0.05245	-1.49965	-0.58959
H	1.87122	0.35009	-0.32020
H	1.22074	0.51609	-1.80297
O	-1.61404	0.57848	2.18667
O	-2.47419	-1.71064	1.42356
H	-1.93742	-0.74556	-3.59938
H	-3.35634	-1.74698	-2.09227
C	-1.06077	-1.35589	-3.82590
H	-1.31698	-2.00342	-4.67318
H	-0.25936	-0.69065	-4.15717
H	-3.45648	-3.49871	-2.34579
C	-3.03400	-2.71395	-1.70514
H	-3.42612	-2.83998	-0.69588
C	-0.65119	-2.18197	-2.64194
C	-1.54979	-2.83434	-1.71607

H	1.89880	-1.40904	-3.61610	H	-2.92673	-1.79316	-0.71396
C	0.68636	-2.70331	-2.38181	H	-3.38899	-0.62333	-2.85823
C	1.89671	-2.42841	-3.22154	H	-4.61838	1.52396	-2.85830
C	-0.77983	-3.66013	-0.82886	Ir	-6.11835	5.60775	0.43700
H	1.90401	-3.10489	-4.08506	H	-4.02605	4.18447	-0.32029
H	-2.08930	-3.98841	0.83208	H	-4.66061	3.56926	1.06250
C	0.60189	-3.61267	-1.27677	O	-9.19057	5.88540	0.86403
C	-1.32589	-4.52343	0.26518	O	-8.90051	3.59476	1.94050
H	2.82683	-2.58833	-2.67277	H	-2.72669	6.72448	0.51215
H	-0.54276	-4.82215	0.96355	H	-3.72314	8.13009	2.00011
H	-1.76731	-5.43297	-0.16023	C	-3.17085	6.88903	-0.47168
C	1.70236	-4.45795	-0.71665	H	-2.69929	7.77908	-0.90569
H	2.68829	-4.11941	-1.03802	H	-2.90282	6.04831	-1.11726
H	1.57589	-5.49019	-1.06420	H	-4.87655	9.46727	1.89903
H	1.67725	-4.47695	0.37509	C	-4.78078	8.37620	1.89344
H	8.84901	1.77255	2.65307	H	-5.31078	7.98226	2.76587
C	8.22671	1.76612	1.76314	C	-4.65502	7.09515	-0.39758
H	7.36720	-0.15453	2.20888	C	-5.35656	7.81822	0.63016
C	7.38872	0.67997	1.51160	H	-4.41731	5.55219	-2.78977
H	8.92888	3.68101	1.06099	C	-5.61059	6.77740	-1.46130
C	8.27211	2.83799	0.86888	C	-5.28190	6.22043	-2.81521
C	6.58234	0.64721	0.36526	C	-6.73880	7.92363	0.23729
C	7.47593	2.81560	-0.27703	H	-5.04014	7.03243	-3.51208
H	6.14860	-1.46015	0.38279	H	-7.51978	8.80414	2.03145
C	6.63712	1.72745	-0.52449	C	-6.88047	7.30645	-1.06029
H	5.41614	-0.58252	-0.95521	C	-7.79896	8.65659	0.98569
C	5.64989	-0.51980	0.11570	H	-6.12627	5.66774	-3.23313
H	7.51297	3.64078	-0.98239	H	-8.74826	8.13088	0.95540
H	6.02745	1.71290	-1.42568	H	-7.93905	9.65864	0.53989
C	4.34131	-0.40854	0.92401	C	-8.12810	7.27209	-1.87943
H	3.92208	-2.53191	0.89006	H	-8.26221	6.29431	-2.34864
C	3.39910	-1.59673	0.65730	H	-8.06458	8.02265	-2.67699
H	3.09861	-1.64063	-0.39313	H	-9.00533	7.48602	-1.26993
H	4.56294	-0.36798	1.99373	H	-9.67873	-1.81756	5.52251
H	3.84668	0.54233	0.67790	C	-8.84921	-1.24184	5.92354
C	2.16968	-1.57350	1.56854	C	-8.75113	0.12201	5.64425
N	0.97151	-1.65627	1.03659	H	-9.50649	0.60285	5.02657
O	2.40986	-1.52107	2.81617	C	-7.88992	-1.86330	6.72550
O	0.90695	-1.62442	3.73912	H	-8.56611	2.79070	5.66620
O	0.05855	-1.80785	2.86620	H	-7.96799	-2.92321	6.94896
O	1.13118	-1.50815	4.89252	C	-7.69695	0.88768	6.16082
C	-4.03234	0.37813	1.14684	C	-6.83505	-1.11163	7.24689
C	-4.41380	1.32545	2.09781	C	-7.57088	2.35829	5.82458
C	-4.97544	-0.18172	0.28208	H	-7.12369	2.89582	6.67016
C	-5.74877	1.72001	2.16765	C	-6.74125	0.25181	6.96539
H	-3.67399	1.73482	2.77476	H	-6.08929	-1.58528	7.87896
C	-6.30181	0.23129	0.35934	H	-5.92128	0.83249	7.38208
H	-4.68349	-0.92986	-0.44305	H	-7.57013	4.51540	3.98581
C	-6.71342	1.18371	1.30492	C	-6.71140	2.59316	4.56541
H	-6.04452	2.45535	2.91078	H	-6.18051	4.65056	5.06278
H	-7.03374	-0.19906	-0.31890	C	-6.59157	4.08189	4.21583
C	-8.16175	1.59216	1.41114	H	-7.16438	2.06155	3.72046
H	-8.67200	1.51900	0.44659	H	-5.71209	2.17218	4.71247
H	-8.69737	0.94183	2.11353	C	-5.65195	4.32380	3.04815
H	-8.26353	2.61778	1.77634	N	-5.98499	5.42351	2.30351

III

E(B3LYP) = -2483.28021086

of imaginary frequency = 0

N	-7.56467	4.25461	-0.19600
C	-7.06986	2.84170	-0.26890
C	-5.60229	2.90249	-0.73596
C	-7.86137	1.95644	-1.22094
H	-7.09280	2.39025	0.73122
N	-4.90920	3.92069	0.11588
H	-5.59921	3.30496	-1.75291
C	-4.85599	1.58400	-0.71548
S	-9.00584	4.43149	0.73132
C	-8.20110	2.39503	-2.50688
C	-8.85210	1.54147	-3.39652
C	-9.16508	0.23500	-3.01247
C	-8.82794	-0.20993	-1.73369
C	-8.18104	0.64768	-0.84255
C	-4.59261	0.91808	0.49230
C	-3.89878	-0.29155	0.48947
C	-3.46512	-0.85043	-0.71509
C	-3.72339	-0.19371	-1.91901
C	-4.41213	1.01971	-1.91770
H	-7.97511	3.41596	-2.80127
H	-9.11681	1.89476	-4.38879
H	-9.66988	-0.43045	-3.70624
H	-9.06793	-1.22368	-1.42754
H	-7.91745	0.29475	0.15079
H	-4.91553	1.33958	1.44107
H	-3.69779	-0.79724	1.42877

TS-S₁

E(B3LYP) = -2483.27039941

of imaginary frequency = 1(-334.58)

N	0.76160	0.28663	0.24937
C	1.90311	-0.35099	-0.47837
C	2.04882	-1.77451	0.09513
C	3.22553	0.38978	-0.33455
H	1.67008	-0.43732	-1.54766
N	0.69343	-2.40246	0.04800
H	2.30918	-1.67695	1.15328
C	3.07848	-2.64999	-0.59225
S	0.19570	1.70054	-0.49784
C	3.68517	0.81791	0.91755
C	4.93457	1.42349	1.04333

C	5.74324	1.60302	-0.08196
C	5.29330	1.17820	-1.33249
C	4.04001	0.57621	-1.45689
C	2.91009	-3.06304	-1.92364
C	3.86591	-3.87589	-2.53253
C	4.99987	-4.28087	-1.82456
C	5.17446	-3.87276	-0.50161
C	4.21633	-3.06434	0.11100
H	3.04964	0.69678	1.79003
H	5.27799	1.75710	2.01824
H	6.71742	2.07253	0.01671
H	5.91576	1.31457	-2.21177
H	3.69468	0.24325	-2.43182
H	2.03068	-2.76384	-2.48836
H	3.72440	-4.19285	-3.56127
H	5.74264	-4.91245	-2.30220
H	6.05400	-4.18301	0.05416
H	4.36073	-2.74206	1.13905
Ir	-0.81665	-1.07418	0.67609
H	0.69055	-3.25412	0.60754
H	0.40637	-2.67882	-0.91658
O	-1.09205	2.00671	0.15906
O	0.21879	1.54855	-1.96924
H	-2.00797	-4.37357	1.33592
H	-4.79479	-2.25099	1.85080
C	-1.54597	-3.94634	2.22837
H	-2.06438	-4.35780	3.10281
H	-0.51224	-4.29820	2.28346
H	-4.31161	-1.51275	0.31709
C	-3.98314	-2.17977	1.11716
H	-3.82933	-3.17126	0.68762
C	-1.63596	-2.44916	2.24530
C	-2.74278	-1.66626	1.77920
H	1.01798	-2.84008	3.25425
C	-0.67680	-1.54325	2.88368
C	0.53708	-1.94913	3.66704
C	-2.48832	-0.28017	2.12307
H	0.26097	-2.18391	4.70233
H	-4.20687	0.63248	1.20303
C	-1.23266	-0.22157	2.82334
C	-3.44081	0.85949	1.94484
H	1.27779	-1.14716	3.69607
H	-2.91750	1.75991	1.62381
H	-3.94515	1.06606	2.89753
C	-0.61687	1.00730	3.40885
H	0.45903	1.03654	3.22043
H	-0.77224	1.02010	4.49454
H	-1.06433	1.90665	2.98584
H	-5.59057	4.06739	-0.32608
C	-5.55905	3.06472	-0.74168
H	-7.65718	2.68492	-0.40292
C	-6.72178	2.28811	-0.78580
H	-3.45501	3.15250	-1.19129
C	-4.36177	2.55663	-1.23606
C	-6.67751	0.99972	-1.32826
C	-4.30174	1.26496	-1.80063
H	-2.27279	1.56726	-2.42692
H	-7.57938	0.39628	-1.36863
C	-5.48072	0.49101	-1.82746
C	-3.00492	0.76512	-2.31701
H	-2.51361	0.09512	-1.46426
H	-5.46680	-0.50716	-2.25412
C	-2.96161	-0.19445	-3.49787
H	-3.73318	-0.96696	-3.41482
H	-3.15560	0.34735	-4.43168
N	-1.68871	-1.14685	-1.07337
C	-1.58141	-0.85101	-3.55133
C	-1.21735	-1.59169	-2.27587
H	-1.48592	-1.57393	-4.36552
H	-0.81083	-0.08175	-3.68977
O	-0.54139	-2.64234	-2.32963
C	1.30970	3.04508	-0.09401
C	1.27009	3.61735	1.17949
C	2.14325	3.56208	-1.08644
C	2.09106	4.70524	1.46063
H	0.59793	3.22823	1.93449
C	2.95651	4.65279	-0.78710
H	2.14606	3.11712	-2.07403
C	2.94670	5.24111	0.48538
H	2.06202	5.15332	2.45016
H	3.60743	5.05600	-1.55781
C	3.80720	6.44272	0.78764
H	3.29097	7.36972	0.50945
H	4.04496	6.50932	1.85280
H	4.74590	6.41413	0.22725

TS-R₁

E(B3LYP) = -2483.25976662			
# of imaginary frequency = 1(-716.53)			
N	-0.53128	0.24584	-0.34168
C	-1.77530	0.08602	0.47055
C	-2.33259	-1.31596	0.15000
C	-2.84326	1.13188	0.17843
H	-1.53974	0.12057	1.54206
N	-1.19984	-2.27831	0.30182
H	-2.60939	-1.32437	-0.90840
C	-3.52846	-1.74297	0.97900
S	0.46361	1.50682	0.18516
C	-3.18650	1.46979	-1.13681
C	-4.22130	2.36929	-1.38971
C	-4.92967	2.93963	-0.32892
C	-4.59409	2.60819	0.98429
C	-3.55534	1.71006	1.23507
C	-3.41543	-1.96634	2.36073
C	-4.52895	-2.36374	3.10057
C	-5.76546	-2.53779	2.47450
C	-5.88533	-2.31598	1.10207
C	-4.77113	-1.92405	0.35925
H	-2.62157	1.04405	-1.96097
H	-4.47454	2.62801	-2.41378
H	-5.73674	3.63889	-0.52609
H	-5.13942	3.04743	1.81434
H	-3.30051	1.45098	2.25917
H	-2.46000	-1.84214	2.86400
H	-4.43003	-2.53765	4.16776
H	-6.63024	-2.84607	3.05412
H	-6.84354	-2.44820	0.60898
H	-4.87121	-1.74402	-0.70806
Ir	0.57065	-1.55743	-0.58523
H	-1.46901	-3.18573	-0.07570
H	-0.93217	-2.43260	1.30136
O	1.73965	1.32453	-0.53608
O	0.47888	1.56281	1.66371
H	0.49882	-5.14290	-0.88387
H	3.89272	-4.10186	-1.59613
C	0.15495	-4.65839	-1.80015
H	0.42240	-5.30924	-2.64133
H	-0.93736	-4.61068	-1.77763
H	3.58945	-3.23287	-0.08260
C	3.11109	-3.78023	-0.89829
H	2.65397	-4.67514	-0.47286
C	0.77670	-3.30714	-1.99137
C	2.10333	-2.92863	-1.60792
H	-1.87046	-2.86247	-2.95364
C	0.17044	-2.18974	-2.71478
C	-1.14214	-2.20954	-3.44150
C	2.33973	-1.58285	-2.09992
H	-1.01018	-2.57914	-4.46572
H	4.31161	-1.28688	-1.30156
C	1.16211	-1.15035	-2.79997
C	3.63307	-0.83368	-2.02642
H	-1.57494	-1.20858	-3.50227
H	3.46706	0.20700	-1.74411
H	4.13149	-0.85655	-3.00368
C	1.01628	0.14044	-3.53733
H	-0.00909	0.51229	-3.48899
H	1.27117	-0.00940	-4.59400
H	1.67910	0.90091	-3.12442
H	6.29390	2.77301	-0.12593
H	5.34074	4.63936	1.21400
C	5.52040	2.57598	0.60986
C	4.98761	3.62403	1.36674
C	5.06458	1.27859	0.81033
H	5.49144	0.46320	0.23260
C	4.00120	3.36241	2.32488
H	3.58821	4.17555	2.91355
C	4.07514	0.99309	1.77615
C	3.54740	2.06513	2.52685
H	4.37254	-1.09417	1.51720
C	3.66251	-0.40630	1.98775
H	2.77213	1.88216	3.26114
H	2.66758	-0.69985	1.32300
H	3.60862	-1.89877	3.54304
C	3.23029	-0.88465	3.38136
H	3.67792	-0.25212	4.15400
N	1.50700	-1.58791	1.15879
H	1.38411	-1.34102	4.47732
C	1.70458	-0.88886	3.53548
C	1.00743	-1.65013	2.42454
H	1.31257	0.13405	3.49732
O	0.02148	-2.37813	2.67789

C	-0.23504	3.05723	-0.38322
C	-0.83898	3.91148	0.53923
C	-0.10120	3.42923	-1.72314
C	-1.32461	5.14386	0.10594
H	-0.92012	3.61256	1.57730
C	-0.59363	4.66237	-2.13820
H	0.39162	2.77045	-2.42762
C	-1.21244	5.54013	-1.23360
H	-1.79733	5.80945	0.82272
H	-0.49024	4.95437	-3.17987
C	-1.71309	6.88858	-1.68863
H	-0.90396	7.62910	-1.67480
H	-2.09769	6.84900	-2.71189
H	-2.50820	7.26183	-1.03778

TS-S₂

E(B3LYP) = -2483.26439623
of imaginary frequency = 1(-361.51)

N	0.85137	0.30309	0.16506
C	1.87492	-0.46635	-0.60570
C	1.70776	-1.95968	-0.24609
C	3.31160	-0.02917	-0.34330
H	1.67127	-0.36225	-1.67909
N	0.23708	-2.22843	-0.27283
H	2.02434	-2.10183	0.79032
C	2.46235	-2.92854	-1.13491
S	0.39202	1.75614	-0.59412
C	3.75961	0.26622	0.94973
C	5.09492	0.59473	1.18184
C	6.00259	0.62880	0.12080
C	5.56552	0.33576	-1.17152
C	4.22770	0.01065	-1.40109
C	2.21821	-2.99160	-2.51592
C	2.89574	-3.91345	-3.31269
C	3.83000	-4.78076	-2.74108
C	4.08293	-4.72231	-1.37034
C	3.39961	-3.80321	-0.57266
H	3.05202	0.25834	1.77284
H	5.42728	0.82775	2.18931
H	7.04229	0.88490	0.30073
H	6.26379	0.36233	-2.00269
H	3.89518	-0.21883	-2.40989
H	1.50477	-2.31603	-2.98356
H	2.69745	-3.95258	-4.37935
H	4.35831	-5.49676	-3.36288
H	4.81056	-5.39064	-0.92051
H	3.60507	-3.75838	0.49388
Ir	-0.79144	-0.79002	0.87661
H	0.00522	-3.17520	0.02916
H	-0.10569	-2.17716	-1.23295
O	-0.77124	2.24916	0.16642
O	0.25570	1.52058	-2.04570
H	-2.06170	-3.89481	1.79335
H	-3.94932	-2.56072	1.67567
C	-1.47977	-3.53497	2.64527
H	-1.95687	-3.89230	3.56547
H	-0.48572	-3.98666	2.60077
H	-4.52531	-1.48412	2.96298
C	-3.90123	-1.54259	2.06302
H	-4.32648	-0.87055	1.31502
C	-1.40710	-2.03804	2.65542
C	-2.50070	-1.14894	2.40529
H	1.30896	-2.72573	3.15510
C	-0.24194	-1.22875	3.00867
C	1.05499	-1.74258	3.55848
C	-2.03282	0.21447	2.57031
H	0.98622	-1.84804	4.64844
H	-3.70241	1.30091	1.76522
C	-0.65878	0.15422	2.98452
C	-2.87553	1.44655	2.46238
H	1.88114	-1.06172	3.34401
H	-2.28837	2.29179	2.10335
H	-3.29982	1.69813	3.44247
C	0.19452	1.31697	3.37316
H	1.17054	1.27522	2.88480
H	0.35511	1.30539	4.45796
H	-0.28167	2.26094	3.10914
H	-5.03607	4.40423	-0.51572
C	-5.16554	3.45438	-1.02614
H	-7.31936	3.59986	-1.09337
C	-6.44937	3.00368	-1.35167
H	-3.05353	3.04068	-1.11164
C	-4.05139	2.69394	-1.36665
C	-6.60718	1.78570	-2.01734
C	-4.19375	1.46180	-2.04028

H	-2.14605	1.36034	-2.67174
H	-7.60046	1.43565	-2.28207
C	-5.49230	1.01808	-2.35114
C	-2.96035	0.69551	-2.37501
H	-2.55240	0.27740	-1.35128
H	-5.63811	0.08314	-2.88257
C	-3.04112	-0.56009	-3.24443
H	-3.73584	-0.42255	-4.08084
H	-2.05569	-0.73272	-3.69119
N	-2.19247	-0.91268	-0.45898
C	-3.44042	-1.79539	-2.42601
C	-2.60458	-2.00854	-1.16394
H	-4.48355	-1.72654	-2.09273
H	-3.36040	-2.71795	-3.00691
O	-2.40139	-3.15012	-0.71336
C	1.71647	2.94255	-0.38106
C	1.81441	3.66475	0.81101
C	2.59261	3.18522	-1.43975
C	2.81736	4.61954	0.94553
H	1.10225	3.49856	1.60985
C	3.59048	4.14557	-1.28659
H	2.48275	2.63992	-2.36946
C	3.72278	4.87471	-0.09692
H	2.89371	5.18530	1.87015
C	4.27432	4.33554	-2.10895
H	4.78509	5.93565	0.04853
H	4.38620	6.92253	-0.21610
H	5.14987	5.99892	1.07773
H	5.63815	5.74181	-0.60701

TS-R₂

E(B3LYP) = -2483.26008147
of imaginary frequency = 1(-648.98)

N	0.65655	-0.10339	-0.38344
C	1.73039	0.44974	0.49639
C	1.52281	1.97852	0.59105
C	3.14280	0.14033	0.01368
H	1.61255	0.04804	1.51138
N	0.05515	2.17791	0.79110
H	1.76136	2.41865	-0.38044
C	2.33417	2.67806	1.66419
S	0.16443	-1.65721	0.07937
C	3.47866	0.20261	-1.34386
C	4.79198	-0.00855	-1.76297
C	5.79036	-0.28423	-0.82607
C	5.46454	-0.35419	0.52896
C	4.14860	-0.14516	0.94450
C	2.17618	2.35908	3.02197
C	2.91024	3.03266	3.99731
C	3.81674	4.02953	3.62812
C	3.98465	4.34985	2.28076
C	3.24419	3.67956	1.30595
H	2.69814	0.39313	-2.07301
H	5.03665	0.03823	-2.82029
H	6.81336	-0.44822	-1.15107
H	6.23295	-0.57431	1.26400
H	3.90395	-0.19858	2.00184
H	1.48551	1.57645	3.32933
H	2.77767	2.77765	5.04424
H	4.38935	4.55211	4.38805
H	4.69004	5.12100	1.98696
H	3.38300	3.92931	0.25717
Ir	-1.02676	1.13176	-0.69244
H	-0.21112	3.16239	0.81786
H	-0.22215	1.81301	1.70304
O	-0.96941	-1.99603	-0.79977
O	-0.02511	-1.69088	1.54543
H	-2.18635	4.40026	-0.64165
H	-4.10233	3.10105	-0.70166
C	-1.67290	4.28175	-1.59935
H	-2.19306	4.89506	-2.34455
H	-0.65951	4.67864	-1.50307
H	-4.78185	2.61774	-2.26892
C	-4.14406	2.29628	-1.43650
H	-4.61619	1.43245	-0.96606
C	-1.66744	2.84616	-2.02836
C	-2.78239	1.95510	-1.95157
H	1.05412	3.56072	-2.47702
C	-0.55449	2.12791	-2.64407
C	0.72605	2.74312	-3.12341
C	-2.38038	0.66893	-2.49713
H	0.58786	3.16029	-4.12872
H	-4.12252	-0.48747	-2.00650
C	-1.02505	0.79279	-2.95211
C	-3.25597	-0.53302	-2.66837

H	1.53236	2.00984	-3.17866	C	0.78146	-1.57699	-5.53216
H	-2.70704	-1.44886	-2.44408	H	1.33889	-2.07100	-6.33744
H	-3.62691	-0.58615	-3.69935	H	1.01916	-0.51190	-5.58442
C	-0.25300	-0.27055	-3.66295	H	0.16300	-5.06712	-4.84094
H	0.81344	-0.20809	-3.44046	C	-0.37859	-4.27487	-4.30761
H	-0.38373	-0.15662	-4.74618	H	-1.05156	-4.72790	-3.58070
H	-0.60596	-1.26091	-3.37359	C	1.17435	-2.17543	-4.21629
H	-4.67712	-5.23526	0.00876	C	0.62160	-3.38010	-3.64625
H	-3.10893	-6.47922	1.48606	H	2.74498	0.19941	-4.24217
C	-4.06062	-4.69945	0.72383	C	2.24609	-1.71773	-3.37120
C	-3.18129	-5.39807	1.55636	C	3.21308	-0.61592	-3.68532
C	-4.15130	-3.31579	0.82151	C	1.32964	-3.65229	-2.40973
H	-4.84646	-2.77443	0.18472	H	4.03448	-1.00110	-4.30209
C	-2.39333	-4.70204	2.48008	H	0.11726	-5.20551	-1.55980
H	-1.70924	-5.24419	3.12564	C	2.35071	-2.64553	-2.27001
C	-3.37078	-2.59830	1.75304	C	1.15431	-4.86369	-1.54891
C	-2.47854	-3.31793	2.57325	H	3.65276	-0.19843	-2.77844
H	-4.49917	-0.83065	1.40063	H	1.43883	-4.65591	-0.51626
C	-3.54913	-1.13758	1.85404	H	1.78384	-5.68016	-1.92381
H	-1.84220	-2.79015	3.27349	C	3.43025	-2.61867	-1.24193
H	-2.78735	-0.53067	1.11236	H	3.65467	-1.59534	-0.93519
H	-4.00666	-0.75003	3.93343	H	4.34270	-3.04574	-1.67751
C	-3.30781	-0.40126	3.16295	H	3.15969	-3.19532	-0.35941
H	-2.29769	-0.61037	3.53046	H	-2.95837	-4.49954	2.76188
N	-2.38015	0.81329	0.70233	H	-4.10095	-6.70468	2.74369
H	-4.54024	1.34304	2.76760	H	-3.88360	-3.00664	2.67096
C	-3.48121	1.09960	2.92801	C	-3.81915	-4.02674	2.27270
C	-2.72983	1.65259	1.71625	C	-5.05094	-6.17798	2.80155
H	-3.16056	1.69560	3.78686	H	-1.41365	-3.61212	0.95095
O	-2.52149	2.87608	1.61291	C	-5.08240	-4.79007	2.60719
C	1.50489	-2.78050	-0.30191	C	-6.21914	-6.88908	3.07761
C	2.23903	-3.34238	0.74238	H	-6.17400	-7.96340	3.23181
C	1.75225	-3.14272	-1.62925	H	-2.33449	-2.14248	0.74937
C	3.24002	-4.26726	0.44757	C	-2.27790	-3.18497	0.42331
H	2.01310	-3.07064	1.76700	C	-6.31659	-4.13144	2.69533
C	2.75575	-4.06478	-1.90407	C	-7.44214	-6.22070	3.16227
H	1.15635	-2.72350	-2.43154	C	-3.56127	-3.96411	0.75254
C	3.51904	-4.63939	-0.87364	C	-7.48755	-4.83835	2.97100
H	3.80853	-4.71168	1.25965	H	-6.35839	-3.05345	2.55556
C	2.94614	-4.35401	-2.93412	H	-8.35188	-6.77199	3.38087
H	4.61714	-5.62387	-1.19058	H	-3.48518	-4.97562	0.34321
H	4.30638	-6.33289	-1.96405	N	-1.45429	-2.08175	-1.57043
H	5.50795	-5.10591	-1.56608	C	-1.93104	-3.26377	-1.05600
H	4.91467	-6.19245	-0.30597	H	-8.43385	-4.30968	3.04244

IV

E(B3LYP) = -2483.27471169
of imaginary frequency = 0

N	0.91989	-0.23693	-0.76413
C	0.33582	1.13869	-0.88943
C	-0.08171	1.35838	-2.35759
C	1.28016	2.24982	-0.44702
H	-0.57592	1.19065	-0.28126
N	-0.81745	0.12395	-2.77635
H	0.82337	1.39051	-2.97101
C	-0.90529	2.60374	-2.61914
S	0.73777	-0.86765	0.83834
C	2.64150	2.22528	-0.77130
C	3.47473	3.28546	-0.41493
C	2.95433	4.38770	0.26676
C	1.59776	4.42113	0.59305
C	0.76705	3.35688	0.24013
C	-2.16441	2.77977	-2.02355
C	-2.92080	3.91889	-2.29546
C	-2.42717	4.89765	-3.16178
C	-1.17535	4.73244	-3.75524
C	-0.42074	3.58941	-3.48704
H	3.05121	1.36042	-1.28225
H	4.53079	3.25074	-0.66625
H	3.60281	5.21326	0.54395
H	1.18519	5.27308	1.12503
H	-0.28841	3.38973	0.49621
H	-2.56143	2.03539	-1.33638
H	-3.89319	4.04396	-1.82929
H	-3.01655	5.78487	-3.37116
H	-0.78513	5.49114	-4.42644
H	0.55722	3.46960	-3.94623
Ir	0.25227	-1.60900	-2.18417
H	-1.01673	0.15196	-3.77638
H	-1.72153	0.03776	-2.29942
O	1.08431	-2.29519	0.74510
O	-0.58939	-0.47243	1.34333
H	-0.28107	-1.71398	-5.74531
H	-0.98233	-3.73619	-5.04081

V

E(B3LYP) = -2483.27571239
of imaginary frequency = 0

N	0.39893	1.25454	-0.27201
C	0.43222	1.72365	1.15527
C	0.24922	0.50295	2.07924
C	-0.43395	2.92596	1.49747
H	1.47181	2.05876	1.26964
N	1.26646	-0.50042	1.60357
H	-0.72626	0.05715	1.87514
C	0.41806	0.72411	3.56843
S	-1.11013	1.09908	-1.06407
C	-1.69477	2.80718	2.09745
C	-2.42003	3.94644	2.44823
C	-1.90168	5.21751	2.19706
C	-0.64794	5.34692	1.59616
C	0.08006	4.20802	1.25758
C	1.46204	1.50669	4.08606
C	1.62263	1.65051	5.46399
C	0.74465	1.01187	6.34249
C	-0.29443	0.22885	5.83754
C	-0.45459	0.08461	4.45922
H	-2.12172	1.82966	2.28739
H	-3.39111	3.83813	2.92189

H	-2.46718	6.10191	2.47460	H	0.29383	1.56504	0.41330
H	-0.23301	6.33168	1.40384	C	0.60025	2.92743	-1.22509
H	1.06335	4.31427	0.80532	S	-2.31264	-0.38219	1.18766
H	2.14650	2.02656	3.41990	C	-2.10235	3.11790	0.79297
H	2.42829	2.26649	5.85172	C	-2.92570	4.18768	1.14257
H	0.86945	1.12630	7.41477	C	-3.99372	4.55496	0.32197
H	-0.98069	-0.27029	6.51455	C	-4.23682	3.84652	-0.85571
H	-1.26373	-0.52903	4.07137	C	-3.40928	2.78144	-1.20804
Ir	1.55783	-0.45510	-0.50524	C	0.24305	3.38039	-2.50470
H	0.97607	-1.46479	1.84637	C	0.79834	4.55191	-3.01878
H	2.15342	-0.31518	2.07207	C	1.71938	5.28150	-2.26337
O	-2.11132	0.53146	-0.13914	C	2.08365	4.83616	-0.99171
O	-0.80638	0.37793	-2.30940	C	1.52856	3.66430	-0.47630
H	4.40086	1.53558	1.01744	H	-1.29221	2.83403	1.45456
H	3.79865	2.87622	-0.67100	H	-2.72909	4.73684	2.05835
C	4.66329	0.53646	0.66406	H	-4.62964	5.39133	0.59607
H	5.72416	0.55231	0.38583	H	-5.06149	4.12793	-1.50347
H	4.56947	-0.16309	1.49951	H	-3.59537	2.24161	-2.13368
H	3.62451	2.83923	-2.42840	H	-0.48709	2.83781	-3.10023
C	3.21084	2.45668	-1.48933	H	0.50685	4.89956	-4.00521
H	2.18052	2.81731	-1.39817	H	2.14800	6.19487	-2.66413
C	3.83674	0.11677	-0.51391	H	2.79691	5.40056	-0.39911
C	3.23845	0.96176	-1.48443	H	1.81302	3.31743	0.51401
H	4.28574	-2.39548	0.79687	Ir	-0.08532	-1.39567	-0.80204
C	3.61938	-1.27247	-0.92810	H	1.78841	0.51661	-0.96110
C	4.23466	-2.48246	-0.29095	H	0.84250	0.60559	-2.28741
C	2.60294	0.12120	-2.49151	O	-1.57740	0.37786	2.20592
H	5.25999	-2.61381	-0.65885	O	-2.37543	-1.84898	1.29324
H	1.62918	1.64495	-3.65156	H	-2.12801	-0.87165	-3.88563
C	2.90912	-1.25174	-2.18299	H	-3.54638	-1.88422	-2.44073
C	1.95992	0.61121	-3.75115	C	-1.22047	-1.45204	-4.06579
H	3.67317	-3.38678	-0.53136	H	-1.41808	-2.12040	-4.91267
H	1.08732	0.01376	-4.01535	H	-0.43466	-0.76072	-4.38203
H	2.68426	0.56611	-4.57400	H	-3.60480	-3.64478	-2.29761
C	2.56121	-2.44856	-3.00720	C	-3.17821	-2.73222	-1.86144
H	2.01535	-3.18572	-2.41101	H	-3.53438	-2.65388	-0.83330
H	3.47392	-2.91868	-3.38956	C	-0.82106	-2.24215	-2.85361
H	1.93468	-2.17604	-3.85736	C	-1.69320	-2.83012	-1.89672
H	-7.59371	-1.28202	2.58531	H	1.70992	-1.48659	-3.89122
C	-6.99184	-2.17553	2.44468	C	0.53387	-2.68146	-2.52707
H	-5.85357	-1.32909	0.82394	C	1.74457	-2.45342	-3.38305
C	-6.01081	-2.20291	1.45251	C	-0.91204	-3.62529	-0.96230
H	-7.97459	-3.27979	4.01634	H	1.79354	-3.22394	-4.16223
C	-7.20744	-3.29719	3.24783	H	-2.28145	-4.02327	0.64172
C	-5.23069	-3.34863	1.24438	C	0.44677	-3.59453	-1.40373
C	-6.43721	-4.44491	3.05052	C	-1.45798	-4.50526	0.11714
H	-4.42790	-2.71975	-0.64824	H	2.67222	-2.50542	-2.80962
C	-5.45750	-4.46786	2.05712	H	-0.68982	-4.74859	0.85333
H	-4.03065	-4.37795	-0.21101	H	-1.81516	-5.44627	-0.32066
C	-4.14238	-3.36368	0.19245	C	1.56690	-4.36829	-0.78521
H	-6.60370	-5.32491	3.66525	H	2.53765	-4.08171	-1.19306
H	-4.86689	-5.36837	1.90407	H	1.42312	-5.43704	-0.98093
C	-2.78513	-2.89171	0.75282	H	1.59044	-4.22320	0.29785
H	-1.89703	-2.19742	-1.12417	H	8.68966	2.43157	3.20597
C	-1.68538	-2.90698	-0.31705	C	8.39286	2.01956	2.24581
H	-1.61215	-3.90035	-0.78338	H	7.03635	0.59462	3.11767
H	-2.89237	-1.87305	1.14196	C	7.45972	0.98375	2.19440
H	-2.48628	-3.52980	1.59011	H	9.68130	3.32165	1.10624
C	-0.31274	-2.61003	0.25894	C	8.95042	2.51946	1.06706
N	0.53184	-2.00436	-0.63784	C	7.06792	0.43010	0.96755
O	0.05756	-2.95923	1.38917	C	8.56993	1.97578	-0.16088
C	-1.63552	2.74759	-1.52333	H	6.16017	-1.34877	1.76504
C	-2.89303	3.18989	-1.11539	C	7.63549	0.93982	-0.20747
C	-0.85079	3.51371	-2.38985	H	6.17084	-1.27007	0.00802
C	-3.35661	4.42353	-1.57138	C	6.02675	-0.66829	0.91449
H	-3.49258	2.57572	-0.45476	H	9.00595	2.35241	-1.08181
C	-1.32635	4.74453	-2.82769	H	7.35195	0.51392	-1.16769
H	0.11550	3.15166	-2.72133	C	4.58820	-0.11489	0.94105
C	-2.58757	5.21922	-2.42986	H	3.69193	-1.95069	1.68681
H	-4.33594	4.77061	-1.25455	C	3.52845	-1.22178	0.88095
H	-0.71608	5.34499	-3.49685	H	3.59224	-1.79669	-0.05244
C	-3.10961	6.53805	-2.94327	H	4.43166	0.47469	1.84880
H	-2.30852	7.27687	-3.03871	H	4.45572	0.57999	0.10047
H	-3.55875	6.41653	-3.93647	C	2.10902	-0.69022	1.06239
H	-3.87890	6.94904	-2.28453	N	1.10896	-1.53594	0.60533
				O	1.85546	0.34445	1.67250
				C	-4.00420	0.21991	1.16440
				C	-4.44565	0.91995	2.28872
				C	-4.89454	-0.12818	0.14670
				C	-5.79094	1.27227	2.38399
				H	-3.74393	1.18229	3.07160
				C	-6.23221	0.23907	0.25566
				H	-4.54730	-0.65926	-0.72976
				C	-6.70589	0.93779	1.37718
				H	-6.13357	1.81776	3.25879
				H	-6.92251	-0.02158	-0.54218

VI

E(B3LYP) = -2483.25475991

of imaginary frequency = 0

N	-1.63933	-0.10844	-0.36294
C	-1.41225	1.29332	-0.86950
C	0.07054	1.63014	-0.65359
C	-2.33844	2.39981	-0.38860
H	-1.58401	1.20396	-1.95068
N	0.81800	0.47294	-1.27519

C	-8.16569	1.29618	1.50415
H	-8.62040	1.48115	0.52677
H	-8.72605	0.47891	1.97447
H	-8.30751	2.18629	2.12289

Ir12

E(B3LYP) = -2484.16092697

of imaginary frequency = 0

N	-7.57265	4.16358	-0.22571
C	-6.97375	2.79920	-0.27747
C	-5.50920	2.95373	-0.75018
C	-7.70836	1.83785	-1.20534
H	-6.94799	2.35784	0.72689
N	-4.88324	4.00261	0.09536
H	-5.53166	3.33896	-1.77595
C	-4.71307	1.65882	-0.72704
S	-8.95958	4.20356	0.70445
C	-8.06709	2.22295	-2.50395
C	-8.68253	1.31966	-3.36943
C	-8.95005	0.01450	-2.94797
C	-8.60101	-0.37687	-1.65505
C	-7.98476	0.53051	-0.79094
C	-4.34887	1.05347	0.48636
C	-3.61766	-0.13477	0.48692
C	-3.24166	-0.73479	-0.71716
C	-3.59930	-0.13841	-1.92676
C	-4.32825	1.05191	-1.92865
H	-7.88348	3.24569	-2.82018
H	-8.95969	1.63477	-4.37191
H	-9.43123	-0.68930	-3.62151
H	-8.80889	-1.38802	-1.31599
H	-7.71297	0.22202	0.21481
H	-4.62372	1.51567	1.43116
H	-3.34040	-0.59187	1.43259
H	-2.67207	-1.65987	-0.71177
H	-3.31183	-0.59724	-2.86863
H	-4.61346	1.50855	-2.87313
Ir	-6.12027	5.71788	0.23717
H	-3.95909	4.22707	-0.26790
H	-4.76562	3.70291	1.10433
O	-9.23874	5.62028	1.03036
O	-8.92239	3.22883	1.81810
H	-2.71378	6.64582	-0.08315
H	-3.45048	7.66110	1.77553
C	-3.27888	6.90779	-0.98127
H	-2.81044	7.79710	-1.42036
H	-3.16701	6.09522	-1.70504
H	-4.27936	9.22527	1.76349
C	-4.43284	8.13861	1.75937
H	-4.94407	7.86450	2.68533
C	-4.72183	7.17825	-0.67108
C	-5.22935	7.71645	0.56116
H	-4.87792	5.92338	-3.21429
C	-5.82562	6.98912	-1.59407
C	-5.72187	6.59635	-3.03901
C	-6.67307	7.87408	0.40600
H	-5.57839	7.47500	-3.68222
H	-7.20568	8.38645	2.42397
C	-7.01980	7.44829	-0.91792
C	-7.60646	8.47955	1.41146
H	-6.62565	6.08401	-3.37782
H	-8.57699	7.98022	1.38991
H	-7.75431	9.54876	1.21261
C	-8.38759	7.52249	-1.51979
H	-8.50438	6.79609	-2.32707
H	-8.55392	8.52145	-1.94330
H	-9.15322	7.32846	-0.76735
H	-10.34614	-1.18702	6.04012
C	-9.35224	-0.83100	6.29798
C	-9.01592	0.50512	6.07721
H	-9.74944	1.18219	5.64562
C	-8.41739	-1.70766	6.85262

H	-8.24198	3.07747	6.30640
H	-8.67894	-2.74740	7.02855
C	-7.74273	0.99249	6.40506
C	-7.14568	-1.23656	7.18338
C	-7.37010	2.43389	6.13138
H	-6.59846	2.75384	6.84388
C	-6.81464	0.10103	6.96035
H	-6.41169	-1.90927	7.61916
H	-5.82289	0.46200	7.22370
H	-7.32548	4.77939	4.59196
C	-6.85781	2.65951	4.69557
H	-5.68857	4.42237	5.15410
C	-6.46338	4.12092	4.43603
H	-7.63209	2.36646	3.97789
H	-5.98633	2.02365	4.50847
C	-5.87892	4.31015	3.03672
N	-6.43489	5.22739	2.24864
O	-4.89126	3.59474	2.70786
C	-10.32825	3.67427	-0.35093
C	-10.98622	2.47940	-0.06369
C	-10.76143	4.48421	-1.40159
C	-12.07536	2.09193	-0.84391
H	-10.64082	1.86841	0.76187
C	-11.85025	4.08497	-2.17226
H	-10.25477	5.41804	-1.61184
C	-12.52581	2.88444	-1.90691
H	-12.58245	1.15639	-0.62138
H	-12.18507	4.71678	-2.99153
C	-13.72617	2.47289	-2.72581
H	-14.65619	2.84421	-2.27701
H	-13.67471	2.87253	-3.74304
H	-13.81061	1.38401	-2.79205
H	-7.29975	5.61186	2.60942

1

E(B3LYP) = -706.20607894

of imaginary frequency = 0

H	-1.16800	3.06344	8.50707
C	-0.62722	2.32102	7.92723
H	-2.38974	1.63162	6.90274
C	-1.31516	1.51322	7.02141
H	1.28698	2.79792	8.79899
C	0.75065	2.17202	8.09197
C	-0.64100	0.54489	6.26585
C	1.43400	1.20994	7.34671
H	-2.40980	-0.47735	5.60026
C	0.74189	0.40435	6.44217
H	-0.90734	-1.28955	5.17912
C	-1.38282	-0.30363	5.25504
H	2.50540	1.08300	7.47251
H	1.28014	-0.34744	5.86948
C	-1.42546	0.34344	3.85787
H	-3.19894	-0.72342	3.18980
C	-2.17574	-0.53796	2.83923
H	-1.68501	-1.50930	2.72632
H	-1.90935	1.32420	3.92172
C	-0.40340	0.51908	3.50340
C	-2.25192	0.07377	1.48711
N	-1.73147	-0.39262	0.40834
O	-2.91221	1.25431	1.32386
C	-2.79573	1.56919	-0.02290
O	-2.07549	0.56558	-0.59183
O	-3.24711	2.53312	-0.55757

CO₂

E(B3LYP) = -188.58093689

of imaginary frequency = 0

C	0.00000	0.00000	-0.00001
O	0.00000	0.00000	1.17008
O	0.00000	0.00000	-1.17007