

Full Kinetic Analysis of a Rhodium-Catalyzed Hydroformylation:

Beyond the Rate-Limiting Step Picture

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Supporting Information

Quantum mechanical calculations.....	2
Cartesian coordinates	3
Complete Reference 9	56
Sample kinetic computation input and output.....	56

Quantum mechanical calculations

Low Layer: All intermediates and transition states containing ligand **1** of the catalytic cycle were fully optimized with the B3LYP functional. The STUTTGART-DRESDEN relativistic core potential²⁶ in conjunction with the D95 double zeta basis set (SDD) was used for rhodium. The full electron 6-31G(d,p) basis set was used for all other atoms. The combination of the B3LYP functional and the 6-31G(d,p) basis set was shown to describe the geometries and energetics of the hydrogen bonds between two tautomeric forms of ligand **9** in the coordination sphere of an late transition metal in good agreement with the experiment.¹ Thermodynamic corrections are calculated at the same level of theory from a harmonic vibrational analysis. Transition states and minimum structures were identified by the presence or absence of one imaginary frequency. All discussed reaction energetics are calculated at standard conditions (1 bar ideal gas for all species and 298.15 K).

High Layer: In order to obtain reliable energies for a model system in which ligand **9** was replaced by PH₃ the following scheme was applied which is based on the nearly identical convergence behavior of CCSD(T) and MP2 towards the basis set limit: 1) Geometry optimizations were performed using the BP86 functional together with the STUTTGART-KÖLN full relativistic ECP28MDF core potential³⁰ and the corresponding aug-cc-pVTZ-PP basis set for Rh. The standard aug-cc-pVTZ basis set was used for all other atoms. This level of theory reproduces the gas phase determined Rh-P bond length in a [(NO)Rh(PF₃)₃] complex with an error of 0.005 Å. 2) A MP2 single point energy calculation with the cc-pwCVDZ basis set (cc-pwCVDZ-PP for Rh) including core valence functions was performed. 3) An additional MP2 single point energy calculation with the aug-cc-pwCVQZ basis set (aug-cc-pwCVQZ-PP for Rh) including diffuse and core valence functions was performed. 4) To account for correlation effects beyond second order perturbation theory a coupled-cluster calculation with single and double substitutions and with inclusion of perturbative triple excitations (CCSD(T)) together with cc-pwCVDZ basis set was performed. 5) The final single point energy was obtained by the equation CCSD(T)/cc-pwCVDZ + MP2/aug-cc-pwCVQZ – MP2/cc-pwCVDZ. In order to check for a possible multiconfigurational character in case of the CCSD(T) computations, the largest T2 amplitudes were investigated and found to be below 0.1.

The high layer was then reoptimized with the B3LYP/SDD-6-31G(d,p) method. The IMOMO energy is obtained by three independent methods (equation 1).

$$\Delta E_{\text{IMOMO (CCSD(T):DFT)}} = \Delta E_{\text{real world (DFT)}} + (\Delta E_{\text{Model (CCSD(T))}} - \Delta E_{\text{Model (DFT)}})$$

All computations were performed using the Gaussian 09 suite of programs.

Cartesian coordinates

1 Low Layer (B3LYP/SDD-6-31G(d,p))

Rh	0.03550	-1.59837	0.21805
H	0.09023	-1.68349	-1.37651
P	1.99635	-0.26160	-0.08518
P	-1.99403	-0.40353	-0.15010
C	-3.55861	-1.39605	-0.06485
C	-4.74869	-0.98554	-0.68708
C	-3.55171	-2.59777	0.65865
C	-5.90459	-1.76002	-0.58138
H	-4.77395	-0.06583	-1.26199
C	-4.71172	-3.36593	0.77164
H	-2.62868	-2.93444	1.12021
C	-5.88981	-2.94953	0.15020
H	-6.81640	-1.43394	-1.07376
H	-4.68901	-4.29405	1.33537
H	-6.79039	-3.55187	0.22860
C	-2.20862	0.57492	-1.70811
C	-2.88827	1.80369	-1.74475
C	-1.70011	0.04932	-2.90588
C	-3.04992	2.48958	-2.94991
H	-3.29365	2.23314	-0.83436
C	-1.87486	0.72995	-4.11083
H	-1.15717	-0.89026	-2.89052
C	-2.54648	1.95345	-4.13569
H	-3.56907	3.44358	-2.95821
H	-1.47654	0.30696	-5.02862
H	-2.67258	2.48840	-5.07256
C	2.82310	0.21747	1.50790
C	2.59079	1.43875	2.15831
C	3.62170	-0.74756	2.14771
C	3.16367	1.69247	3.40728
H	1.95663	2.19042	1.70405
C	4.18973	-0.48858	3.39418
H	3.80636	-1.70460	1.66924
C	3.96500	0.73518	4.02834
H	2.97435	2.64579	3.89239
H	4.80706	-1.24591	3.86925
H	4.40636	0.93671	5.00021
C	3.38516	-1.08615	-0.99575
C	3.14685	-2.24230	-1.74954
C	4.68851	-0.55763	-0.96207
C	4.18294	-2.85719	-2.45814
H	2.14812	-2.66364	-1.77248

C	5.72209	-1.17346	-1.66586
H	4.89582	0.33514	-0.38028
C	5.47117	-2.32567	-2.41675
H	3.98000	-3.75510	-3.03478
H	6.72396	-0.75516	-1.62684
H	6.27837	-2.80646	-2.96214
C	1.84326	1.34447	-1.02579
C	2.46119	1.56402	-2.25385
C	2.25223	2.79830	-2.88979
H	3.08900	0.80875	-2.70650
C	1.48687	3.77151	-2.27817
H	2.71152	2.99333	-3.85516
H	1.31970	4.74859	-2.71601
C	-2.31609	0.89334	1.14185
C	-3.36370	0.89481	2.03111
C	-3.42173	1.91613	3.01877
H	-4.12530	0.12890	1.97882
C	-1.40716	2.95151	2.11786
C	-2.48358	2.91167	3.07331
H	-4.23880	1.90703	3.73567
H	-2.51858	3.70738	3.80774
N	1.04619	2.27012	-0.44648
C	0.00909	-1.47716	2.16152
O	-0.01240	-1.41906	3.31195
C	0.91028	3.47254	-1.02524
O	0.20504	4.41742	-0.41286
O	-0.54324	3.85249	2.04132
N	-1.37321	1.88284	1.22849
H	-0.01861	4.16284	0.53469
C	0.10459	-3.50464	0.06705
O	0.15357	-4.65303	-0.07209
H	-0.54094	1.87118	0.61330

1 High Layer (BP86/aug-cc-pVTZ)

Rh	-0.14053	0.13614	0.00000
H	-1.75482	0.18561	0.00000
P	-0.52640	-1.16054	1.90422
P	-0.52640	-1.16054	-1.90422
C	1.78250	0.05408	0.00000
O	2.93765	-0.00740	0.00000
H	0.54243	-1.73449	-2.65392
H	-1.19598	-0.57707	-3.01973
H	-1.32789	-2.34231	-1.86659
H	0.54243	-1.73449	2.65392
H	-1.32789	-2.34231	1.86659
H	-1.19598	-0.57707	3.01973
C	-0.35857	2.02673	0.00000
O	-0.52640	3.17326	0.00000

1 High Layer (B3LYP/SDD-6-31G(d,p))

Rh	-0.17653	0.08691	0.00000
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H	-1.72833	-0.31682	0.00000
P	-0.17653	-1.26918	1.93255
P	-0.17653	-1.26918	-1.93255
C	1.71048	0.56814	0.00000
O	2.82875	0.84463	0.00000
H	1.00216	-1.50463	-2.68379
H	-0.99135	-0.89628	-3.02867
H	-0.60070	-2.62212	-1.88720
H	1.00216	-1.50463	2.68379
H	-0.60070	-2.62212	1.88720
H	-0.99135	-0.89628	3.02867
C	-0.91849	1.85593	0.00000
O	-1.40430	2.90323	0.00000

2 Low Layer (B3LYP/SDD-6-31G(d,p))

Rh	0.01141	-0.78970	-0.32940
P	-2.24008	-0.40408	0.03252
P	2.26826	-0.42408	0.00812
C	3.57766	-1.48189	-0.76418
C	4.88185	-1.56948	-0.25010
C	3.24486	-2.23752	-1.89960
C	5.83351	-2.38060	-0.87038
H	5.15455	-1.01151	0.63953
C	4.19961	-3.04376	-2.52012
H	2.23590	-2.19807	-2.29485
C	5.49576	-3.11680	-2.00744
H	6.83780	-2.43988	-0.46045
H	3.92576	-3.62092	-3.39849
H	6.23693	-3.75026	-2.48630
C	2.88157	-0.21303	1.74101
C	3.77156	0.80317	2.11870
C	2.45491	-1.13627	2.70787
C	4.22321	0.89362	3.43786
H	4.11231	1.52991	1.38816
C	2.92059	-1.05430	4.01917
H	1.73997	-1.90519	2.43269
C	3.80308	-0.03636	4.38863
H	4.90226	1.69356	3.71883
H	2.58224	-1.77697	4.75614
H	4.15433	0.03559	5.41395
C	-3.20075	-1.73040	0.89106
C	-2.51237	-2.68922	1.65021
C	-4.60067	-1.81252	0.80214
C	-3.20884	-3.69935	2.31620
H	-1.42982	-2.63579	1.70845
C	-5.29413	-2.82310	1.46883
H	-5.14930	-1.08931	0.20689
C	-4.59983	-3.76814	2.22774
H	-2.66218	-4.43643	2.89769
H	-6.37655	-2.87452	1.39129
H	-5.14112	-4.55749	2.74173

C	-2.44360	1.09792	1.10928
C	-3.32615	1.14090	2.18365
C	-1.74900	3.27165	1.45873
C	-3.39368	2.32897	2.92991
H	-3.93925	0.28636	2.43935
C	-2.60956	3.40735	2.57323
H	-4.06490	2.39896	3.78166
H	-2.62681	4.34737	3.11261
C	-3.31430	-0.02826	-1.42547
C	-3.41750	-0.99976	-2.43533
C	-4.20744	-0.77363	-3.56056
H	-2.87578	-1.93724	-2.34127
C	-4.89750	0.43338	-3.70083
H	-4.27718	-1.53573	-4.33144
H	-5.50667	0.61398	-4.58186
C	2.60346	1.25013	-0.73709
C	3.75105	1.62285	-1.38979
C	3.83702	2.93724	-1.93039
H	4.56861	0.92224	-1.49679
C	1.59497	3.46056	-1.10316
C	2.80879	3.82711	-1.79540
H	4.74042	3.23206	-2.45823
H	2.84966	4.83110	-2.20076
C	0.01159	-0.75969	-2.23891
O	-0.00318	-0.76878	-3.39744
C	-4.79493	1.40705	-2.70804
O	0.61964	4.21453	-0.94237
N	1.57681	2.15321	-0.61754
C	-4.01110	1.17866	-1.57368
H	-3.93968	1.94748	-0.81267
H	-5.32405	2.35010	-2.81175
N	-1.65832	2.13722	0.75413
O	-1.00858	4.32127	1.12144
H	-0.46025	4.15074	0.30301
H	-0.05993	-0.85105	1.29309
H	0.68208	1.83183	-0.22837

2 High Layer (BP86/aug-cc-pVTZ)

Rh	0.00000	0.00000	0.19720
H	0.00000	0.00000	1.84276
P	0.00000	2.22799	0.59031
H	0.00000	3.21806	-0.43676
H	-1.06699	2.77446	1.35917
H	1.06699	2.77446	1.35917
P	0.00000	-2.22799	0.59031
H	0.00000	-3.21806	-0.43676
H	1.06699	-2.77446	1.35917
H	-1.06699	-2.77446	1.35917
C	0.00000	0.00000	-1.69265
O	0.00000	0.00000	-2.85417

2 High Layer (B3LYP/SDD-6-31G(d,p))

Rh	0.00000	0.00000	0.20004
H	0.00000	0.00000	1.83735
P	0.00000	2.25322	0.59324
H	0.00000	3.23271	-0.43059
H	-1.06347	2.78775	1.35633
H	1.06347	2.78775	1.35633
P	0.00000	-2.25322	0.59324
H	0.00000	-3.23271	-0.43059
H	1.06347	-2.78775	1.35633
H	-1.06347	-2.78775	1.35633
C	0.00000	0.00000	-1.71065
O	0.00000	0.00000	-2.86708

TS-1prolinear Low Layer (B3LYP/SDD-6-31G(d,p))

C	-0.24517900	-3.48376300	1.05522600
Rh	0.01137900	-1.06517900	0.00666900
H	-0.09681900	-0.74685600	1.58384500
C	0.47369000	-3.89527100	-0.01123600
P	-2.12753600	-0.19081900	0.14855500
P	2.14444800	-0.18913300	0.22468500
C	3.62026200	-1.31109600	0.09001700
C	4.63473200	-1.36425700	1.05680300
C	3.67438800	-2.21006300	-0.99128400
C	5.67841400	-2.28725600	0.94198300
H	4.61611300	-0.68553800	1.90226200
C	4.72635800	-3.11619400	-1.11411100
H	2.89024200	-2.19637800	-1.74276500
C	5.73108000	-3.16085400	-0.14325300
H	6.45292400	-2.31627200	1.70332800
H	4.75664900	-3.79343200	-1.96304900
H	6.54507400	-3.87446200	-0.23230800
C	2.57791500	0.87473800	1.68342600
C	3.56650900	1.87006900	1.59653500
C	1.93710300	0.66929800	2.91278100
C	3.89854800	2.64083900	2.71078800
H	4.07854000	2.04756100	0.65605200
C	2.27879000	1.43308500	4.03046200
H	1.15566000	-0.07990600	2.98307900
C	3.25701300	2.42276300	3.93173400
H	4.65758800	3.41294900	2.62288500
H	1.77005600	1.26029200	4.97458700
H	3.51470900	3.02505400	4.79824100
C	-3.11766300	-0.11473200	-1.41565900
C	-3.76358100	1.04505900	-1.86706200
C	-3.23652900	-1.29064400	-2.17488700
C	-4.50431100	1.02809600	-3.05172400
H	-3.68505200	1.96788900	-1.30429200
C	-3.98687900	-1.30987100	-3.34928200
H	-2.73386800	-2.19553900	-1.84492100
C	-4.62051200	-0.14702100	-3.79375800

H	-4.98928800	1.93857200	-3.39221200
H	-4.06735800	-2.22935400	-3.92218300
H	-5.19598400	-0.15675900	-4.71501100
C	-3.33159900	-0.99620300	1.31564300
C	-2.85694200	-1.53657600	2.52219600
C	-4.70733700	-1.07361000	1.04339300
C	-3.73185600	-2.12832500	3.43424500
H	-1.79470800	-1.49142600	2.73945800
C	-5.58045000	-1.67560500	1.95170300
H	-5.10123000	-0.66176000	0.12049000
C	-5.09667100	-2.20335000	3.14975600
H	-3.34471700	-2.53827400	4.36306200
H	-6.64092800	-1.72891800	1.72130600
H	-5.77733600	-2.67205900	3.85487000
C	-2.15798400	1.58284300	0.72662800
C	-2.93921000	2.00919400	1.79659900
C	-2.89053000	3.36742100	2.15122900
H	-3.56918600	1.31715800	2.33925800
C	-2.11038800	4.23861000	1.41935100
H	-3.47763400	3.73143700	2.99026200
H	-2.04948300	5.29822400	1.63897400
C	2.47225800	1.00660300	-1.16888800
C	3.60845000	1.05099600	-1.93956900
C	3.69128300	2.00570100	-2.99061100
H	4.42147000	0.36348000	-1.75086500
C	1.49315400	2.88868600	-2.39991100
C	2.67746800	2.89253200	-3.22265500
H	4.58265500	2.02889900	-3.61257200
H	2.71712500	3.63279600	-4.01275100
N	-1.36742000	2.41832700	0.01729500
C	0.09304300	-1.31595700	-1.88897800
O	0.16690300	-1.47273800	-3.03566900
C	-1.36906700	3.72113300	0.33160400
O	-0.65222300	4.57643800	-0.38687100
O	0.54643900	3.69012000	-2.52230100
N	1.45987300	1.89530500	-1.42281800
H	-1.32382800	-3.60447300	1.09156400
H	-0.25895200	4.14573800	-1.20573700
H	0.57355300	1.81867000	-0.90372700
H	1.55931900	-3.83023500	0.03315800
H	0.24261400	-3.14958100	1.96324500
C	-0.10597700	-4.57141500	-1.22291800
H	0.25191400	-4.12680200	-2.15723700
H	0.19117700	-5.62812400	-1.24091000
H	-1.19961600	-4.52984500	-1.21860500

TS-1probranched Low Layer (B3LYP/SDD-6-31G(d,p))

C	-0.41749900	-4.08726700	-0.56975900
Rh	0.01188100	-0.91917900	-0.18481800
H	-0.07559800	-0.80180900	1.42617600
C	0.28588200	-3.72876300	0.51567600

P	-2.12881500	-0.09305600	0.10726900
P	2.20859800	-0.28631200	0.11724100
C	3.60386200	-1.44710000	-0.28177200
C	4.78351500	-1.52634000	0.47385500
C	3.44539500	-2.31370600	-1.37747900
C	5.78106000	-2.44482800	0.13702400
H	4.92714500	-0.87295600	1.32743200
C	4.44840200	-3.21964200	-1.72040100
H	2.53230700	-2.27684800	-1.96368300
C	5.61867500	-3.29008100	-0.96080900
H	6.68635100	-2.49621100	0.73545300
H	4.31097400	-3.87650100	-2.57458800
H	6.39576400	-4.00319500	-1.22056300
C	2.73114400	0.43789600	1.74171900
C	3.65279000	1.49377000	1.82882100
C	2.21896400	-0.10999100	2.92710800
C	4.04601100	1.99172400	3.07255300
H	4.06606800	1.93248400	0.92621600
C	2.62531900	0.37800700	4.16916100
H	1.48349900	-0.90559800	2.87018600
C	3.53632800	1.43311100	4.24534100
H	4.75023700	2.81733300	3.12175600
H	2.21845400	-0.05833600	5.07695900
H	3.84198300	1.82217200	5.21236300
C	-3.15059700	0.25681600	-1.39719800
C	-3.80799900	1.47640200	-1.61497600
C	-3.28241100	-0.76001300	-2.35674200
C	-4.57503500	1.67199300	-2.76620500
H	-3.71874400	2.28093300	-0.89401800
C	-4.05737000	-0.56809900	-3.49930100
H	-2.76889600	-1.70580300	-2.21032800
C	-4.70414200	0.65199800	-3.70876100
H	-5.06972200	2.62621800	-2.92383300
H	-4.14659500	-1.36673900	-4.23024600
H	-5.29943900	0.80772100	-4.60392900
C	-3.31105700	-1.07292700	1.15282600
C	-2.80138400	-1.86630100	2.19347500
C	-4.69992700	-1.04618500	0.94667100
C	-3.65703000	-2.60523100	3.01211800
H	-1.72827600	-1.90025300	2.35123900
C	-5.55409900	-1.79247000	1.76090000
H	-5.11771500	-0.44173700	0.14840400
C	-5.03610100	-2.57286600	2.79588400
H	-3.24480700	-3.21201100	3.81375600
H	-6.62582400	-1.76217000	1.58492600
H	-5.70216000	-3.15409100	3.42735500
C	-2.10128500	1.56231300	0.96358600
C	-2.86626000	1.83399700	2.09366100
C	-2.77272300	3.11556800	2.66107900
H	-3.51589700	1.08262700	2.52280100
C	-1.96341100	4.06674800	2.07450800

H	-3.34627300	3.35905100	3.55151300
H	-1.86586100	5.07397700	2.46276800
C	2.56694600	1.12728800	-1.04207000
C	3.70041900	1.26362100	-1.80475700
C	3.81425700	2.38485600	-2.67314200
H	4.48715500	0.52361200	-1.74668500
C	1.64847100	3.22651500	-1.91744500
C	2.83222600	3.33338200	-2.73556600
H	4.70289200	2.48533600	-3.29124000
H	2.89553800	4.19811500	-3.38527100
N	-1.28557100	2.47412000	0.39096200
C	0.06109800	-0.99819600	-2.09602400
O	0.09802800	-1.06051700	-3.25330000
C	-1.23965000	3.70664200	0.91377000
O	-0.48975700	4.64040800	0.34085900
O	0.72847700	4.06606600	-1.89569800
N	1.58546900	2.08119100	-1.12528900
H	0.09234800	-4.12235900	-1.53270400
H	-0.09644900	4.32702100	-0.52827400
H	0.69680500	1.93535400	-0.62679100
H	-0.17150100	-3.70725600	1.50088300
H	1.34828700	-3.52002200	0.46113400
C	-1.86045500	-4.50204100	-0.57168300
H	-2.44267700	-3.92752600	-1.30166500
H	-1.95762300	-5.55755100	-0.85780900
H	-2.32040300	-4.36785700	0.41099500

TS-1 High Layer (BP86/aug-cc-pVTZ)

C	-1.91361	2.57561	0.39455
Rh	0.15383	-0.26635	-0.20067
H	0.13742	-0.09303	-1.83433
C	-0.67627	2.73187	-0.09058
P	-1.78613	-1.33333	-0.69933
P	2.32232	0.23913	-0.57129
C	0.22784	-0.58606	1.66272
O	0.29542	-0.82098	2.79879
H	-2.11352	2.57759	1.46717
H	-0.47882	2.74750	-1.16286
H	0.17573	2.90044	0.56896
H	-2.77215	2.43290	-0.26389
H	3.31036	0.23697	0.45841
H	2.70039	1.48877	-1.15067
H	3.03403	-0.58239	-1.49045
H	-1.69591	-2.47031	-1.55187
H	-2.63286	-1.92864	0.28327
H	-2.82111	-0.67193	-1.42460

TS-1 High Layer (BP86/aug-cc-pVTZ)

C	-1.16631	2.79843	0.22824
Rh	0.06384	-0.28707	-0.19345
H	0.07573	-0.16704	-1.82338

C	0.12013	2.88307	-0.12004
P	-2.07723	-0.95627	-0.66190
P	2.31504	-0.32243	-0.57899
C	0.06799	-0.52498	1.70348
O	0.07558	-0.68243	2.85006
H	-1.47585	2.75932	1.26889
H	0.42654	2.93030	-1.16057
H	0.90901	2.92941	0.62521
H	-1.95610	2.76876	-0.51720
H	3.27387	-0.48998	0.45201
H	2.95500	0.76657	-1.22298
H	2.80513	-1.33334	-1.43708
H	-2.22800	-2.09084	-1.49202
H	-3.00614	-1.34770	0.33540
H	-2.95440	-0.10643	-1.38040

3prolinear Low Layer (B3LYP/SDD-6-31G(d,p))

C	-0.74774800	-3.56038200	-0.01688000
Rh	0.07898700	-1.51165300	-0.16931300
H	0.07722100	-1.59142900	1.43011200
C	0.65392200	-3.69423800	0.01906000
P	-1.96773700	-0.29062800	0.11446800
P	1.98117800	-0.17461300	0.19653200
C	3.60008500	-1.06158800	0.37023700
C	4.38192900	-0.98189200	1.53144100
C	4.02552500	-1.90729800	-0.66938700
C	5.56144800	-1.72283700	1.64598400
H	4.07549300	-0.34136600	2.35073400
C	5.21386300	-2.62833100	-0.56246300
H	3.42398800	-1.99858200	-1.56839700
C	5.98468900	-2.54155700	0.59992100
H	6.15122300	-1.65134800	2.55553200
H	5.53143300	-3.26622200	-1.38246000
H	6.90490400	-3.11163300	0.68869100
C	2.01533500	1.00137400	1.63110100
C	2.87147500	2.11635800	1.64059600
C	1.19690800	0.77004200	2.74472500
C	2.90180600	2.97812000	2.73622500
H	3.51809500	2.31306300	0.79084700
C	1.23502000	1.62904300	3.84529200
H	0.52605700	-0.08196900	2.74009200
C	2.08413500	2.73542800	3.84245500
H	3.56325400	3.83962800	2.72453000
H	0.59274300	1.43573200	4.69966800
H	2.10733700	3.40849100	4.69478400
C	-2.98665900	-0.09936500	-1.42387100
C	-3.58205300	1.10557700	-1.82396700
C	-3.18267000	-1.24237400	-2.21779700
C	-4.34663300	1.16511500	-2.99206700
H	-3.44562000	2.00513400	-1.23614000
C	-3.95659400	-1.18397100	-3.37554100

H	-2.72477700	-2.18236900	-1.92556300
C	-4.53829700	0.02324200	-3.76921500
H	-4.79100800	2.11005000	-3.29156300
H	-4.09667600	-2.07943700	-3.97441700
H	-5.13244600	0.07333200	-4.67716700
C	-3.18598200	-1.09348800	1.26810500
C	-4.57161200	-1.03421100	1.04601200
C	-2.72071800	-1.75609100	2.41537000
C	-5.46329900	-1.62088400	1.94581000
H	-4.95844800	-0.52750800	0.16843100
C	-3.61332600	-2.33361400	3.31997700
H	-1.65179600	-1.82642800	2.59012200
C	-4.98798200	-2.27050600	3.08612800
H	-6.53134600	-1.56770600	1.75378900
H	-3.23202400	-2.84187100	4.20133400
H	-5.68315600	-2.72793900	3.78441900
C	-1.93713300	1.45166700	0.78082200
C	-2.61306900	1.83330400	1.93567300
C	-2.52890100	3.17547300	2.34099700
H	-3.19626200	1.11976100	2.50191000
C	-1.82324600	4.08103200	1.57601800
H	-3.03688500	3.50229200	3.24448200
H	-1.74752900	5.13183100	1.83012500
C	2.35544200	1.01521400	-1.19328600
C	3.51548000	1.07130100	-1.92829800
C	3.61123600	2.00581300	-2.99576500
H	4.34140700	0.41338200	-1.69913700
C	1.39375200	2.87091500	-2.47744000
C	2.59148000	2.87237300	-3.27692000
H	4.52194900	2.03339000	-3.58881300
H	2.64662100	3.60272200	-4.07522100
N	-1.20688800	2.32099700	0.04463400
C	0.16036700	-1.47354200	-2.09797000
O	0.24744300	-1.46519400	-3.25060400
C	-1.18400500	3.61322800	0.40493600
O	-0.54413500	4.49987000	-0.34591400
H	-0.24184300	4.11362600	-1.22671200
O	0.44926600	3.67773800	-2.60466100
N	1.33916700	1.88171500	-1.49897800
H	0.44705400	1.84929500	-0.97681000
H	-1.33523900	-3.60620800	0.89353300
H	-1.28110000	-3.86719000	-0.91493100
H	1.12740700	-3.77703800	0.99514000
C	1.41479800	-4.36603900	-1.10296600
H	2.44876100	-4.01954800	-1.16959000
H	1.45268100	-5.45181800	-0.93271200
H	0.93331200	-4.20392900	-2.07300800

3probranched Low Layer (B3LYP/SDD-6-31G(d,p))

C	0.74771500	-3.56016200	-0.00757400
Rh	-0.07922800	-1.51247800	0.15873600

H	-0.07662400	-1.58099000	-1.44115500
C	-0.65387900	-3.69387300	-0.04518100
P	1.96808600	-0.28995600	-0.11516800
P	-1.98122700	-0.17314200	-0.19899300
C	-3.59984200	-1.05916100	-0.38000800
C	-4.38063300	-0.97189000	-1.54138000
C	-4.02613400	-1.91182900	0.65356200
C	-5.55991100	-1.71225400	-1.66196500
H	-4.07355000	-0.32586600	-2.35610900
C	-5.21424200	-2.63233400	0.54073200
H	-3.42545400	-2.00892700	1.55253600
C	-5.98398800	-2.53798800	-0.62177200
H	-6.14883900	-1.63481100	-2.57157700
H	-5.53246900	-3.27569600	1.35619200
H	-6.90401300	-3.10763200	-0.71520000
C	-2.01459300	1.01276600	-1.62538500
C	-2.87130600	2.12736200	-1.62792100
C	-1.19492800	0.78972600	-2.73976700
C	-2.90104600	2.99674700	-2.71751400
H	-3.51884900	2.31778700	-0.77744000
C	-1.23242900	1.65639300	-3.83433800
H	-0.52354800	-0.06188900	-2.74045700
C	-2.08216300	2.76224900	-3.82462300
H	-3.56297300	3.85780200	-2.70042600
H	-0.58918200	1.46939000	-4.68939400
H	-2.10490500	3.44124300	-4.67225000
C	2.98632800	-0.10961700	1.42488400
C	3.58209100	1.09230000	1.83346900
C	3.18152400	-1.25811600	2.21104800
C	4.34626300	1.14349000	3.00221100
H	3.44620900	1.99592300	1.25176600
C	3.95504900	-1.20799700	3.36945100
H	2.72330000	-2.19587500	1.91221400
C	4.53714800	-0.00377900	3.77157900
H	4.79094100	2.08615200	3.30835600
H	4.09449600	-2.10760400	3.96224100
H	5.13100300	0.03983300	4.68006100
C	3.18680000	-1.08455700	-1.27398300
C	2.72194700	-1.73888900	-2.42614700
C	4.57233400	-1.02697700	-1.05087800
C	3.61489100	-2.30997000	-3.33450700
H	1.65308600	-1.80786800	-2.60182400
C	5.46434300	-1.60723800	-1.95450000
H	4.95883800	-0.52662200	-0.16951400
C	4.98944700	-2.24863000	-3.09964200
H	3.23392100	-2.81191500	-4.21962100
H	6.53232000	-1.55550100	-1.76168300
H	5.68488300	-2.70107600	-3.80092000
C	1.93764600	1.45705700	-0.76905300
C	2.61393200	1.84687000	-1.92096100
C	2.53003900	3.19190100	-2.31672500

H	3.19719000	1.13732500	-2.49214700
C	1.82428600	4.09205900	-1.54548700
H	3.03831100	3.52508400	-3.21772400
H	1.74876800	5.14465700	-1.79209700
C	-2.35656200	1.00694600	1.19880000
C	-3.51730700	1.05808000	1.93304900
C	-3.61395100	1.98506700	3.00698600
H	-4.34311400	0.40191100	1.69849100
C	-1.39578300	2.85340100	2.49697600
C	-2.59430500	2.84938700	3.29527300
H	-4.52524900	2.00863800	3.59931200
H	-2.65009300	3.57403900	4.09871100
N	1.20729000	2.32118700	-0.02685800
C	-0.16161000	-1.48755100	2.08767700
O	-0.24908700	-1.48693300	3.24029900
C	1.18469200	3.61593000	-0.37797000
O	0.54455800	4.49729500	0.37890600
O	-0.45116700	3.65890600	2.63106300
N	-1.34043700	1.87111400	1.51156900
H	1.28066900	-3.87305600	0.88861700
H	0.24154500	4.10466800	1.25653300
H	-0.44785600	1.84220900	0.99000300
H	-1.12681800	-3.76996700	-1.02207900
H	1.33573200	-3.59965300	-0.91795600
C	-1.41534800	-4.37337800	1.07180200
H	-2.44934800	-4.02734700	1.14021600
H	-1.45311000	-5.45796100	0.89404900
H	-0.93435100	-4.21791100	2.04316600

3 High Layer (BP86/aug-cc-pVTZ)

C	-0.46506	2.19958	0.70822
Rh	-0.15664	0.13906	0.00000
H	-1.77378	0.08206	0.00000
C	-0.46506	2.19958	-0.70822
P	-0.46506	-1.19337	1.86469
P	-0.46506	-1.19337	-1.86469
C	1.75695	0.20858	0.00000
O	2.91674	0.22179	0.00000
H	0.40658	2.56518	-1.25190
H	-1.40748	2.27635	1.25067
H	0.40658	2.56518	1.25190
H	-1.40748	2.27635	-1.25067
H	0.62015	-1.75940	-2.59998
H	-1.14787	-0.66520	-3.00155
H	-1.23167	-2.39658	-1.79391
H	0.62015	-1.75940	2.59998
H	-1.23167	-2.39658	1.79391
H	-1.14787	-0.66520	3.00155

3 High Layer (B3LYP/SDD-6-31G(d,p))

C	-0.46441	2.20530	0.70468
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Rh	-0.16189	0.12881	0.00000
H	-1.76609	0.08129	0.00000
C	-0.46441	2.20530	-0.70468
P	-0.46441	-1.20300	1.89657
P	-0.46441	-1.20300	-1.89657
C	1.77425	0.23184	0.00000
O	2.92715	0.29141	0.00000
H	0.40454	2.56261	-1.24980
H	-1.40149	2.26997	1.24856
H	0.40454	2.56261	1.24980
H	-1.40149	2.26997	-1.24856
H	0.61710	-1.74274	-2.63986
H	-1.16254	-0.66940	-3.00900
H	-1.21089	-2.40730	-1.82149
H	0.61710	-1.74274	2.63986
H	-1.21089	-2.40730	1.82149
H	-1.16254	-0.66940	3.00900

TS-2prolinear Low Layer (B3LYP/SDD-6-31G(d,p))

C	-0.85037	-3.23992	-1.35304
Rh	0.12449	-1.35009	-0.76389
H	0.11514	-2.18578	0.65329
C	-0.19301	-3.59807	-0.14676
P	-1.94128	-0.24437	-0.02287
P	1.97866	-0.20228	0.05120
C	3.61262	-1.08184	-0.04113
C	4.66090	-0.84651	0.86221
C	3.80358	-2.01674	-1.07055
C	5.87146	-1.53037	0.73478
H	4.53487	-0.13262	1.66916
C	5.01935	-2.68817	-1.20529
H	2.98621	-2.21710	-1.75708
C	6.05517	-2.44914	-0.30008
H	6.67141	-1.34266	1.44555
H	5.15250	-3.40479	-2.01088
H	6.99825	-2.97952	-0.39714
C	1.97102	0.44152	1.78877
C	2.56320	1.66157	2.15203
C	1.37326	-0.34063	2.78817
C	2.55213	2.08756	3.48175
H	3.03552	2.28535	1.39994
C	1.37630	0.07812	4.11858
H	0.89707	-1.27746	2.51482
C	1.96193	1.29634	4.46803
H	3.00537	3.03922	3.74376
H	0.91185	-0.54205	4.88012
H	1.95398	1.62941	5.50184
C	-3.05676	0.41001	-1.35731
C	-4.06648	1.35133	-1.09487
C	-2.91062	-0.06840	-2.66690
C	-4.90061	1.80285	-2.11731

H	-4.20164	1.73679	-0.08935
C	-3.75133	0.37759	-3.68928
H	-2.12880	-0.78650	-2.88674
C	-4.74599	1.31669	-3.41765
H	-5.67014	2.53775	-1.89785
H	-3.61843	-0.00273	-4.69813
H	-5.39413	1.67252	-4.21356
C	-3.06247	-1.42788	0.86933
C	-4.30802	-1.83170	0.36462
C	-2.60287	-2.02628	2.05828
C	-5.07101	-2.79642	1.02941
H	-4.69041	-1.38906	-0.54853
C	-3.37258	-2.97438	2.73110
H	-1.63717	-1.73736	2.46384
C	-4.61062	-3.36760	2.21492
H	-6.03152	-3.09459	0.61819
H	-3.00306	-3.41143	3.65489
H	-5.20706	-4.11343	2.73239
C	-1.93508	1.23189	1.12192
C	-2.64588	1.29772	2.31727
C	-2.59255	2.48979	3.05787
H	-3.23772	0.46007	2.66112
C	-1.87902	3.56722	2.57442
H	-3.13180	2.56906	3.99827
H	-1.82565	4.51721	3.09320
C	2.34922	1.34197	-0.91489
C	3.49671	1.56476	-1.63634
C	3.60076	2.75254	-2.41108
H	4.29977	0.84110	-1.62146
C	1.41439	3.49310	-1.62383
C	2.60130	3.68609	-2.41777
H	4.49898	2.91909	-3.00027
H	2.66234	4.60428	-2.98964
N	-1.19991	2.26867	0.65728
C	0.48423	-0.89083	-2.57009
O	0.71698	-0.65539	-3.68416
C	-1.20347	3.42246	1.34120
O	-0.55125	4.47720	0.86899
H	-0.23297	4.34659	-0.07822
O	0.48820	4.32258	-1.51212
N	1.35043	2.27900	-0.94545
H	0.45876	2.11233	-0.44732
H	-1.93371	-3.15859	-1.35292
H	-0.41009	-3.56111	-2.29337
H	-0.85128	-3.76920	0.70485
C	1.06328	-4.44341	-0.12549
H	1.69632	-4.21855	0.73746
H	0.78745	-5.50533	-0.06636
H	1.65942	-4.29274	-1.02812

TS-2probranched Low Layer (B3LYP/SDD-6-31G(d,p))

C	-0.94540400	-3.43353700	-0.60033300
Rh	0.07608700	-1.45627700	-0.43269100
H	0.08254500	-1.97632700	1.11850200
C	-0.20252100	-3.49657500	0.61130400
P	-1.92124100	-0.16558100	0.09319900
P	2.00047800	-0.26648600	0.13817700
C	3.57230600	-1.24885900	0.24754100
C	4.68748200	-0.82233500	0.98662400
C	3.64301900	-2.46736900	-0.44419200
C	5.84719000	-1.59770900	1.02650000
H	4.65099000	0.11237500	1.53665900
C	4.80705600	-3.23728000	-0.41045400
H	2.77164300	-2.80391800	-0.99931200
C	5.91048700	-2.80489600	0.32688300
H	6.70112100	-1.25837300	1.60612100
H	4.84772500	-4.17717800	-0.95375400
H	6.81387300	-3.40728900	0.36135300
C	2.05246600	0.71782400	1.70849900
C	2.63924600	1.98940600	1.79980400
C	1.50352100	0.14538900	2.86633600
C	2.66926300	2.67144400	3.01844400
H	3.07498500	2.45589400	0.92238300
C	1.54840000	0.81990600	4.08581100
H	1.03535900	-0.83276600	2.80691200
C	2.12748000	2.08825500	4.16394900
H	3.11776900	3.65943500	3.06842900
H	1.12288000	0.35896600	4.97279700
H	2.15223000	2.61991900	5.11076100
C	-3.05341800	0.21296200	-1.33011000
C	-3.98120100	1.26730000	-1.29725500
C	-3.00401200	-0.60060400	-2.47135100
C	-4.82898300	1.50216200	-2.37989100
H	-4.04230300	1.91049600	-0.42540100
C	-3.85923100	-0.37153900	-3.55112500
H	-2.28535900	-1.41156600	-2.51419700
C	-4.77121200	0.68317200	-3.50962700
H	-5.53362100	2.32820000	-2.34081600
H	-3.80205300	-1.01110300	-4.42738200
H	-5.42967900	0.87013500	-4.35318700
C	-3.05204800	-1.07275900	1.25656700
C	-2.55408000	-1.45053700	2.51805900
C	-4.34967800	-1.47799500	0.90866000
C	-3.33427300	-2.18726000	3.40826500
H	-1.54930000	-1.15403800	2.80639000
C	-5.12478200	-2.23271500	1.79416600
H	-4.76229500	-1.20135900	-0.05531400
C	-4.62383400	-2.58674100	3.04623800
H	-2.93330700	-2.45555800	4.38200900
H	-6.12597000	-2.53748800	1.50200400
H	-5.22917400	-3.16983200	3.73427000
C	-1.82718800	1.52661500	0.87828900

C	-2.50955000	1.88314000	2.03821200
C	-2.39546200	3.20550300	2.49721200
H	-3.12482300	1.16637400	2.56546200
C	-1.65091800	4.11895200	1.77969500
H	-2.91126700	3.51212500	3.40346200
H	-1.54955200	5.15650200	2.07583300
C	2.44798500	1.01558200	-1.12740000
C	3.60437800	1.02742200	-1.86827200
C	3.76060400	2.01439300	-2.88001100
H	4.37432100	0.28969200	-1.68938600
C	1.60632600	2.99879500	-2.29588700
C	2.80259900	2.96575000	-3.09882300
H	4.66552800	2.01139200	-3.48233100
H	2.90397000	3.73428200	-3.85573000
N	-1.06168800	2.40349500	0.18757600
C	0.40165800	-1.30916400	-2.30284900
O	0.61210200	-1.23202700	-3.44234500
C	-1.00569500	3.67796400	0.60172300
O	-0.32032900	4.57534900	-0.09567100
H	-0.01372900	4.22691600	-0.98978500
O	0.71454600	3.86820400	-2.37814300
N	1.49070600	1.96556000	-1.37001900
H	0.59183100	1.94472000	-0.85826500
H	0.75135600	-4.01820800	0.62426500
H	-2.02091200	-3.30271500	-0.48703600
H	-0.74996100	-3.55236100	1.54956600
C	-0.54556700	-4.27427600	-1.79856500
H	-0.94735400	-5.29233200	-1.69871900
H	-0.93058200	-3.86565300	-2.73718300
H	0.54248600	-4.35017700	-1.88840200

TS-2 High Layer (BP86/aug-cc-pVTZ)

C	1.58978	-1.57723	-0.54567
Rh	0.04064	-0.09975	-0.12850
H	0.61946	0.40699	-1.59160
C	1.19927	-1.08946	-1.82826
P	1.37554	1.56296	0.88116
P	-1.93095	0.89267	-0.75975
C	-0.75979	-1.11988	1.24975
O	-1.27734	-1.72963	2.09552
H	2.57546	-1.31591	-0.15684
H	1.20977	-2.54496	-0.21979
H	1.94073	-0.55354	-2.42671
H	0.48480	-1.65548	-2.42618
H	1.43026	1.66457	2.30548
H	2.79938	1.62965	0.71486
H	1.18529	2.96811	0.67780
H	-2.14814	2.30503	-0.66830
H	-3.16865	0.52254	-0.15605
H	-2.38301	0.78359	-2.11048

TS-2 High Layer (B3LYP/6-31G(d,p))

C	1.57223	-1.58157	-0.62728
Rh	0.02554	-0.09684	-0.13643
H	0.51497	0.40147	-1.62692
C	1.18307	-1.06535	-1.88988
P	1.39012	1.62473	0.82342
P	-2.02793	0.81982	-0.69979
C	-0.63667	-1.11811	1.33005
O	-1.04335	-1.73564	2.22247
H	2.55342	-1.33115	-0.23314
H	1.18247	-2.54490	-0.31582
H	1.90932	-0.49760	-2.46704
H	0.46371	-1.60678	-2.49582
H	1.51205	1.72084	2.23467
H	2.79068	1.71619	0.57625
H	1.15318	3.01390	0.62684
H	-2.27782	2.21886	-0.65186
H	-3.20549	0.43756	-0.01070
H	-2.54362	0.63647	-2.00869

4prolinear Low Layer (B3LYP/SDD-6-31G(d,p))

C	-1.64834600	-2.72108000	-1.34690100
Rh	-0.03280500	-1.40994500	-0.75754400
H	-0.59371700	-4.52894000	-0.76762000
C	-1.54511000	-4.02682200	-0.54764700
P	-1.76999700	0.02572300	0.06793700
P	1.92145000	-0.35130600	0.05060600
C	3.41754200	-1.42879000	0.24130900
C	4.66505800	-0.89598500	0.61145900
C	3.29144400	-2.81719300	0.09793000
C	5.76424500	-1.73137500	0.79957500
H	4.77784800	0.17396900	0.75649700
C	4.39272700	-3.65457200	0.29610400
H	2.32693500	-3.24063500	-0.16160300
C	5.63052000	-3.11386500	0.64004700
H	6.72362800	-1.30476300	1.07823500
H	4.27789500	-4.72830100	0.17978700
H	6.48750600	-3.76407600	0.79097400
C	1.95561700	0.50821500	1.69256500
C	2.51510800	1.77332500	1.91905200
C	1.43038300	-0.20450100	2.78268800
C	2.54159700	2.31403000	3.20693600
H	2.92595300	2.34922600	1.09666300
C	1.46860800	0.33131400	4.06900800
H	0.99973900	-1.18991500	2.62210200
C	2.02226100	1.59544700	4.28371000
H	2.97084000	3.29929400	3.36433700
H	1.06345400	-0.23609000	4.90212300
H	2.04699700	2.01768100	5.28407500
C	-2.76466000	0.72932800	-1.32591800
C	-3.77243100	1.68177900	-1.09685900

C	-2.48369200	0.34274200	-2.64348000
C	-4.49505200	2.21773600	-2.16197400
H	-3.98822400	2.01419300	-0.08574700
C	-3.20582100	0.88489000	-3.70907300
H	-1.69098500	-0.37626900	-2.82348000
C	-4.21356400	1.81908400	-3.47107600
H	-5.27083900	2.95356700	-1.97012400
H	-2.97355700	0.57851100	-4.72493900
H	-4.77261100	2.24262700	-4.30064400
C	-2.98471200	-0.87770100	1.13620400
C	-4.35221900	-0.98551000	0.84789900
C	-2.48291200	-1.53801300	2.27152100
C	-5.19742900	-1.72293200	1.68148600
H	-4.76212400	-0.49921000	-0.03018500
C	-3.32963500	-2.26126600	3.11075700
H	-1.42238300	-1.48327400	2.50048600
C	-4.69171000	-2.35727600	2.81584100
H	-6.25360300	-1.80005100	1.43925400
H	-2.92415700	-2.75923500	3.98700400
H	-5.35117300	-2.92876500	3.46255900
C	-1.49952100	1.60430700	1.03714700
C	-2.11218800	1.87188700	2.25616000
C	-1.91722600	3.13953400	2.83121200
H	-2.73436400	1.13262900	2.74266200
C	-1.16002700	4.08511300	2.17175200
H	-2.38101000	3.37923000	3.78433600
H	-1.00090000	5.08437600	2.55983900
C	2.49075400	0.95546500	-1.13589600
C	3.57454900	0.85480300	-1.97522500
C	3.79215500	1.88000000	-2.93608400
H	4.24060500	0.00551600	-1.91093200
C	1.85619000	3.11281800	-2.11450700
C	2.97196700	2.97312300	-3.01442300
H	4.63733600	1.79187400	-3.61398100
H	3.12963000	3.77146200	-3.72969700
N	-0.71922200	2.50802800	0.40271900
C	0.86863900	-2.28299500	-2.12913800
O	1.34125200	-2.73676900	-3.08781000
C	-0.57505500	3.73098800	0.93415800
O	0.14192300	4.65098800	0.30307900
H	0.41311800	4.37675500	-0.62983400
O	1.08850200	4.09708900	-2.06463500
N	1.66458400	2.04163700	-1.24789700
H	0.79425800	2.09672900	-0.68649000
H	-2.62696900	-2.26428700	-1.16634900
H	-1.61651000	-2.94393400	-2.42042500
H	-1.53336700	-3.81206000	0.52933600
C	-2.70192400	-4.99872300	-0.84021100
H	-2.60331900	-5.92758700	-0.26546100
H	-3.66683900	-4.54683400	-0.58356200
H	-2.73238200	-5.26426600	-1.90336600

4probranched Low Layer (B3LYP/SDD-6-31G(d,p))

C	-1.09396300	-3.07030900	-1.66372000
Rh	0.08160600	-1.38908200	-0.94035500
H	-0.00449500	-4.14882200	-0.09070600
C	-1.03107500	-4.00488700	-0.45092400
P	-1.79644300	-0.22444200	0.03903800
P	1.92995000	-0.28391200	0.08661100
C	3.46154800	-1.32385700	0.18723800
C	4.60581800	-0.86792600	0.86550200
C	3.47973300	-2.60313800	-0.38582500
C	5.74550100	-1.66604500	0.94710900
H	4.60443600	0.11065800	1.33560100
C	4.62096800	-3.40459600	-0.29659000
H	2.59541300	-2.96874700	-0.89715000
C	5.75549600	-2.93695900	0.36514400
H	6.62369600	-1.29880500	1.47052800
H	4.61809400	-4.39385600	-0.74497700
H	6.64288800	-3.55971200	0.43399300
C	1.86318300	0.35687800	1.82257200
C	2.24543700	1.64787600	2.21086700
C	1.42135700	-0.54397600	2.80623500
C	2.18423300	2.02862300	3.55415700
H	2.58702900	2.36621800	1.47320300
C	1.37248000	-0.16596100	4.14673000
H	1.12474000	-1.55062400	2.52067600
C	1.75198100	1.12463500	4.52400600
H	2.47792800	3.03503600	3.83806000
H	1.03642100	-0.87722800	4.89600000
H	1.70912400	1.42284400	5.56747800
C	-2.82500300	0.59143300	-1.27183900
C	-3.94503300	1.37525800	-0.94545600
C	-2.43277600	0.49867500	-2.61291400
C	-4.67125200	2.02336200	-1.94360700
H	-4.24459200	1.49225900	0.09179900
C	-3.15589100	1.15557100	-3.61124200
H	-1.55113000	-0.08338400	-2.86134100
C	-4.27872100	1.91314200	-3.28008400
H	-5.53601800	2.62420800	-1.67636400
H	-2.83529800	1.07683400	-4.64610700
H	-4.84057000	2.42523400	-4.05611500
C	-2.98807000	-1.22293200	1.05496900
C	-2.47866800	-1.86462300	2.19854700
C	-4.33393400	-1.42874000	0.72087700
C	-3.29556800	-2.66406200	2.99724700
H	-1.43468300	-1.73138800	2.46966100
C	-5.14863200	-2.24266500	1.51276500
H	-4.75256200	-0.95851500	-0.16169400
C	-4.63585500	-2.85807200	2.65406100
H	-2.88296100	-3.14363800	3.88045700
H	-6.18752300	-2.39272200	1.23279500

H	-5.27164200	-3.48848200	3.26888400
C	-1.59425400	1.29526200	1.13201900
C	-2.20465800	1.43412400	2.37409400
C	-2.09415800	2.66783300	3.03697700
H	-2.76788800	0.62355500	2.81499200
C	-1.41895500	3.71109200	2.43980100
H	-2.56099500	2.80354600	4.00896600
H	-1.32830100	4.69052700	2.89464700
C	2.49450900	1.17562100	-0.90561500
C	3.67186700	1.25725600	-1.60908700
C	3.88531600	2.38129700	-2.45377800
H	4.41248600	0.47347300	-1.53116200
C	1.74408700	3.33758600	-1.78508100
C	2.96358500	3.38837400	-2.55045300
H	4.80693400	2.43843300	-3.02732300
H	3.11223000	4.25740600	-3.18016400
N	-0.89004000	2.29756800	0.55819400
C	0.99039000	-1.58745600	-2.54350800
O	1.45061000	-1.58855600	-3.61208100
C	-0.82806600	3.48686100	1.17584500
O	-0.18771400	4.50319800	0.61137800
H	0.10542400	4.32617700	-0.33657900
O	0.87205200	4.23110900	-1.75481200
N	1.57421600	2.18152700	-1.03050000
H	0.65656400	2.10635100	-0.55275000
H	-1.41538700	-5.00429700	-0.71600200
H	-1.63632500	-3.64460800	0.38642900
H	-0.50076600	-3.53180000	-2.45950100
C	-2.51082500	-2.92383300	-2.21302000
H	-2.53976800	-2.29919800	-3.11021800
H	-2.91277300	-3.91157100	-2.49233200
H	-3.20619300	-2.49532500	-1.48632600

4 High Layer (BP86/aug-cc-pVTZ)

Rh	-0.07169	0.06028	-0.03814
P	-2.23799	-0.51048	0.46732
H	-2.67088	-0.47473	1.83187
H	-3.34736	0.22253	-0.05212
H	-2.78042	-1.80473	0.18649
C	-0.46083	1.85629	-0.34383
O	-0.71474	2.95484	-0.62229
P	0.68518	-2.08108	-0.41112
H	1.10104	-2.34847	-1.74637
H	1.87144	-2.54862	0.23166
H	-0.08591	-3.27131	-0.23193
C	2.00814	0.56600	-0.27892
H	2.55497	-0.21105	-0.83955
H	2.10925	1.48274	-0.87413
C	2.63152	0.75391	1.10852
H	2.56227	-0.15398	1.72768
H	3.70451	1.00917	1.03271

H	2.14418	1.56347	1.67048
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4 High Layer (B3LYP/SDD-6-31G(d,p))

Rh	-0.08773	0.06942	-0.09209
P	-2.37020	-0.22839	0.33792
H	-3.23386	0.88809	0.44911
H	-3.20114	-0.97819	-0.53825
H	-2.79560	-0.87438	1.52991
C	-0.17563	1.93245	-0.20394
O	-0.21799	3.08472	-0.29316
P	0.46041	-2.21498	-0.19729
H	0.80755	-2.70786	-1.47685
H	1.62190	-2.64019	0.48902
H	-0.37950	-3.29333	0.18234
C	2.03083	0.32437	-0.40054
H	2.43458	-0.51835	-0.97971
H	2.20666	1.20818	-1.02120
C	2.79250	0.45725	0.92443
H	2.65928	-0.41858	1.57116
H	3.87397	0.57110	0.75677
H	2.45848	1.32812	1.49789

5prolinear Low Layer (B3LYP/SDD-6-31G(d,p))

P	-2.02473700	-0.23535200	-0.03823400
P	2.02818200	0.02881700	-0.00387700
C	3.66895300	-0.72515500	-0.42013800
C	4.80546700	-0.55019800	0.38688700
C	3.78803200	-1.45453600	-1.61184900
C	6.03190200	-1.09626700	0.00710200
H	4.73344600	0.01134000	1.31294700
C	5.01778700	-1.99371500	-1.99385700
H	2.90630900	-1.60639400	-2.22749900
C	6.14068600	-1.81766800	-1.18444100
H	6.90231900	-0.95730800	0.64201300
H	5.09330300	-2.55837100	-2.91858300
H	7.09632200	-2.24363700	-1.47699300
C	2.09596800	0.12654200	1.84629500
C	1.82799400	1.30315800	2.56324700
C	2.34336400	-1.05693900	2.56607400
C	1.80967000	1.29495700	3.95980100
H	1.63415400	2.23690900	2.04884800
C	2.32601000	-1.05979100	3.96070100
H	2.57034700	-1.97716600	2.03811900
C	2.05612800	0.11616000	4.66315900
H	1.60429800	2.21813300	4.49383300
H	2.52695200	-1.98329700	4.49655300
H	2.04251100	0.11379900	5.74916300
C	-3.23359700	0.45782400	-1.26658800
C	-3.23494200	-0.05137100	-2.57547800
C	-4.16921200	1.44898900	-0.93166600
C	-4.14976900	0.41266800	-3.52187200

H	-2.51521000	-0.81485800	-2.85263100
C	-5.07315400	1.92305000	-1.88337000
H	-4.19627400	1.85752200	0.07252800
C	-5.06797600	1.40621700	-3.17966500
H	-4.13475900	0.00396700	-4.52818300
H	-5.78250400	2.69852900	-1.60827400
H	-5.77201900	1.77779700	-3.91863000
C	-2.98331000	-1.63226300	0.71541900
C	-4.09290200	-2.20164900	0.07227400
C	-2.54477900	-2.20537700	1.92331000
C	-4.74910500	-3.30447500	0.62390300
H	-4.45405300	-1.78305300	-0.86030800
C	-3.20936500	-3.29848400	2.47869800
H	-1.68717800	-1.78887300	2.44151100
C	-4.31301300	-3.85457700	1.82900500
H	-5.60802700	-3.72685400	0.11011600
H	-2.85795500	-3.71923000	3.41672000
H	-4.82708900	-4.70950100	2.25873300
C	-2.11378500	1.06855500	1.30222200
C	-2.93446000	0.94782700	2.42097500
C	-2.96761800	2.00327400	3.34500700
H	-3.54240300	0.06653200	2.57230600
C	-2.22400700	3.13989000	3.10788900
H	-3.59242800	1.93060700	4.23127500
H	-2.22725900	3.99532000	3.77338700
C	2.32453400	1.78865600	-0.53675600
C	3.47600300	2.23656800	-1.13802000
C	3.52632800	3.56844000	-1.63132700
H	4.32521800	1.57821800	-1.24865400
C	1.26261800	3.98105000	-0.83452100
C	2.46269000	4.41702600	-1.49725400
H	4.43333900	3.91238100	-2.12174400
H	2.47667700	5.43725800	-1.86095200
N	-1.36094600	2.16942900	1.06964500
C	0.04611300	0.52415100	-2.42529200
O	0.04480200	1.31976100	-3.26024500
C	-1.44236100	3.19605000	1.93203600
O	-0.75873000	4.31185500	1.71006400
O	0.26569300	4.70121000	-0.61702200
N	1.26406300	2.65132000	-0.41685700
Rh	0.10364000	-0.91755600	-1.13429400
C	0.02228300	-2.27312000	-2.45888100
O	-0.05023300	-3.09746900	-3.27137300
C	0.21646000	-2.63885500	0.20751100
H	0.27767900	-2.22286700	1.21861200
H	-0.75240200	-3.13849200	0.12806500
C	1.32599100	-3.67683300	0.01523800
H	1.25517400	-4.12719400	-0.98249100
H	2.31571400	-3.20619600	0.05277800
C	1.26648700	-4.79908100	1.06516500
H	0.30606000	-5.32547700	1.02407800

H	2.06083100	-5.53844200	0.90906100
H	1.37642100	-4.40045400	2.08120300
H	-0.43396700	4.39676800	0.75647700
H	0.36820400	2.32830900	-0.01503000

5probranched Low Layer (B3LYP/SDD-6-31G(d,p))

P	-1.97559800	-0.16449800	0.00623400
P	2.02392000	-0.13939500	0.12895900
C	3.62031900	-1.07833200	0.04660500
C	4.61135300	-0.97773400	1.03475700
C	3.85315400	-1.89859600	-1.06850600
C	5.80889500	-1.68470900	0.90821800
H	4.45133900	-0.34909200	1.90432200
C	5.05566800	-2.59289000	-1.19925000
H	3.08211800	-1.99971400	-1.82590900
C	6.03505900	-2.49039700	-0.20888100
H	6.56523900	-1.60235800	1.68366300
H	5.22077100	-3.22307100	-2.06838000
H	6.96729000	-3.03962400	-0.30494600
C	1.96753500	0.39935100	1.90124900
C	2.36376700	1.66969000	2.34580400
C	1.48855400	-0.52613400	2.84534400
C	2.27605900	2.00760000	3.69865900
H	2.74502800	2.40268700	1.64299000
C	1.41739100	-0.19168200	4.19733500
H	1.17880800	-1.51463500	2.52205100
C	1.80569300	1.07940000	4.62739400
H	2.58127100	2.99818200	4.02334300
H	1.05525400	-0.92343200	4.91406800
H	1.74179500	1.34346200	5.67895300
C	-3.23707800	0.22337200	-1.30200200
C	-3.27514400	-0.57849000	-2.45408300
C	-4.17403300	1.26050600	-1.17255500
C	-4.22992100	-0.35494900	-3.44731500
H	-2.54486700	-1.37336100	-2.57224200
C	-5.11851500	1.49183200	-2.17372900
H	-4.16970700	1.89395600	-0.29230900
C	-5.15113900	0.68448000	-3.31186700
H	-4.24293300	-0.98640800	-4.33107600
H	-5.82877300	2.30623100	-2.06223600
H	-5.88632500	0.86801800	-4.09019700
C	-2.92543700	-1.25611600	1.16454500
C	-4.14780500	-1.84511500	0.80938300
C	-2.37854400	-1.55429700	2.42585900
C	-4.80404900	-2.70946000	1.68893300
H	-4.59368300	-1.62924700	-0.15524300
C	-3.03867100	-2.41192400	3.30504700
H	-1.44491000	-1.09272500	2.73400800
C	-4.25250900	-2.99704300	2.93713500
H	-5.75063100	-3.15418600	1.39514300
H	-2.60367100	-2.62396200	4.27778900

H	-4.76433200	-3.66882800	3.62014300
C	-1.97196200	1.44562600	0.97277500
C	-2.80395000	1.63518900	2.07428500
C	-2.81299200	2.89008500	2.70260900
H	-3.44114300	0.83988400	2.43380100
C	-2.03169300	3.90653400	2.19908600
H	-3.44772000	3.06042500	3.56805500
H	-2.01179700	4.90206600	2.62674400
C	2.53232000	1.42714100	-0.73715000
C	3.74996600	1.62173700	-1.34369600
C	3.96520400	2.80553200	-2.10059800
H	4.52646100	0.87530500	-1.25879100
C	1.72035800	3.58773000	-1.56877900
C	2.99119700	3.75679400	-2.22310900
H	4.92548700	2.94899100	-2.58922800
H	3.12703000	4.66535800	-2.79722000
N	-1.17672200	2.42750800	0.48514700
C	0.02163700	0.24544700	-2.40571200
O	-0.04195500	0.94938300	-3.31673100
C	-1.23311100	3.64100300	1.06283200
O	-0.52022500	4.65048200	0.58707400
O	0.78944700	4.41865300	-1.60202600
N	1.57142800	2.39929300	-0.85757300
Rh	0.08527000	-1.13407300	-1.04452400
C	0.31392700	-2.48074100	-2.34169700
O	0.49938900	-3.28699400	-3.15592800
C	-0.03417500	-2.91062200	0.28507500
H	-0.32394500	-2.45950500	1.23756700
C	1.26973000	-3.68398600	0.49921200
H	1.65650700	-4.10542300	-0.43545000
H	2.06914600	-3.07721800	0.93054500
H	-0.09662200	4.47046200	-0.31300300
H	0.63605800	2.25950300	-0.44186900
H	1.09879300	-4.53121100	1.18277200
C	-1.13876000	-3.89467900	-0.12192700
H	-2.09553600	-3.40620900	-0.31459200
H	-0.86529200	-4.45418600	-1.02357800
H	-1.30445300	-4.63517800	0.67615900

5 High Layer (BP86/aug-cc-pVTZ)

Rh	0.14444	0.13324	-0.00186
P	0.95208	-0.89297	1.95538
P	-0.24182	-1.57221	-1.57874
C	1.86422	0.59122	-0.69811
O	2.90617	0.86743	-1.12062
H	0.81418	-2.23158	-2.27635
H	-1.04151	-1.33138	-2.73807
H	-0.92937	-2.75989	-1.18012
H	2.33614	-0.95442	2.29343
H	0.66247	-2.25787	2.27171
H	0.50930	-0.37366	3.20937

C	-0.55212	1.90054	-0.02973
O	-0.96032	2.98691	-0.03339
C	-1.82090	-0.41180	0.81936
H	-1.92558	0.13113	1.76935
H	-1.77212	-1.48453	1.06627
C	-3.03687	-0.14190	-0.06679
H	-3.14825	0.92609	-0.29950
H	-2.98511	-0.67500	-1.02869
H	-3.96662	-0.47026	0.43042

5 High Layer (B3LYP/SDD-6-31G(d,p))

Rh	0.14308	0.12953	-0.01138
P	1.01648	-0.78159	2.01014
P	-0.24523	-1.66182	-1.53515
C	1.86269	0.60304	-0.76288
O	2.88598	0.88760	-1.21164
H	0.79903	-2.31159	-2.24099
H	-1.09055	-1.47815	-2.65874
H	-0.87835	-2.84041	-1.06248
H	2.39822	-0.78335	2.32475
H	0.77017	-2.12778	2.39134
H	0.57267	-0.20685	3.22737
C	-0.60404	1.88961	-0.10041
O	-1.06136	2.95089	-0.13144
C	-1.79441	-0.40593	0.85653
H	-1.88985	0.15648	1.79153
H	-1.73575	-1.46781	1.12751
C	-3.03695	-0.16976	-0.00603
H	-3.16676	0.88795	-0.25502
H	-3.00040	-0.71887	-0.95416
H	-3.94658	-0.49712	0.51743

5prolinear Low Layer (B3LYP/SDD-6-31G(d,p))

5probranched Low Layer (B3LYP/SDD-6-31G(d,p))

P	-1.95096100	-0.11785300	0.01721600
P	1.99372400	-0.02700100	0.09750500
C	3.60691100	-0.93736400	0.02718500
C	4.60411200	-0.79032100	1.00464200
C	3.84665300	-1.78983900	-1.06287900
C	5.81037600	-1.48432100	0.89433300
H	4.44169200	-0.13423800	1.85310300
C	5.05801300	-2.47285500	-1.17634700
H	3.08053100	-1.92298900	-1.81917800
C	6.04116700	-2.32491300	-0.19608300
H	6.57051800	-1.36407200	1.66111200
H	5.22630500	-3.12791900	-2.02614500
H	6.98042700	-2.86416300	-0.27947200
C	1.95311900	0.54805900	1.85848700
C	2.20244800	1.86533700	2.26904900
C	1.62069400	-0.41025400	2.83294300

C	2.11443700	2.21595400	3.61917700
H	2.46759500	2.62583600	1.54248800
C	1.55222300	-0.06273800	4.18122200
H	1.42660900	-1.43728800	2.53413800
C	1.79286700	1.25558400	4.57782700
H	2.30437500	3.24282400	3.91803800
H	1.30711300	-0.81938400	4.92135600
H	1.72965300	1.53032300	5.62664300
C	-3.31125200	0.18668300	-1.20791000
C	-3.36769300	-0.61444400	-2.35956600
C	-4.30441700	1.15930400	-1.01292900
C	-4.39548500	-0.45178500	-3.28983300
H	-2.59521700	-1.35896900	-2.52734200
C	-5.32312100	1.32941600	-1.95145800
H	-4.28573500	1.78971100	-0.13052300
C	-5.37292700	0.52402900	-3.09053200
H	-4.42186600	-1.08002800	-4.17556200
H	-6.07739000	2.09458800	-1.79105600
H	-6.16573200	0.66023300	-3.82055000
C	-2.73988900	-1.28286400	1.22257500
C	-3.95152900	-1.93859400	0.95990200
C	-2.06468800	-1.57310400	2.42228900
C	-4.47516600	-2.85767400	1.87269700
H	-4.49271800	-1.73002200	0.04351700
C	-2.59392700	-2.48416300	3.33593500
H	-1.13187000	-1.06610300	2.65377800
C	-3.80012600	-3.13363600	3.06159000
H	-5.41586900	-3.35420300	1.65205000
H	-2.06320800	-2.68768500	4.26192600
H	-4.21007900	-3.84694300	3.77071700
C	-1.97176100	1.48489900	0.98063200
C	-2.73185700	1.65044100	2.13567600
C	-2.75225500	2.91522400	2.74501400
H	-3.30352300	0.83038600	2.54835700
C	-2.05286900	3.95735500	2.17494000
H	-3.33186300	3.07356600	3.65050500
H	-2.04865100	4.95874900	2.58930000
C	2.43790800	1.52348500	-0.82700100
C	3.64960000	1.74682500	-1.43541300
C	3.81887200	2.91195600	-2.23167200
H	4.45587600	1.03640500	-1.32116300
C	1.54626900	3.62734400	-1.72145600
C	2.80949100	3.82168900	-2.38373000
H	4.77344900	3.07686800	-2.72473200
H	2.91282500	4.71715600	-2.98459100
N	-1.25299400	2.48969700	0.42906400
C	-0.05803500	0.00321800	-2.58261100
O	-0.08849500	0.61212900	-3.56657900
C	-1.31811400	3.70809400	0.99245600
O	-0.67470600	4.73214300	0.45327000
O	0.58954800	4.42830700	-1.76548500

N	1.43760800	2.44904800	-0.98627900
Rh	0.06504900	-1.08366100	-1.05206700
C	0.51695100	-2.68682000	-1.86264100
O	0.85728700	-3.54078300	-2.59475300
C	-0.00754400	-3.28676400	0.03719600
H	-0.33328300	-2.64931300	0.85822200
C	1.27242200	-4.01286800	0.43688700
H	1.66408000	-4.62251500	-0.38378300
H	2.06302700	-3.32628100	0.74949400
H	-0.27245700	4.52705100	-0.45114000
H	0.50627000	2.28922900	-0.56936900
H	1.06321600	-4.69221600	1.27614100
C	-1.13970700	-4.23729600	-0.33820200
H	-2.05919300	-3.70034100	-0.58145700
H	-0.86876400	-4.86386800	-1.19432500
H	-1.35920000	-4.90608700	0.50627000

TS-3prolinear Low Layer (B3LYP/SDD-6-31G(d,p))

P	-1.94113500	-0.17270400	-0.01985800
P	1.97409500	0.14188700	0.03421500
C	3.61770800	-0.68230600	-0.16569400
C	4.67443900	-0.48662900	0.73865200
C	3.81896000	-1.50739600	-1.28272800
C	5.90674300	-1.10586300	0.52659000
H	4.53568900	0.14763800	1.60830500
C	5.05564900	-2.11989300	-1.49542200
H	2.99674100	-1.66837400	-1.97471600
C	6.09977600	-1.92219200	-0.59060400
H	6.71606700	-0.94972300	1.23417400
H	5.19773100	-2.75697400	-2.36353700
H	7.05959500	-2.40455700	-0.75204000
C	1.89478100	0.42715000	1.86165100
C	1.81563000	1.69601800	2.45271600
C	1.84412300	-0.70821900	2.69150700
C	1.68610100	1.82560900	3.83806800
H	1.85162100	2.59207200	1.84328900
C	1.72279400	-0.57522800	4.07399200
H	1.91994500	-1.70190400	2.25857400
C	1.63934800	0.69429800	4.65174400
H	1.62448800	2.81709400	4.27703900
H	1.69591300	-1.46313600	4.69935900
H	1.54124700	0.79884800	5.72826200
C	-3.26692800	0.28050100	-1.23675100
C	-3.22346900	-0.27232400	-2.52616100
C	-4.33154400	1.13482400	-0.90596100
C	-4.22110000	0.01676700	-3.45934300
H	-2.40557500	-0.92980900	-2.79962000
C	-5.32073400	1.43192100	-1.84361600
H	-4.39099700	1.57346000	0.08443100
C	-5.26923200	0.87331800	-3.12229200
H	-4.16925200	-0.42164400	-4.45174600

H	-6.13191800	2.10216700	-1.57339600
H	-6.03963300	1.10770400	-3.85140600
C	-2.73135400	-1.52597600	0.96812200
C	-3.88124500	-2.20344000	0.53638500
C	-2.10277100	-1.95715500	2.15109200
C	-4.39327700	-3.27619500	1.27121700
H	-4.38289000	-1.89321400	-0.37384100
C	-2.62511600	-3.01694000	2.89121400
H	-1.20668800	-1.45249200	2.50323500
C	-3.77193700	-3.68336500	2.45153100
H	-5.28478600	-3.78796200	0.91975000
H	-2.13203300	-3.32697400	3.80844100
H	-4.17450900	-4.51411400	3.02385000
C	-2.04949600	1.27612000	1.15673700
C	-2.79964000	1.24633300	2.32993800
C	-2.86880900	2.41231500	3.10833300
H	-3.32763100	0.35125900	2.62950600
C	-2.22647300	3.55622300	2.68278400
H	-3.44320800	2.41693000	4.03088400
H	-2.26371700	4.49030900	3.23107300
C	2.31629500	1.82736800	-0.66302200
C	3.50958400	2.20526000	-1.22819800
C	3.59886600	3.47175300	-1.86792200
H	4.36058500	1.53945100	-1.20191100
C	1.28350900	3.96384800	-1.28419300
C	2.53038900	4.32367500	-1.90858800
H	4.53880400	3.76158200	-2.33038800
H	2.57322000	5.29430400	-2.38785800
N	-1.38577300	2.38205000	0.74560600
C	0.31387800	0.13633600	-2.67198200
O	0.38660200	0.76321100	-3.64333200
C	-1.49994100	3.50609500	1.47154200
O	-0.90707700	4.62399700	1.07297200
O	0.27794800	4.69988500	-1.22259000
N	1.25258100	2.69233900	-0.71365700
Rh	0.14507500	-0.95873200	-1.15408900
C	-0.23972200	-2.57557100	-1.97701500
O	-0.53124700	-3.42402100	-2.73839700
C	0.18221600	-3.14914100	-0.13770800
H	0.39489600	-2.55293000	0.75187900
H	-0.80637700	-3.58730200	0.00823700
C	1.26676400	-4.20074100	-0.35624800
H	1.05177100	-4.76722500	-1.26929800
H	2.23449900	-3.71092600	-0.51104900
C	1.37350500	-5.17542700	0.82667100
H	0.42490900	-5.69674300	0.99695400
H	2.14323200	-5.93336500	0.64286000
H	1.63570600	-4.65411800	1.75509500
H	-0.54107200	4.57103700	0.13494800
H	0.33373900	2.41915500	-0.32579200

TS-3probranched Low Layer (B3LYP/SDD-6-31G(d,p))

P	-1.95096100	-0.11785300	0.01721600
P	1.99372400	-0.02700100	0.09750500
C	3.60691100	-0.93736400	0.02718500
C	4.60411200	-0.79032100	1.00464200
C	3.84665300	-1.78983900	-1.06287900
C	5.81037600	-1.48432100	0.89433300
H	4.44169200	-0.13423800	1.85310300
C	5.05801300	-2.47285500	-1.17634700
H	3.08053100	-1.92298900	-1.81917800
C	6.04116700	-2.32491300	-0.19608300
H	6.57051800	-1.36407200	1.66111200
H	5.22630500	-3.12791900	-2.02614500
H	6.98042700	-2.86416300	-0.27947200
C	1.95311900	0.54805900	1.85848700
C	2.20244800	1.86533700	2.26904900
C	1.62069400	-0.41025400	2.83294300
C	2.11443700	2.21595400	3.61917700
H	2.46759500	2.62583600	1.54248800
C	1.55222300	-0.06273800	4.18122200
H	1.42660900	-1.43728800	2.53413800
C	1.79286700	1.25558400	4.57782700
H	2.30437500	3.24282400	3.91803800
H	1.30711300	-0.81938400	4.92135600
H	1.72965300	1.53032300	5.62664300
C	-3.31125200	0.18668300	-1.20791000
C	-3.36769300	-0.61444400	-2.35956600
C	-4.30441700	1.15930400	-1.01292900
C	-4.39548500	-0.45178500	-3.28983300
H	-2.59521700	-1.35896900	-2.52734200
C	-5.32312100	1.32941600	-1.95145800
H	-4.28573500	1.78971100	-0.13052300
C	-5.37292700	0.52402900	-3.09053200
H	-4.42186600	-1.08002800	-4.17556200
H	-6.07739000	2.09458800	-1.79105600
H	-6.16573200	0.66023300	-3.82055000
C	-2.73988900	-1.28286400	1.22257500
C	-3.95152900	-1.93859400	0.95990200
C	-2.06468800	-1.57310400	2.42228900
C	-4.47516600	-2.85767400	1.87269700
H	-4.49271800	-1.73002200	0.04351700
C	-2.59392700	-2.48416300	3.33593500
H	-1.13187000	-1.06610300	2.65377800
C	-3.80012600	-3.13363600	3.06159000
H	-5.41586900	-3.35420300	1.65205000
H	-2.06320800	-2.68768500	4.26192600
H	-4.21007900	-3.84694300	3.77071700
C	-1.97176100	1.48489900	0.98063200
C	-2.73185700	1.65044100	2.13567600
C	-2.75225500	2.91522400	2.74501400
H	-3.30352300	0.83038600	2.54835700

C	-2.05286900	3.95735500	2.17494000
H	-3.33186300	3.07356600	3.65050500
H	-2.04865100	4.95874900	2.58930000
C	2.43790800	1.52348500	-0.82700100
C	3.64960000	1.74682500	-1.43541300
C	3.81887200	2.91195600	-2.23167200
H	4.45587600	1.03640500	-1.32116300
C	1.54626900	3.62734400	-1.72145600
C	2.80949100	3.82168900	-2.38373000
H	4.77344900	3.07686800	-2.72473200
H	2.91282500	4.71715600	-2.98459100
N	-1.25299400	2.48969700	0.42906400
C	-0.05803500	0.00321800	-2.58261100
O	-0.08849500	0.61212900	-3.56657900
C	-1.31811400	3.70809400	0.99245600
O	-0.67470600	4.73214300	0.45327000
O	0.58954800	4.42830700	-1.76548500
N	1.43760800	2.44904800	-0.98627900
Rh	0.06504900	-1.08366100	-1.05206700
C	0.51695100	-2.68682000	-1.86264100
O	0.85728700	-3.54078300	-2.59475300
C	-0.00754400	-3.28676400	0.03719600
H	-0.33328300	-2.64931300	0.85822200
C	1.27242200	-4.01286800	0.43688700
H	1.66408000	-4.62251500	-0.38378300
H	2.06302700	-3.32628100	0.74949400
H	-0.27245700	4.52705100	-0.45114000
H	0.50627000	2.28922900	-0.56936900
H	1.06321600	-4.69221600	1.27614100
C	-1.13970700	-4.23729600	-0.33820200
H	-2.05919300	-3.70034100	-0.58145700
H	-0.86876400	-4.86386800	-1.19432500
H	-1.35920000	-4.90608700	0.50627000

TS-3 High Layer (BP86/aug-cc-pVTZ)

P	-1.01913	-1.07343	1.91107
P	-1.28103	2.01721	-0.03292
C	-1.12912	-0.70140	-1.56796
O	-1.71041	-1.12880	-2.47947
Rh	-0.16576	-0.07598	-0.08771
C	1.47041	-0.92634	-0.34824
O	2.33167	-1.66257	-0.66849
C	1.98692	0.62396	0.72626
H	1.35103	1.34641	1.25507
H	2.44846	-0.01103	1.49115
C	3.00351	1.32785	-0.16169
H	3.64008	0.60930	-0.69563
H	2.51175	1.96428	-0.90936
H	3.66203	1.97012	0.44610
H	-0.28391	-1.17887	3.13599
H	-1.35828	-2.45758	1.85321

H	-2.23670	-0.66912	2.54443
H	-1.73410	2.64444	-1.23054
H	-0.53423	3.13395	0.45529
H	-2.46498	2.29717	0.72238

TS-3 High Layer (B3LYP/SDD-6-31G(d,p))

P	-1.02237	-1.08913	1.95347
P	-1.24687	2.08514	-0.03708
C	-1.17180	-0.71443	-1.55959
O	-1.77015	-1.14570	-2.45166
Rh	-0.16902	-0.07038	-0.09620
C	1.44964	-0.93472	-0.39474
O	2.29631	-1.66883	-0.74230
C	2.00666	0.58157	0.73738
H	1.39708	1.31166	1.27371
H	2.44945	-0.07836	1.48568
C	3.04767	1.27274	-0.13525
H	3.66007	0.54736	-0.67837
H	2.57628	1.93302	-0.86917
H	3.72025	1.88233	0.48206
H	-0.20312	-1.29724	3.09671
H	-1.46408	-2.43131	1.85541
H	-2.14855	-0.62784	2.68905
H	-1.74055	2.67507	-1.22534
H	-0.43716	3.17779	0.36735
H	-2.36739	2.41964	0.77092

6prolinear Low Layer (B3LYP/SDD-6-31G(d,p))

Rh	-0.00454200	0.51404400	-0.80926100
P	2.21546900	0.03230500	-0.23432200
P	-2.22210900	0.03933700	-0.27740400
C	-3.59472600	0.45628000	-1.44304800
C	-4.95215500	0.28607500	-1.11594600
C	-3.26243600	0.97478200	-2.70310700
C	-5.94728400	0.61148800	-2.03705400
H	-5.23105600	-0.09150400	-0.13722500
C	-4.26056100	1.30029000	-3.62436100
H	-2.21823900	1.12796200	-2.95720400
C	-5.60304200	1.11698900	-3.29384300
H	-6.99180100	0.47449300	-1.77206900
H	-3.98614900	1.70061000	-4.59587800
H	-6.38029700	1.37259100	-4.00826800
C	-2.90083300	0.56084800	1.36379400
C	-2.61301700	-0.14977200	2.53877600
C	-3.61533000	1.76677600	1.46183300
C	-3.04807100	0.32495700	3.77662700
H	-2.04315100	-1.07147500	2.50736100
C	-4.04580200	2.23875600	2.70141000
H	-3.84712400	2.33779700	0.56811800
C	-3.76540500	1.51792700	3.86319300
H	-2.81738200	-0.24095500	4.67430600

H	-4.60106600	3.17085400	2.75661100
H	-4.09976800	1.88596300	4.82873900
C	2.91888400	-1.44487100	-1.11019500
C	2.59380500	-2.75579600	-0.72476500
C	3.69988400	-1.25250700	-2.26216800
C	3.06033100	-3.84335400	-1.46547300
H	1.97704300	-2.93285200	0.14851700
C	4.15807800	-2.34378800	-3.00110400
H	3.95866400	-0.24930100	-2.58538100
C	3.84276800	-3.64375200	-2.60350400
H	2.80434200	-4.84973600	-1.14652700
H	4.76270600	-2.17413600	-3.88768800
H	4.20094400	-4.49325600	-3.17810300
C	3.56813800	1.27465300	-0.42925700
C	4.90536800	0.97874500	-0.10903600
C	3.26200200	2.54218400	-0.94158900
C	5.90282600	1.93725000	-0.28042300
H	5.16625500	-0.00445200	0.27067000
C	4.26279700	3.50180500	-1.11754200
H	2.23594100	2.77282600	-1.20863200
C	5.58282400	3.20180100	-0.78378900
H	6.93106200	1.69656000	-0.02566800
H	4.00827000	4.47936300	-1.51670100
H	6.36237900	3.94607600	-0.91933900
C	2.25756900	-0.42539000	1.56658900
C	3.01559400	0.24747000	2.51753900
C	2.89355500	-0.15168200	3.85698600
H	3.66260200	1.06883800	2.24097200
C	2.06356300	-1.20458400	4.19078100
H	3.45801100	0.36369600	4.62922100
H	1.94859800	-1.56020800	5.20811000
C	-2.31270000	-1.82246400	-0.18245400
C	-3.30034800	-2.59942700	-0.73490300
C	-3.21637800	-4.01318100	-0.61160800
H	-4.12335700	-2.14245200	-1.26544100
C	-1.16135100	-3.81102100	0.68617700
C	-2.19198200	-4.60745000	0.07169700
H	-3.98977300	-4.62694200	-1.06626500
H	-2.11171100	-5.68168400	0.18752200
N	1.41701000	-1.43306400	1.88201900
C	0.03374800	-0.47342100	-2.47328100
O	0.06765400	-0.88011300	-3.55621200
C	1.34741400	-1.83904700	3.15472200
O	0.56462300	-2.87427400	3.46269600
H	0.30161400	-3.37008600	2.63341900
O	-0.21510300	-4.26766900	1.35965700
N	-1.27612600	-2.43692900	0.47522800
H	-0.46815500	-1.88304700	0.79265700
C	-0.00161900	1.99785900	0.61740900
C	-0.34191200	3.37182500	-0.02959100
H	-1.43716700	3.46036600	0.02250800

H	-0.09336400	3.36048200	-1.09947900
C	0.30753700	4.56612800	0.68264200
H	0.07246600	4.49702200	1.74931400
H	1.39910500	4.48130900	0.60735800
C	-0.14631500	5.91597200	0.11921600
H	0.33413800	6.74846600	0.64494600
H	0.09916700	6.01094200	-0.94538300
H	-1.23073100	6.04359900	0.21811000
O	0.19935900	1.94699300	1.81768600

6probranched Low Layer (B3LYP/SDD-6-31G(d,p))

Rh	-0.30135500	-1.53817400	-0.12012700
P	-1.72851700	0.45756800	-0.15494500
P	1.94800700	-0.57479600	0.06333400
C	3.29867800	-1.81873700	-0.17169400
C	4.19714400	-2.15386000	0.85138300
C	3.39758700	-2.48868700	-1.40373300
C	5.17338600	-3.13144800	0.64458400
H	4.13712200	-1.65699400	1.81296800
C	4.38306900	-3.45256900	-1.61227300
H	2.70063600	-2.26282400	-2.20412400
C	5.27267700	-3.77944500	-0.58618900
H	5.85722700	-3.38280200	1.45031900
H	4.44505500	-3.95713700	-2.57201500
H	6.03281900	-4.53890900	-0.74453400
C	2.18036100	0.01745400	1.79712300
C	3.21938100	0.88903900	2.16301600
C	1.29119800	-0.43864000	2.78345600
C	3.36185700	1.29984600	3.48832900
H	3.91874700	1.24930000	1.41457600
C	1.44338500	-0.03137100	4.11029200
H	0.47340100	-1.10533200	2.51875600
C	2.47475000	0.83944900	4.46403900
H	4.16381800	1.98128900	3.75690600
H	0.74755900	-0.39092200	4.86256700
H	2.58607000	1.16250700	5.49516700
C	-1.49176400	1.34077400	-1.76163600
C	-1.81226500	2.69713600	-1.93622700
C	-1.00870000	0.61294500	-2.85978900
C	-1.64533900	3.30890100	-3.17843300
H	-2.18537200	3.28131100	-1.10234500
C	-0.84978900	1.22528800	-4.10476700
H	-0.75284300	-0.43431200	-2.72625000
C	-1.16422300	2.57503200	-4.26524200
H	-1.88650800	4.36141500	-3.29470600
H	-0.47482700	0.64709600	-4.94458200
H	-1.03287100	3.05547500	-5.23066000
C	-3.56588800	0.18376900	-0.09139000
C	-4.13119400	-0.48426700	1.01101500
C	-4.41479900	0.59091600	-1.13169200
C	-5.50614000	-0.71310700	1.07750700

H	-3.49689500	-0.84491600	1.81299400
C	-5.78859700	0.34515600	-1.06921400
H	-4.00871000	1.10135100	-1.99722400
C	-6.34054900	-0.30185200	0.03588600
H	-5.92176700	-1.22368800	1.94179000
H	-6.42611300	0.66599600	-1.88834700
H	-7.40950500	-0.48850100	0.08431500
C	-1.50399900	1.84514000	1.08589700
C	-2.36369300	2.05568100	2.15933900
C	-2.06262700	3.09070800	3.05885900
H	-3.24941800	1.45137800	2.29575800
C	-0.96564900	3.89934900	2.83920000
H	-2.71031100	3.26925300	3.91295500
H	-0.71071500	4.73197900	3.48419900
C	2.62288500	0.87245700	-0.90358900
C	3.68502800	0.81795800	-1.77590000
C	4.06214200	1.99646700	-2.47444000
H	4.23086500	-0.10362200	-1.91851600
C	2.34380800	3.27130500	-1.31218500
C	3.42020900	3.18619500	-2.26388700
H	4.89175500	1.94756300	-3.17532500
H	3.70480500	4.10232200	-2.76740300
N	-0.40561000	2.60588500	0.88517300
C	0.14407500	-2.90717600	-1.28547800
O	0.36007300	-3.68206500	-2.12787500
C	-0.16624200	3.64198400	1.70428000
O	0.84834700	4.45909900	1.45030200
O	1.75890000	4.32690600	-0.98766100
N	1.97295900	2.06352900	-0.72875700
H	1.16798900	4.37085900	0.49656700
H	1.12641700	2.13105900	-0.13047700
C	-1.68403600	-2.67180700	0.77590500
C	-2.49140500	-3.85960600	0.22721900
H	-1.71309300	-4.58391400	-0.05812700
C	-3.38785000	-4.49367800	1.29830900
H	-2.81687800	-4.75208500	2.19327300
H	-4.18384800	-3.80391000	1.59675900
O	-1.68455700	-2.39512900	1.96952900
H	-3.85801300	-5.40259200	0.90861000
C	-3.27422300	-3.49740300	-1.04453100
H	-4.09940200	-2.81702800	-0.81420700
H	-2.63253400	-3.01406900	-1.78533300
H	-3.69545500	-4.40248000	-1.49377700

6 High Layer (BP86/aug-cc-pVTZ)

Rh	0.48908	-0.02705	0.03691
P	0.04709	-2.12922	-0.74202
P	0.76986	2.17622	-0.49219
C	2.25148	-0.36866	0.70561
O	3.28411	-0.57202	1.19455
C	-1.51757	0.32887	-0.28669

C	-2.20062	0.49159	1.09513
H	-2.36527	1.57711	1.21467
H	-1.50927	0.19244	1.90014
C	-3.53133	-0.26466	1.18927
H	-4.19250	0.02276	0.36183
H	-3.37417	-1.35147	1.13408
O	-2.17191	0.41353	-1.31239
H	0.29877	3.25877	0.31680
H	0.18780	2.62682	-1.71242
H	2.07911	2.69622	-0.69843
H	-0.65502	-3.13547	-0.00579
H	1.12928	-2.96211	-1.14429
H	-0.73267	-2.22159	-1.93084
H	-4.03843	-0.04639	2.13926

6 High Layer (B3LYP/SDD-6-31G(d,p))

Rh	-0.56268	0.00000	0.02001
P	-0.34967	-2.29966	0.17312
P	-0.34966	2.29968	0.17292
C	-2.45065	0.00000	-0.32193
O	-3.57251	0.00000	-0.60156
C	1.52239	0.00000	0.30133
C	2.43524	0.00000	-0.93723
H	2.15384	0.86887	-1.54833
H	2.15383	-0.86913	-1.54819
C	3.93325	0.00000	-0.62300
H	4.21042	0.87959	-0.03560
H	4.21042	-0.87961	-0.03546
O	2.01487	0.00011	1.41872
H	0.63081	3.00259	-0.56932
H	-0.00859	2.80209	1.45017
H	-1.43303	3.16822	-0.09671
H	0.63070	-3.00265	-0.56916
H	-1.43309	-3.16819	-0.09631
H	-0.00847	-2.80195	1.45038
H	4.52363	-0.00013	-1.54468

6'prolinear Low Layer (B3LYP/SDD-6-31G(d,p))

Rh	-0.00333900	-1.06465200	-1.01644700
P	-2.09773000	-0.24296700	-0.00366400
P	1.93732100	0.18847200	-0.21634300
C	3.52638700	-0.46339700	-0.91438200
C	4.67169500	-0.69121600	-0.13716900
C	3.55721000	-0.81070500	-2.27703700
C	5.82178200	-1.23850200	-0.71267100
H	4.67195000	-0.44910400	0.91917600
C	4.71293600	-1.33520100	-2.85306000
H	2.66676200	-0.68521300	-2.88501200
C	5.84964500	-1.55380300	-2.07039500
H	6.69630100	-1.41576900	-0.09316700
H	4.71869100	-1.58856800	-3.90919100

H	6.74569800	-1.97651200	-2.51534600
C	2.34673800	0.57686700	1.55186600
C	3.32596900	1.53772900	1.86804500
C	1.65597300	-0.05423300	2.59525100
C	3.62015300	1.84033400	3.19565300
H	3.85634300	2.05470300	1.07375500
C	1.95503300	0.25240100	3.92632700
H	0.87217200	-0.76866600	2.38067300
C	2.93665400	1.19377500	4.22931300
H	4.37684800	2.58566500	3.42307800
H	1.40677800	-0.24260600	4.72217500
H	3.16318300	1.43377000	5.26418700
C	-3.04577500	0.91351600	-1.11718000
C	-2.88932200	2.30835700	-1.11074700
C	-3.87493000	0.33642500	-2.09666100
C	-3.56027300	3.10027100	-2.04618900
H	-2.24819100	2.78651200	-0.38150900
C	-4.53731100	1.13137800	-3.03115100
H	-4.01324300	-0.73965800	-2.12757000
C	-4.38504400	2.51896500	-3.00828900
H	-3.42773000	4.17803600	-2.01565300
H	-5.17521900	0.66280200	-3.77546100
H	-4.90225900	3.13876400	-3.73521200
C	-3.40633400	-1.50821900	0.33550600
C	-3.20864600	-2.84598400	-0.02588700
C	-4.64738900	-1.13036900	0.87793200
C	-4.22005500	-3.79123000	0.16240600
H	-2.26177600	-3.14356400	-0.46108300
C	-5.65439400	-2.07471800	1.07136600
H	-4.83007500	-0.09395700	1.14476900
C	-5.44188100	-3.40920800	0.71499200
H	-4.04907400	-4.82496600	-0.12417500
H	-6.60691400	-1.76727800	1.49375000
H	-6.22829300	-4.14405800	0.86258400
C	-1.95144100	0.67846300	1.60773800
C	-2.38958400	0.16387100	2.82432000
C	-2.19898700	0.94230200	3.97657200
H	-2.85616500	-0.81002400	2.87996400
C	-1.62231300	2.19535900	3.88178200
H	-2.52345400	0.56474100	4.94259000
H	-1.48202000	2.84314700	4.73915900
C	1.89998000	1.93667700	-0.85322200
C	2.76896100	2.50623700	-1.75074200
C	2.57066000	3.86531400	-2.12306900
H	3.58791100	1.93104200	-2.16097400
C	0.67393500	4.04715600	-0.60113200
C	1.56536800	4.61793000	-1.57845700
H	3.24660900	4.31439300	-2.84632000
H	1.41108400	5.65887600	-1.83610700
N	-1.32383400	1.87297200	1.51544400
C	-0.25608300	0.15184000	-2.54197400

O	-0.38625700	0.80639500	-3.47904100
C	-1.20676500	2.63850800	2.60905500
O	-0.67333900	3.85306200	2.50026900
O	-0.23007700	4.66257500	0.00263900
N	0.88071900	2.69544300	-0.34326100
H	-0.56200200	4.12151400	1.54147200
C	0.13958000	-2.58008700	-2.16796000
O	0.19949200	-3.45525900	-2.92585200
C	0.22853600	-2.41336700	0.58726200
C	1.36552700	-3.44726300	0.53587300
H	1.05790100	-4.19466700	-0.21113300
H	2.25857600	-2.97435800	0.11025700
C	1.67708100	-4.13002000	1.87167700
H	1.98996100	-3.37100700	2.59944200
H	0.75780300	-4.56959600	2.27214600
C	2.76491000	-5.20080200	1.74118300
H	3.70295300	-4.77489800	1.36634900
H	2.97685400	-5.67140200	2.70714900
H	2.46264900	-5.99255800	1.04582900
O	-0.51074800	-2.39876900	1.55922400
H	0.17589300	2.27614100	0.28601100

6'probranched Low Layer (B3LYP/SDD-6-31G(d,p))

P	-1.95187900	0.06468300	0.03452600
P	2.02515700	-0.08807200	0.12030200
C	3.47928500	-1.22927900	0.09049500
C	4.53369200	-1.11937500	1.01080600
C	3.54385100	-2.21702100	-0.90234600
C	5.62978700	-1.97939600	0.93362300
H	4.49839900	-0.36527200	1.79007200
C	4.64382100	-3.07233700	-0.98141200
H	2.72410500	-2.31550200	-1.60659200
C	5.68782000	-2.95643900	-0.06247800
H	6.43733100	-1.88644500	1.65429200
H	4.67847200	-3.83386900	-1.75515400
H	6.54060400	-3.62703700	-0.11836900
C	2.03320800	0.52373100	1.87605100
C	2.46616400	1.80831500	2.24125100
C	1.58700300	-0.35075800	2.88387900
C	2.44161600	2.21346100	3.57816100
H	2.83051600	2.50369600	1.49384700
C	1.57543000	0.05669900	4.21798300
H	1.25807500	-1.34727600	2.61118600
C	1.99706000	1.34054500	4.57039500
H	2.77729800	3.21315700	3.83882300
H	1.23543600	-0.63456500	4.98433600
H	1.98221200	1.65646300	5.60961800
C	-3.30001100	0.48512900	-1.17225000
C	-3.43320500	-0.29704000	-2.33035700
C	-4.21059500	1.53170000	-0.95765700
C	-4.45474700	-0.04524400	-3.24737900

H	-2.72383600	-1.09813100	-2.51423200
C	-5.22313500	1.79077700	-1.88268400
H	-4.13158500	2.15035300	-0.07033200
C	-5.34967300	1.00288300	-3.02792800
H	-4.54093700	-0.66126000	-4.13787500
H	-5.91242000	2.61173000	-1.70665500
H	-6.13729700	1.20834900	-3.74718600
C	-2.82958600	-0.99370400	1.27324500
C	-4.12590000	-1.48530700	1.06006000
C	-2.16157200	-1.33829400	2.46149000
C	-4.74172100	-2.29823300	2.01552800
H	-4.66176500	-1.23089600	0.15228700
C	-2.78417000	-2.13848200	3.41776900
H	-1.15617500	-0.97415000	2.64303400
C	-4.07590300	-2.62333300	3.19731000
H	-5.74615000	-2.67038100	1.83441400
H	-2.25534500	-2.39105900	4.33230600
H	-4.55741500	-3.25215800	3.94065800
C	-1.79419900	1.68188500	0.97266800
C	-2.54516000	1.92106700	2.12059500
C	-2.46093600	3.18500800	2.72575400
H	-3.18892900	1.15655900	2.53291100
C	-1.66617800	4.15648500	2.15873100
H	-3.03224200	3.39700800	3.62540500
H	-1.57358400	5.15510100	2.56923900
C	2.69581500	1.38786400	-0.78312400
C	3.91670700	1.45869400	-1.40710100
C	4.22898600	2.61252700	-2.17803600
H	4.62000000	0.64208600	-1.32029800
C	2.06941500	3.60617800	-1.63556600
C	3.34650900	3.65095500	-2.29954000
H	5.19201500	2.66351500	-2.67958900
H	3.56206100	4.53634500	-2.88537500
N	-0.98074600	2.61587500	0.42309900
C	-0.07385600	0.68049000	-2.37658100
O	-0.19592800	1.45211600	-3.22022700
C	-0.94291600	3.83625200	0.98591200
O	-0.20404300	4.80445300	0.46443200
O	1.20772300	4.50743100	-1.67380800
N	1.82791700	2.44405300	-0.90709900
Rh	0.00042500	-0.86182400	-1.14046400
C	-0.05743300	-2.61633400	0.02257700
O	0.51093400	-2.68219700	1.10189200
C	-0.77043600	-3.90244300	-0.47953100
H	-1.43588900	-3.62936800	-1.30413700
C	-1.58886000	-4.57193500	0.63385100
H	-0.95142000	-4.79309500	1.49401700
H	-2.40896900	-3.93458200	0.97227700
H	0.22943900	4.58578400	-0.41926500
H	0.89125500	2.38570900	-0.48235200
H	-2.01777100	-5.51218900	0.26981700

C	0.30996700	-4.86978500	-1.00605500
H	0.91823100	-4.42607800	-1.79895900
H	0.97664700	-5.16587800	-0.19013100
H	-0.16048000	-5.77097500	-1.41311600
C	0.10966200	-1.97215200	-2.67655000
O	0.17606200	-2.55114800	-3.68001900

TS-4prolinear Low Layer (B3LYP/SDD-6-31G(d,p))

Rh	-0.02603500	0.79184300	-1.29113500
H	-0.61751600	1.82440500	-2.42344800
H	0.46061200	1.90250500	-2.39882400
P	2.06758800	0.14891100	-0.20546100
P	-1.99737500	-0.15495600	-0.26046000
C	0.09904100	-0.63109900	-2.64489400
O	0.14692200	-1.39357500	-3.50593800
C	-0.14673700	2.41273300	0.02450900
O	0.23404300	2.35049300	1.17990200
C	-0.74256800	3.74222300	-0.48646000
H	-0.13741500	4.05750500	-1.34822800
H	-1.73277200	3.51958600	-0.90775700
C	-0.82456800	4.85623400	0.56064600
H	0.17740300	5.04614400	0.96138200
H	-1.42054500	4.50713600	1.41142000
C	-2.47316700	0.28518000	1.47763200
C	-3.00842800	1.56710800	1.69194000
C	-2.27994800	-0.55487400	2.58269900
C	-3.34900800	1.99271800	2.97370600
H	-3.17141700	2.23584400	0.85211200
C	-2.61792600	-0.12295300	3.86795800
H	-1.86646000	-1.54910800	2.46708300
C	-3.15256700	1.14825300	4.06856200
H	-3.76520700	2.98586400	3.11631100
H	-2.45947200	-0.79064200	4.70969300
H	-3.41412100	1.48051700	5.06896800
C	-3.59432800	0.15209200	-1.15579200
C	-4.83577600	-0.10488800	-0.54703900
C	-3.57437700	0.62688700	-2.47378000
C	-6.02399000	0.10857700	-1.24463700
H	-4.87347200	-0.46821200	0.47486100
C	-4.76567000	0.83705900	-3.17292400
H	-2.62084600	0.84342500	-2.94459500
C	-5.99160600	0.57981300	-2.56002200
H	-6.97545600	-0.09080100	-0.75986900
H	-4.73151900	1.20723500	-4.19354300
H	-6.91854600	0.74861900	-3.10067200
C	-1.97207600	-2.01919100	-0.23711400
C	-2.87205100	-2.82563100	-0.89301400
C	-2.68969100	-4.23429800	-0.85550000
H	-3.70285300	-2.39360000	-1.43198700
C	-0.74548500	-3.97768900	0.58693500
H	-0.18276500	-2.03290000	0.86806500

C	-1.66739700	-4.80343700	-0.14566600
H	-3.39023200	-4.86779900	-1.39352400
H	-1.52190000	-5.87539500	-0.08620800
C	3.44013000	1.39426700	-0.28568400
C	3.22267300	2.66991900	-0.81847400
C	4.73175300	1.06255200	0.16285900
C	4.26316900	3.60028500	-0.89245100
H	2.23773100	2.92841300	-1.18987200
C	5.76938400	1.98993300	0.09045800
H	4.92708400	0.07346200	0.56572200
C	5.53653200	3.26371400	-0.43639400
H	4.07494600	4.58523200	-1.31027200
H	6.76080400	1.71723400	0.44102500
H	6.34649700	3.98531400	-0.49492500
C	2.90210000	-1.31611800	-0.99399200
C	2.75508200	-2.63489300	-0.53821500
C	3.62740400	-1.09054900	-2.17807400
C	3.33408000	-3.69446100	-1.24186500
H	2.18892400	-2.84876200	0.35958000
C	4.20090100	-2.15159900	-2.87714200
H	3.75330300	-0.07975900	-2.55430500
C	4.05812300	-3.45979300	-2.41000000
H	3.21000000	-4.70634700	-0.86675400
H	4.76018700	-1.95339800	-3.78729200
H	4.50490600	-4.28698300	-2.95426400
C	2.01338300	-0.26323300	1.60983400
C	2.60912000	0.51982600	2.59323600
C	1.20419000	-1.76557200	3.18445500
C	2.45562000	0.13089300	3.93133800
H	3.15947900	1.41402500	2.33615100
C	1.76304600	-1.02495100	4.24342100
H	2.89511500	0.73227800	4.72236300
H	1.64305300	-1.38078200	5.25999600
N	1.28895300	-1.36253800	1.90923900
O	0.55494200	-2.89812800	3.46289700
H	0.44864000	-3.45809100	2.63607600
N	-0.92989900	-2.60556600	0.43148500
O	0.17040200	-4.40086500	1.32648200
C	-1.41960200	6.15072600	-0.00320400
H	-1.46826700	6.93307100	0.76184200
H	-0.81893200	6.53822400	-0.83463300
H	-2.43705800	5.99302000	-0.38067100

TS-4probranched Low Layer (B3LYP/SDD-6-31G(d,p))

Rh	0.00950800	-0.78924700	-1.29697000
P	-1.93885700	0.00166800	-0.06200800
P	2.01455000	-0.15844200	-0.01620500
C	3.49080200	-1.26078200	-0.17281300
C	4.55546500	-1.21091400	0.74111200
C	3.56179700	-2.15320200	-1.25115600
C	5.66901000	-2.03448200	0.57261600

H	4.51413400	-0.53220800	1.58671600
C	4.67845000	-2.97326700	-1.42031100
H	2.73253400	-2.20537800	-1.94974900
C	5.73326700	-2.91645800	-0.50834600
H	6.48470800	-1.98866200	1.28861900
H	4.71819300	-3.66205400	-2.25933200
H	6.59930200	-3.55991100	-0.63518600
C	2.00389300	0.23147300	1.80166100
C	2.41730800	1.46680300	2.32456600
C	1.56978600	-0.76853900	2.69084100
C	2.38565600	1.70192000	3.70152800
H	2.77059700	2.25556400	1.67036000
C	1.55023300	-0.53007100	4.06517500
H	1.25671200	-1.72824900	2.29418500
C	1.95287200	0.70580000	4.57585100
H	2.70578500	2.66631100	4.08554900
H	1.21938500	-1.31609600	4.73858200
H	1.93240600	0.88956400	5.64632100
C	-3.28483600	0.61888300	-1.18596800
C	-4.21131700	1.59454800	-0.78378600
C	-3.40576600	0.06773800	-2.47076500
C	-5.22558800	2.00960300	-1.64742400
H	-4.14326100	2.03610600	0.20455400
C	-4.42805100	0.47518800	-3.32967200
H	-2.68825300	-0.67835100	-2.79780200
C	-5.33820800	1.45073000	-2.92172300
H	-5.92713700	2.77277600	-1.32260300
H	-4.50367000	0.03683800	-4.32072800
H	-6.12708300	1.77740900	-3.59322800
C	-2.83089800	-1.22819600	0.99689100
C	-4.11623900	-1.69657400	0.68767600
C	-2.17861700	-1.74316100	2.13115800
C	-4.73747400	-2.65137200	1.49706900
H	-4.63998300	-1.31365900	-0.18128900
C	-2.80747800	-2.68398000	2.94512000
H	-1.17985000	-1.40263900	2.38248800
C	-4.08893600	-3.14329600	2.62969000
H	-5.73326300	-3.00303600	1.24214500
H	-2.29080300	-3.06644000	3.82068900
H	-4.57522500	-3.88155800	3.26088000
C	-1.77198300	1.46103200	1.10352200
C	-2.48887000	1.52738200	2.29526700
C	-2.39327800	2.69426300	3.07022300
H	-3.11525800	0.70570000	2.61394300
C	-1.62312400	3.74541500	2.62318200
H	-2.93784900	2.77111700	4.00741700
H	-1.52542400	4.67701400	3.16811100
C	2.65890400	1.43136800	-0.72779500
C	3.88066800	1.60038800	-1.33045400
C	4.17463200	2.84620100	-1.95088800
H	4.59848900	0.79190900	-1.34142400

C	1.99760200	3.72814300	-1.29595600
C	3.27458600	3.87639600	-1.94535000
H	5.13778800	2.97561700	-2.43794000
H	3.47668200	4.83222400	-2.41353400
N	-0.98175200	2.47195300	0.66935700
C	0.01022600	0.79280700	-2.47576400
O	-0.04474300	1.57078500	-3.32193600
C	-0.93413200	3.60097500	1.39648400
O	-0.21659700	4.63902700	0.99104700
O	1.12451400	4.61595500	-1.21760900
N	1.77143200	2.47807200	-0.72530200
C	-0.03262000	-2.66265300	-0.38092300
C	-0.76919400	-3.84509200	-1.08023600
C	-1.37806300	-4.81607800	-0.05963600
H	-0.60348000	-5.20812700	0.60468300
H	-2.13526100	-4.32588400	0.55731600
O	0.55563800	-2.91144800	0.66173600
H	-0.52746600	-1.61413600	-2.60823600
H	0.50375700	-1.67394700	-2.59441200
H	0.18653100	4.54041600	0.07269800
H	0.83372200	2.35312200	-0.31413000
H	-1.85216000	-5.65834500	-0.57582800
H	-1.56555900	-3.42487100	-1.70337900
C	0.23162800	-4.57869600	-1.99467800
H	0.66669200	-3.91540600	-2.74877400
H	1.04858700	-5.00247300	-1.40094100
H	-0.26923100	-5.39870900	-2.52012500

TS4 High Lyer (BP86/aug-cc-pVTZ)

Rh	0.48328	-0.08265	-0.35771
H	0.03363	-0.87071	-1.74694
H	0.12023	0.16278	-1.96040
P	0.72849	2.04750	0.62775
H	-0.19495	3.06464	0.26137
H	0.59714	2.21652	2.03720
H	1.91796	2.82097	0.47672
P	0.33647	-1.63223	1.39114
H	1.48042	-2.34213	1.85948
H	-0.14071	-1.22188	2.67256
H	-0.51030	-2.77577	1.27873
C	2.36353	-0.33505	-0.75172
O	3.48059	-0.48737	-1.00986
C	-1.57384	0.20655	0.00028
O	-1.98555	0.83023	0.97024
C	-2.58011	-0.39582	-0.99289
H	-2.35730	0.06223	-1.97127
H	-2.31982	-1.45962	-1.11806
C	-4.04827	-0.21184	-0.61002
H	-4.30204	0.85168	-0.51154
H	-4.70238	-0.65480	-1.37426
H	-4.27221	-0.68969	0.35307

TS4 High Layer (B3LYP/SDD-6-31G(d,p))

Rh	0.47866	-0.09649	-0.35557
P	0.76858	2.09227	0.58331
P	0.28812	-1.60242	1.47419
C	2.38402	-0.40307	-0.73332
O	3.48940	-0.58435	-0.99780
C	-1.56634	0.24282	-0.06021
C	-2.58459	-0.46880	-0.96630
H	-2.33111	-1.53652	-0.97815
H	-2.38616	-0.11793	-1.98803
C	-4.04534	-0.24129	-0.57566
H	-4.24944	-0.61861	0.43051
H	-4.29064	0.82382	-0.57877
O	-1.97166	0.98443	0.82155
H	0.15131	0.10420	-1.95563
H	0.04691	-0.92772	-1.70572
H	-0.71210	-2.60484	1.44033
H	1.35751	-2.45385	1.84424
H	-0.01030	-1.13056	2.77784
H	0.58874	2.31402	1.96933
H	1.98693	2.80563	0.44964
H	-0.09625	3.11111	0.13109
H	-4.71383	-0.75299	-1.27532

7prolinear Low Layer (B3LYP/SDD-6-31G(d,p))

P	1.85943300	-0.25227800	-0.06083300
P	-1.99428200	0.30949300	-0.05851600
C	-3.40726400	1.49375900	-0.19530400
C	-4.47892800	1.44572600	0.71189900
C	-3.43618100	2.43863200	-1.23001900
C	-5.55674000	2.32101600	0.58002000
H	-4.47103400	0.72764600	1.52525600
C	-4.51656800	3.31305800	-1.35983300
H	-2.60674400	2.49250100	-1.92657000
C	-5.57799000	3.25697200	-0.45624800
H	-6.37722900	2.27366600	1.29035700
H	-4.52160500	4.04292100	-2.16422300
H	-6.41572800	3.94149700	-0.55492500
C	-1.97689600	-0.06193700	1.75948800
C	-2.42601100	-1.27370800	2.30576300
C	-1.50788300	0.94239500	2.62560500
C	-2.39617800	-1.48199200	3.68712500
H	-2.80289500	-2.06462700	1.66746000
C	-1.48914300	0.73011000	4.00398000
H	-1.17244200	1.88635700	2.20854300
C	-1.92880900	-0.48248300	4.53956900
H	-2.74425700	-2.42815100	4.09141300
H	-1.13138000	1.51819800	4.66087500
H	-1.91052300	-0.64546900	5.61344300
C	3.07613900	-1.15399200	-1.13595300

C	3.31625700	-0.70562900	-2.44443900
C	3.79908600	-2.26189800	-0.66329000
C	4.25260100	-1.34672600	-3.25753300
H	2.76655200	0.14662400	-2.82833600
C	4.72780600	-2.90653400	-1.48071800
H	3.64026800	-2.62807100	0.34491700
C	4.95767100	-2.45158200	-2.78006700
H	4.42107500	-0.98480600	-4.26769900
H	5.27009400	-3.76712800	-1.09959900
H	5.67884900	-2.95685800	-3.41605900
C	2.93144100	0.92658500	0.88059800
C	4.28851100	1.11505600	0.58133200
C	2.35062300	1.69699400	1.90343200
C	5.04700300	2.05207800	1.28789500
H	4.75831700	0.53166000	-0.20265800
C	3.11383800	2.62200500	2.61498400
H	1.30019400	1.57478200	2.14433400
C	4.46418300	2.80528700	2.30656300
H	6.09617600	2.18730500	1.04074200
H	2.64949900	3.20597400	3.40440600
H	5.05562100	3.53217000	2.85582000
C	1.49576100	-1.57497900	1.20743900
C	2.11223700	-1.60699800	2.45355600
C	1.86177400	-2.70724700	3.29057900
H	2.77969100	-0.81530900	2.76551400
C	1.04637800	-3.72824300	2.85135500
H	2.32560900	-2.75978500	4.27178100
H	0.83655900	-4.60957100	3.44607300
C	-2.73063400	-1.23817200	-0.77556500
C	-3.94877900	-1.31952900	-1.40330300
C	-4.32053000	-2.54383700	-2.02536300
H	-4.60521200	-0.46097400	-1.43228000
C	-2.24013200	-3.58680600	-1.29880600
C	-3.50431100	-3.64097600	-1.98683000
H	-5.27767600	-2.60261700	-2.53713900
H	-3.77034500	-4.58411800	-2.44881300
N	0.65945800	-2.54931800	0.77948900
C	-0.13797900	-0.61788700	-2.67755800
O	-0.21922900	-1.26332000	-3.62609300
C	0.46185800	-3.61750100	1.56819700
O	-0.31113700	-4.61634200	1.16553000
O	-1.45204400	-4.54545500	-1.16320700
N	-1.92155500	-2.34549800	-0.75452800
Rh	0.06462900	0.82459700	-1.34843700
H	1.19727800	1.36762200	-2.28881400
C	0.24844300	2.68755300	-0.44239700
O	-0.43519700	3.01283400	0.52126200
C	1.22562400	3.71499200	-1.02835400
H	0.95164700	3.83503700	-2.08544600
H	2.21858700	3.24579100	-1.04276600
C	1.26763500	5.06575200	-0.30886400

H	0.26006400	5.49654300	-0.28969700
H	1.54627900	4.90661100	0.73897000
C	2.24540400	6.04710800	-0.96371700
H	3.26805200	5.65176400	-0.96158100
H	1.97279200	6.24656300	-2.00686000
H	2.26042200	7.00733900	-0.43660300
H	-0.80067000	1.71411100	-2.32616300
H	-0.62715600	-4.53179600	0.21154800
H	-0.98464800	-2.29503700	-0.32124300

7probranched Low Layer (B3LYP/SDD-6-31G(d,p))

P	1.90722900	0.02609300	-0.04621000
P	-1.98889900	0.11274300	-0.01736900
C	-3.53175800	1.12615000	-0.11981300
C	-4.57215000	0.95265700	0.80803800
C	-3.69254500	2.06095300	-1.15178000
C	-5.74749800	1.69595700	0.70011700
H	-4.46444500	0.23990100	1.61890900
C	-4.87042200	2.80242700	-1.25805700
H	-2.88989200	2.21210500	-1.86514500
C	-5.89944300	2.62281400	-0.33321000
H	-6.54221200	1.55252800	1.42667400
H	-4.97746000	3.52611100	-2.06093000
H	-6.81345000	3.20439700	-0.41353800
C	-1.90842700	-0.28874800	1.79245700
C	-2.19294800	-1.55898700	2.31583300
C	-1.56156800	0.74905600	2.67661900
C	-2.12123700	-1.79035800	3.69198300
H	-2.47339500	-2.37805600	1.66355900
C	-1.50070400	0.51249500	4.04981000
H	-1.35293800	1.73614900	2.27742700
C	-1.77594300	-0.75722500	4.56228700
H	-2.34125500	-2.78141200	4.07828100
H	-1.23914800	1.32609400	4.72080400
H	-1.72508900	-0.93872800	5.63212800
C	3.22769500	-0.68004000	-1.14581200
C	3.41702700	-0.15398800	-2.43362200
C	4.07752200	-1.71083800	-0.71134200
C	4.42725100	-0.64387600	-3.26322700
H	2.76854300	0.63902000	-2.78931700
C	5.08052800	-2.20528600	-1.54557900
H	3.96051900	-2.13391500	0.28012200
C	5.25902700	-1.67384700	-2.82373500
H	4.55442900	-0.22390900	-4.25684100
H	5.72126400	-3.00892100	-1.19403800
H	6.03853000	-2.06228300	-3.47287000
C	2.82731200	1.29043200	0.94364500
C	4.15607800	1.64456800	0.66857600
C	2.15739600	1.93998500	1.99517800
C	4.80080500	2.62377600	1.42862300
H	4.69323700	1.15608200	-0.13673600

C	2.80942800	2.90508400	2.76216600
H	1.12586200	1.68912200	2.21758100
C	4.13265100	3.25281200	2.47864000
H	5.82927500	2.88818200	1.19959800
H	2.27886600	3.39216100	3.57527700
H	4.63659000	4.01091400	3.07122300
C	1.71282700	-1.37506000	1.17655100
C	2.33993400	-1.37333400	2.41798400
C	2.23254200	-2.52229800	3.21915100
H	2.90960000	-0.51756900	2.75336900
C	1.54246500	-3.61947700	2.75040300
H	2.70864700	-2.54996100	4.19548500
H	1.44609700	-4.53879700	3.31609700
C	-2.55003800	-1.49524600	-0.76065600
C	-3.76116700	-1.70646900	-1.37149500
C	-3.99570400	-2.95070700	-2.02026200
H	-4.51555300	-0.93208500	-1.36809600
C	-1.79131900	-3.75340200	-1.35695500
C	-3.05309900	-3.94206300	-2.02523600
H	-4.94858000	-3.11129100	-2.51799500
H	-3.21255900	-4.89811000	-2.50923900
N	0.99655200	-2.42935300	0.72049300
C	-0.02828600	-0.56273400	-2.65061700
O	-0.01779300	-1.20490300	-3.60492700
C	0.93699600	-3.53849400	1.47478200
O	0.28686600	-4.61069800	1.04483600
O	-0.89032700	-4.61241800	-1.26356000
N	-1.61469700	-2.49814400	-0.78100400
Rh	-0.01772500	0.88820100	-1.31678100
H	1.02914100	1.57577200	-2.25941300
C	-0.07514500	2.75869500	-0.39753500
O	-0.78058200	2.95502500	0.58519100
C	0.72624700	3.95714900	-0.96783900
H	1.72671900	3.57338500	-1.20443700
C	0.84271400	5.10464300	0.04373900
H	-0.14478800	5.49575700	0.30434800
H	1.32433400	4.77414300	0.96766800
H	-1.00906900	1.64376000	-2.28282200
H	-0.04969100	-4.53636800	0.09697200
H	-0.68380800	-2.34582500	-0.35912000
H	1.43723500	5.92235900	-0.37846000
C	0.08654400	4.44872800	-2.28053400
H	0.02453600	3.65217600	-3.02506600
H	-0.92576300	4.82763500	-2.09659400
H	0.67856700	5.26891600	-2.70042300

7 High Layer (BP86/aug-cc-pVTZ)

Rh	0.47594	-0.13758	-0.31088
H	0.07194	-1.50947	-1.00477
H	0.18587	0.40159	-1.78366
P	0.73186	2.12013	0.40009

H	-0.12235	3.07764	-0.20310
H	0.50164	2.49179	1.75529
H	1.96521	2.81809	0.23295
P	0.44963	-1.24216	1.77189
H	1.42104	-2.23815	2.07699
H	0.53225	-0.54677	3.01653
H	-0.69559	-2.02018	2.10451
C	2.30015	-0.50755	-0.85346
O	3.31684	-0.78719	-1.32513
C	-1.59082	0.19521	-0.12064
O	-2.01436	1.13350	0.54767
C	-2.57413	-0.73948	-0.82597
H	-2.29586	-0.72466	-1.89278
H	-2.33154	-1.76509	-0.49905
C	-4.05145	-0.40914	-0.61516
H	-4.28541	0.60297	-0.97105
H	-4.68709	-1.12164	-1.15958
H	-4.32217	-0.44914	0.44849

7 High Layer (B3LYP/SDD-6-31G(d,p))

Rh	0.46958	-0.14438	-0.31763
H	0.07631	-1.50711	-1.00444
H	0.19331	0.38852	-1.77941
P	0.73640	2.15058	0.41116
H	-0.08164	3.10124	-0.22792
H	0.46499	2.51972	1.74837
H	1.97619	2.82575	0.28088
P	0.44303	-1.25659	1.80673
H	1.44394	-2.19832	2.14330
H	0.45321	-0.54482	3.03271
H	-0.67299	-2.07496	2.09472
C	2.32322	-0.51692	-0.86731
O	3.33445	-0.78604	-1.34326
C	-1.58479	0.18801	-0.14023
O	-2.00032	1.13730	0.51130
C	-2.58301	-0.74929	-0.82465
H	-2.32099	-0.75066	-1.89041
H	-2.35821	-1.76849	-0.48208
C	-4.05282	-0.39154	-0.60159
H	-4.27051	0.61705	-0.96329
H	-4.70443	-1.09478	-1.12996
H	-4.31062	-0.41741	0.46105

TS-5prolinear Low Layer (B3LYP/SDD-6-31G(d,p))

P	1.80687600	-0.35797700	-0.10403000
P	-1.97219300	0.36072100	-0.02369500
C	-3.32771000	1.59300700	-0.26655700
C	-4.30386600	1.82586600	0.71389900
C	-3.40240700	2.29279000	-1.48119800
C	-5.32977500	2.74393200	0.48463800
H	-4.26192500	1.29565100	1.65918400

C	-4.43286700	3.20534500	-1.70934300
H	-2.64873900	2.12612500	-2.24423100
C	-5.39673200	3.43529000	-0.72603000
H	-6.07512700	2.91913500	1.25515600
H	-4.47650000	3.74098200	-2.65326200
H	-6.19431200	4.15164100	-0.90114400
C	-1.97333200	0.08404700	1.80488300
C	-2.50082200	-1.06622900	2.40971100
C	-1.41973500	1.09117200	2.61603600
C	-2.46629700	-1.21270000	3.79860900
H	-2.94012800	-1.85501800	1.80920400
C	-1.39966800	0.94266300	4.00272600
H	-1.02629400	1.99163800	2.15422100
C	-1.91751600	-0.21015900	4.59775500
H	-2.87340700	-2.11218900	4.25126500
H	-0.97795700	1.73186900	4.61896600
H	-1.89558900	-0.32487300	5.67777800
C	2.90562100	-1.40136300	-1.18026400
C	3.01612300	-1.12863700	-2.55150000
C	3.66467300	-2.45541300	-0.64316800
C	3.86132500	-1.88682000	-3.36468100
H	2.43897100	-0.32067300	-2.98545000
C	4.50319000	-3.21596800	-1.45748000
H	3.60331900	-2.68737100	0.41476700
C	4.60379700	-2.93470000	-2.82146800
H	3.92879400	-1.66019600	-4.42483100
H	5.07597200	-4.03108800	-1.02436800
H	5.25401500	-3.53081000	-3.45537400
C	3.01495000	0.76742100	0.73910700
C	4.35895200	0.86357900	0.35077900
C	2.54777800	1.60968300	1.76435800
C	5.21511300	1.77650600	0.97352800
H	4.74280600	0.22701600	-0.43867800
C	3.40803800	2.50690700	2.39572700
H	1.50663300	1.56533500	2.06779700
C	4.74533300	2.59646900	1.99892000
H	6.25224100	1.83948700	0.65623000
H	3.03019500	3.14415200	3.19020100
H	5.41289100	3.30244700	2.48447800
C	1.42254400	-1.60048300	1.23950500
C	2.04608700	-1.59505500	2.48305900
C	1.76395300	-2.64538900	3.37240400
H	2.74353100	-0.81468800	2.75459400
C	0.91283800	-3.65954900	2.98739100
H	2.23307500	-2.66679000	4.35235200
H	0.67963400	-4.50467600	3.62442700
C	-2.76229400	-1.18879700	-0.67754900
C	-4.01162900	-1.25451800	-1.24343900
C	-4.44449200	-2.48525200	-1.81023900
H	-4.64640300	-0.37990200	-1.26849100
C	-2.36372900	-3.56426100	-1.13880100

C	-3.65639400	-3.60245300	-1.77363400
H	-5.42548400	-2.53234600	-2.27597900
H	-3.96817600	-4.55194000	-2.19203600
N	0.55214000	-2.56624900	0.86608000
C	-0.43273100	-0.26622000	-2.80758500
O	-0.64812000	-0.81715400	-3.80062500
C	0.32542700	-3.59021700	1.70320200
O	-0.47986300	-4.58129200	1.34586000
O	-1.60466000	-4.54482400	-0.99502200
N	-1.98264700	-2.31505800	-0.65637400
Rh	0.07406800	0.82040100	-1.29520400
H	1.28726600	1.22437400	-2.20827500
C	0.30864600	2.87229500	-0.46724400
O	-0.33333100	3.23642900	0.51242700
C	1.50608600	3.68673000	-0.96095100
H	1.40107200	3.81032900	-2.04666300
H	2.40045400	3.06470700	-0.82457900
C	1.68314500	5.03910700	-0.26416300
H	0.78006700	5.64385400	-0.41036000
H	1.76587000	4.87736100	0.81556700
C	2.91197100	5.79900200	-0.77336400
H	3.83094200	5.22901800	-0.59413900
H	2.84719900	5.99070700	-1.85091100
H	3.01729500	6.76663300	-0.27114200
H	-0.41933900	2.39577400	-1.52167500
H	-0.78806900	-4.52472400	0.38779300
H	-1.02832900	-2.28204100	-0.25684500

TS-5probranched Low Layer (B3LYP/SDD-6-31G(d,p))

P	1.87813500	-0.01576400	-0.11666200
P	-1.97008600	0.08772900	0.05907400
C	-3.50718300	1.10144600	-0.09833100
C	-4.47197300	1.15247500	0.91863600
C	-3.73176900	1.81570200	-1.28593900
C	-5.63398700	1.90771500	0.75230500
H	-4.31598800	0.60821400	1.84370700
C	-4.89758300	2.56392000	-1.45158000
H	-2.98953900	1.78913500	-2.07740000
C	-5.84956100	2.61453800	-0.43160200
H	-6.36930600	1.94358100	1.55103400
H	-5.05682500	3.11245300	-2.37547600
H	-6.75336000	3.20373700	-0.55788000
C	-1.88563100	-0.28249600	1.86913700
C	-2.21634100	-1.53155500	2.41484800
C	-1.47180600	0.75146600	2.72852200
C	-2.12462100	-1.74733900	3.79200300
H	-2.54586800	-2.34397600	1.77676400
C	-1.39422700	0.53169400	4.10365700
H	-1.23351000	1.72593600	2.31351300
C	-1.71480000	-0.71802200	4.63899900
H	-2.37834200	-2.72222900	4.19812500

H	-1.08234600	1.34119300	4.75778500
H	-1.64806000	-0.88732600	5.70996600
C	3.09600200	-0.81316100	-1.27293600
C	3.14973800	-0.42399400	-2.61951300
C	4.00109200	-1.78917900	-0.82162100
C	4.08073900	-0.99266900	-3.49125300
H	2.45974100	0.32557400	-2.98889200
C	4.92573400	-2.36151100	-1.69488200
H	3.98768500	-2.10720100	0.21530400
C	4.96837100	-1.96570100	-3.03308900
H	4.10181100	-0.67849600	-4.53081900
H	5.61144100	-3.11981900	-1.32765500
H	5.68617200	-2.41548200	-3.71309900
C	2.92407600	1.22603400	0.77909500
C	4.24823500	1.50892300	0.41453500
C	2.35178500	1.94049300	1.84679000
C	4.98340900	2.47817500	1.10300900
H	4.71201800	0.97231300	-0.40559500
C	3.09444100	2.89161400	2.54539700
H	1.32262200	1.75052600	2.13467000
C	4.41293900	3.16695700	2.17256600
H	6.00654900	2.68673400	0.80301600
H	2.63870900	3.42537500	3.37461700
H	4.98751500	3.91549500	2.71049800
C	1.72204300	-1.37814800	1.15568800
C	2.36437200	-1.34316900	2.38919500
C	2.26880800	-2.47153500	3.22063000
H	2.93766600	-0.47930000	2.69595900
C	1.57732400	-3.58377100	2.78959700
H	2.75721100	-2.47261100	4.19134900
H	1.49243500	-4.48850500	3.38009900
C	-2.52415900	-1.53037200	-0.66805300
C	-3.76274500	-1.76402500	-1.21284200
C	-4.01141700	-3.01572900	-1.84112400
H	-4.52828700	-1.00179800	-1.17560700
C	-1.76816000	-3.78361200	-1.27325900
C	-3.05580200	-3.99318500	-1.88437400
H	-4.98538900	-3.19348300	-2.28975800
H	-3.22500800	-4.95622800	-2.35096500
N	1.00412000	-2.44647600	0.73917000
C	-0.38627600	-0.16632700	-2.76924500
O	-0.51839900	-0.69470400	-3.78861200
C	0.95800800	-3.53719600	1.51948200
O	0.30933800	-4.62155200	1.11702000
O	-0.85970900	-4.63678500	-1.20144600
N	-1.57634700	-2.51775600	-0.72613400
Rh	-0.04799500	0.93030700	-1.21357200
H	1.06990500	1.56860800	-2.11210900
C	-0.16908000	2.95444600	-0.30411100
O	-0.84857300	3.13634300	0.70010200
C	0.81378900	4.04215000	-0.78691100

H	1.78881500	3.54868700	-0.89075000
C	0.40188000	4.56814800	-2.17561000
H	0.36066400	3.76655300	-2.91746900
H	-0.58253600	5.04940400	-2.13364200
H	-0.81929800	2.39079500	-1.38807800
H	-0.02446700	-4.56266200	0.16776100
H	-0.62910000	-2.35447800	-0.34224700
H	1.12317800	5.31583800	-2.52130100
C	0.92527800	5.18529000	0.22784400
H	1.24171500	4.81960100	1.20708000
H	1.65692000	5.92421700	-0.11579600
H	-0.03783000	5.68862200	0.35612900

TS5 High Layer (BP86/aug-cc-pVTZ))

P	-0.27336	-1.37746	1.69243
P	-0.89467	1.99004	0.64778
C	-2.26118	-0.44594	-0.99143
O	-3.29830	-0.67758	-1.45640
Rh	-0.52400	-0.16880	-0.26426
H	-0.17950	-1.55008	-0.96717
C	1.62834	0.41229	-0.41151
O	1.99497	1.47250	0.09172
C	2.63208	-0.65725	-0.84291
H	2.52521	-0.76107	-1.93679
H	2.29553	-1.62615	-0.44081
C	4.07729	-0.35228	-0.45267
H	4.40953	0.60266	-0.88015
H	4.18844	-0.27595	0.63735
H	0.61352	0.49935	-1.32576
H	4.74740	-1.14560	-0.81179
H	-0.29794	2.34925	1.88955
H	-2.21217	2.45302	0.93348
H	-0.45173	3.11556	-0.09760
H	-0.34764	-0.78626	2.99167
H	0.93172	-2.10395	1.93630
H	-1.15456	-2.46369	1.96865

TS5 High Layer (B3LYP/SDD-6-31G(d,p))

P	-0.40160	-1.43653	1.70872
P	-0.87534	2.02163	0.68999
C	-2.23657	-0.39886	-1.08383
O	-3.23967	-0.59746	-1.61931
Rh	-0.50219	-0.16395	-0.26779
H	-0.15259	-1.52321	-0.98106
C	1.63895	0.37894	-0.36513
O	2.00499	1.42132	0.16164
C	2.64612	-0.69174	-0.78621
H	2.48912	-0.87950	-1.85651
H	2.36374	-1.62938	-0.29077
C	4.09959	-0.32203	-0.48993
H	4.38045	0.60472	-0.99752

H	4.25824	-0.16719	0.58079
H	0.61557	0.50071	-1.31133
H	4.77267	-1.11696	-0.82560
H	-0.30289	2.34870	1.94017
H	-2.18843	2.48160	0.95464
H	-0.41497	3.14211	-0.03187
H	-0.57632	-0.87319	2.99994
H	0.78493	-2.14988	2.01311
H	-1.28801	-2.52595	1.88792

Ethene (BP86/aug-cc-pVTZ)

C	0.00000	0.00000	0.66677
H	0.00000	0.92871	1.24059
H	0.00000	-0.92871	1.24059
C	0.00000	0.00000	-0.66677
H	0.00000	-0.92871	-1.24059
H	0.00000	0.92871	-1.24059

Ethene (B3LYP/ 6-31G(d,p))

C	0.66508	0.00000	0.00291
H	1.23756	0.92364	0.00000
H	1.23842	-0.92303	0.01089
C	-0.66506	0.00000	-0.00291
H	-1.23799	0.92324	-0.01091
H	-1.23813	-0.92341	0.00000

Propene (B3LYP/ 6-31G(d,p))

C	1.28263	0.22048	-0.00241
H	2.24346	-0.28537	0.00068
H	1.30404	1.30790	-0.01051
C	0.13378	-0.45506	0.00325
H	0.16473	-1.54516	0.01117
C	-1.23445	0.16280	-0.00043
H	-1.81010	-0.14397	0.88205
H	-1.18192	1.25556	-0.00927
H	-1.81194	-0.15822	-0.87658

CO (BP86/aug-cc-pVTZ)

C	0.00000	0.00000	-0.65015
O	0.00000	0.00000	0.48761

CO (B3LYP/ 6-31G(d,p))

C	0.00000	0.00000	-0.65025
O	0.00000	0.00000	0.48769

H₂ (BP86/aug-cc-pVTZ)

H	0.00000000	0.00000000	0.37531200 Hatree
H	0.00000000	0.00000000	-0.37531200 Hatree

H₂ (B3LYP/6-31G(d,p))

H	0.00000	0.00000	0.37138
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H	0.00000	0.00000	-0.37138
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n-butanal (B3LYP/6-31G(d,p))

C	1.02088800	0.50282600	-0.14809900
H	0.84205500	0.86959500	-1.16632800
H	0.99998700	1.38533800	0.50490600
C	2.39956500	-0.15888000	-0.07268600
H	2.45824100	-1.02855300	-0.73583100
H	3.18886300	0.53945400	-0.36770900
H	2.61901000	-0.50181600	0.94453500
C	-0.11895200	-0.45289800	0.25119200
H	-0.17944600	-1.31303600	-0.42288600
H	0.07282800	-0.83141200	1.26701000
C	-1.46343900	0.23623200	0.27161200
H	-1.50570400	1.14806700	0.91377200
O	-2.44052500	-0.12891500	-0.34369900

iso-butanal (B3LYP/6-31G(d,p))

C	-0.44605000	1.47220300	0.04184500
H	-0.28265600	1.54267500	1.12158000
H	0.34589800	2.04607800	-0.44560800
C	-0.42790300	0.01263300	-0.41255900
H	-0.59140500	-0.03676400	-1.50238500
C	0.92628700	-0.63644100	-0.19120700
H	0.97315200	-1.71188200	-0.48500800
O	1.90145100	-0.07979800	0.26266600
H	-1.40860100	1.93757000	-0.19059800
C	-1.52408200	-0.84305500	0.25141300
H	-2.51598300	-0.45905700	-0.00343000
H	-1.47533400	-1.88755400	-0.07498300
H	-1.42619300	-0.82472000	1.34215700

propanal (BP86/aug-cc-pVTZ)

C	-0.93182600	0.42421700	0.00015100
O	-1.41833500	-0.69007100	0.00000000
C	0.54742700	0.72545600	0.00000000
H	0.73597000	1.37965100	0.87168200
H	0.73536100	1.37915200	-0.87245800
C	1.45401500	-0.50155900	0.00000000
H	1.27051200	-1.12543500	0.88457900
H	1.26849900	-1.12727200	-0.88275900
H	-1.59257300	1.33102400	0.00039400
H	2.51122500	-0.20523000	-0.00137400

propanal (B3LYP/6-31G(d,p))

C	-0.93113900	0.42531100	0.00011700
O	-1.40350700	-0.69032200	-0.00005200
C	0.54829700	0.73312100	-0.00005500
H	0.74383500	1.37724900	0.87075200
H	0.74364600	1.37694600	-0.87113800
C	1.44007300	-0.50527900	0.00003000

H	1.24726600	-1.12379100	0.88054200
H	1.24667300	-1.12431700	-0.87997800
H	-1.59355600	1.32172000	0.00007500
H	2.49680200	-0.22414900	-0.00039500

Complete Reference 9

Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

Sample kinetic computation input and output

Enthalpy and topology of the reactive cycle file

```

13 species
1  14.83743127
2  22.37160942
3  14.35675135
4  24.81460886
5  14.78681927
6  5.325925143
7  18.03580972
8  8.616465985
9  12.46766476
10 7.999096375
11 15.98614152
12 0.0
13 -2.221248643
25 reactions
1 2
2 1
2 3
3 2
3 4
4 3
4 5
5 4
5 6
6 5

```


6 7
 7 6
 7 8
 8 7
 8 9
 9 8
 9 10
 10 9
 10 11
 11 10
 11 1
 1 12
 12 1
 8 13
 13 8

specify the output reaction

11 1

Gellrich thesis chapter 9.3.2, cycle involving
 the preliminary step and an additional shuffle
 reaction, propene as substrate,
 partial correction of translational DOFs, linear cycle only

Concentration input file

5 reactions involving educt species of constant concentration

1 2 2.91 E

8 9 0.01843 H2

5 6 0.04336 CO

1 12 0.04336 CO

8 13 0.04336 CO

1 3.88d-4 initial catalyst conditions

Output

reaction rates:

2	1	0.7360E+13
11	1	0.7360E+13
12	1	0.4828E+04
1	2	0.4653E+09
3	2	0.8061E+08
2	3	0.7360E+13
4	3	0.7360E+13
3	4	0.2479E+07
5	4	0.4576E+07
4	5	0.7360E+13
6	5	0.1027E+08
5	6	0.3191E+12
7	6	0.7360E+13
6	7	0.1001E+06
8	7	0.1089E+08
7	8	0.7360E+13
9	8	0.7360E+13

13	8	0.1443E+07
8	9	0.5609E+09
10	9	0.1262E+11
9	10	0.7360E+13
11	10	0.7360E+13
10	11	0.8386E+08
1	12	0.3191E+12
8	13	0.3191E+12

k matrix eigenvalues

1	-0.31937451D+12
2	-0.31915947D+12
3	-0.14721079D+14
4	-0.14727443D+14
5	-0.14720805D+14
6	-0.14720808D+14
7	-0.14720801D+14
8	-0.31943385D+12
9	-0.63459533D+10
10	-0.41512976D+08
11	-0.50154599D+05
12	0.00000000D+00
13	-0.85023475D+01

initial conditions fulfilled ?

reaction no, c given, c computed

1	3.8799999999999999E-004	3.8799999999999999E-004
2	0.0000000000000000	-1.44668943950166389E-024
3	0.0000000000000000	7.94668436096376477E-023
4	0.0000000000000000	7.50574996587294847E-027
5	0.0000000000000000	-3.47199772493113484E-025
6	0.0000000000000000	-2.06795153138256919E-024
7	0.0000000000000000	-1.76261108510319825E-030
8	0.0000000000000000	3.23117426778526435E-027
9	0.0000000000000000	0.0000000000000000
10	0.0000000000000000	2.01948391736579022E-028
11	0.0000000000000000	-2.15704153771370416E-031
12	0.0000000000000000	2.71050543121376109E-020
13	0.0000000000000000	8.47032947254300339E-022

concentration limit for infinite t (2 methods):

1	5.79700425201858693E-012	5.79700494800871138E-012
2	3.61051400954530189E-016	3.61051444302473120E-016
3	3.24724578957456735E-011	3.24724617943990161E-011
4	5.50087857719544859E-018	5.50087923763263341E-018
5	1.01524146608681229E-013	1.01524158797701690E-013
6	3.15235945658860348E-009	3.15235983506185558E-009
7	3.74432072949991663E-017	3.74432117904422266E-017
8	2.16282672850855866E-011	2.16282698817820516E-011
9	1.64261970216127704E-015	1.64261989937470691E-015
10	9.54492629430985616E-013	9.54492744027665986E-013

11 5.43775643475741533E-018 5.43775708761613592E-018
12 3.83213046453933831E-004 3.83213092462610788E-004
13 4.78369364741676136E-006 4.78369422174850156E-006

0.10315482049234903 = turnover per s
371.35735377245652 = turnover per hour

12 = most-abundant species

¹ U. Gellrich, J. Huang, W. Seiche, M. Keller, M. Meuwly, B. Breit, *J. Am. Chem. Soc.* **2011**, *133*, 964.