

How phenyl makes a difference: mechanistic insights into ruthenium(II)-catalysed isomerisation of allylic alcohols

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GENERAL CONSIDERATIONS:

All reagents were used as received, complexes **M**₁₀ and [RuCl₂(PPh₃)₃] were purchased from Umicore AG and used as received. Complexes **1**, **14** and **15** have been synthesised according to previously reported procedures.^{1, 2} Compounds **2**, **6**, **9**, **10**, **18**, **19**, **20**, **21**, **22**, **23**, and **24** were purchased from Sigma Aldrich and Alfa Aesar and used as received. Compounds **7** and **8** were synthesised according to reported procedures in the literature.^{3, 4} Compounds **11**, **12**, **13**, **2-d**₁, **25**, **26** and **27** were synthesised *via* reduction of the corresponding aldehyde according to the reported procedure.⁵ Compound **16** was synthesised according to the reported procedure.⁶ Toluene was dispensed from a solvent purification system from Innovative Technology, while 2-methyltetrahydrofuran, cyclopentyl methyl ether and *isobutyl* methyl ketone were dried and degassed as reported in the literature.⁷ Elemental analyses were performed at the London Metropolitan University. Catalyst syntheses were performed in an MBraun glovebox containing dry argon and less than 1 ppm oxygen and water. ¹H, ³¹P{¹H}, and ¹³C{¹H} Nuclear Magnetic Resonance (NMR) spectra were recorded on a Bruker Avance 300 or Bruker Avance II 400 Ultrashield NMR spectrometers.

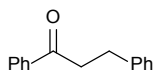
GENERAL PROCEDURE FOR THE OPTIMISATION OF THE ISOMERISATION OF ALLYLIC ALCOHOLS

In a vial fitted with a screw cap, in the glovebox, *trans*-1,3-diphenyl-2-propen-1-ol (**2**) (0.5 mmol), **1** (0.00125 mmol) and base (0.02 mmol) were charged and dissolved in organic solvent (1 mL). The solution was stirred for 1 h. The solvent was removed under vacuum and the crude reaction was analyzed by ¹H NMR spectroscopy.

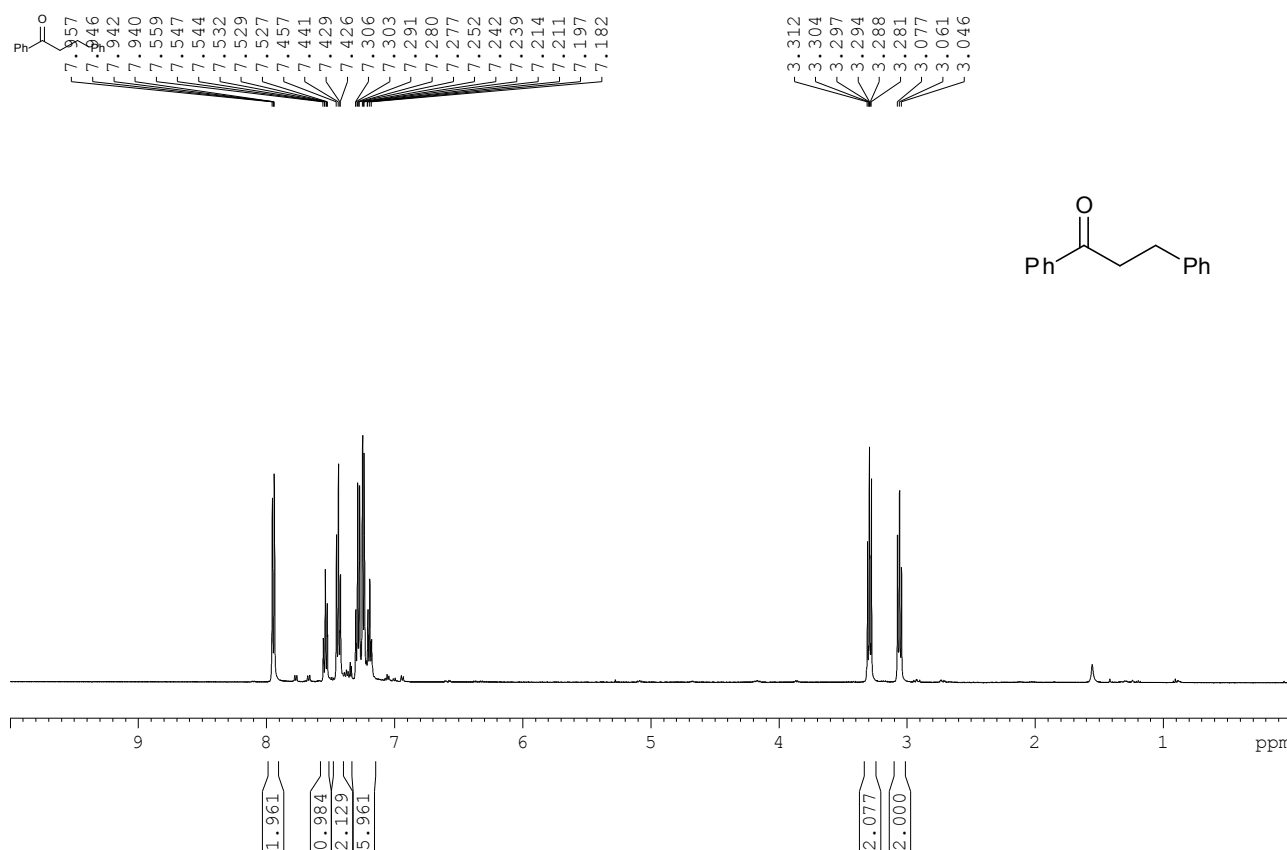
REPRESENTATIVE PROCEDURE FOR ISOMERISATION OF ALLYLIC ALCOHOLS

In a vial fitted with a screw cap, in the glovebox, allylic alcohol (1 mmol), **1** (0.0025 mmol) and NaO^tBu (0.04 mmol) were charged and dissolved in toluene (2 mL). The solution was stirred for 1 h. The solvent was removed under vacuum and the crude reaction was analysed by ¹H NMR spectroscopy. For lower catalyst loadings a stock solution of **1** (2 mg in 2.5 mL) in toluene was used.

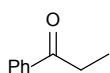
1,3-diphenyl-1,4-propanedione



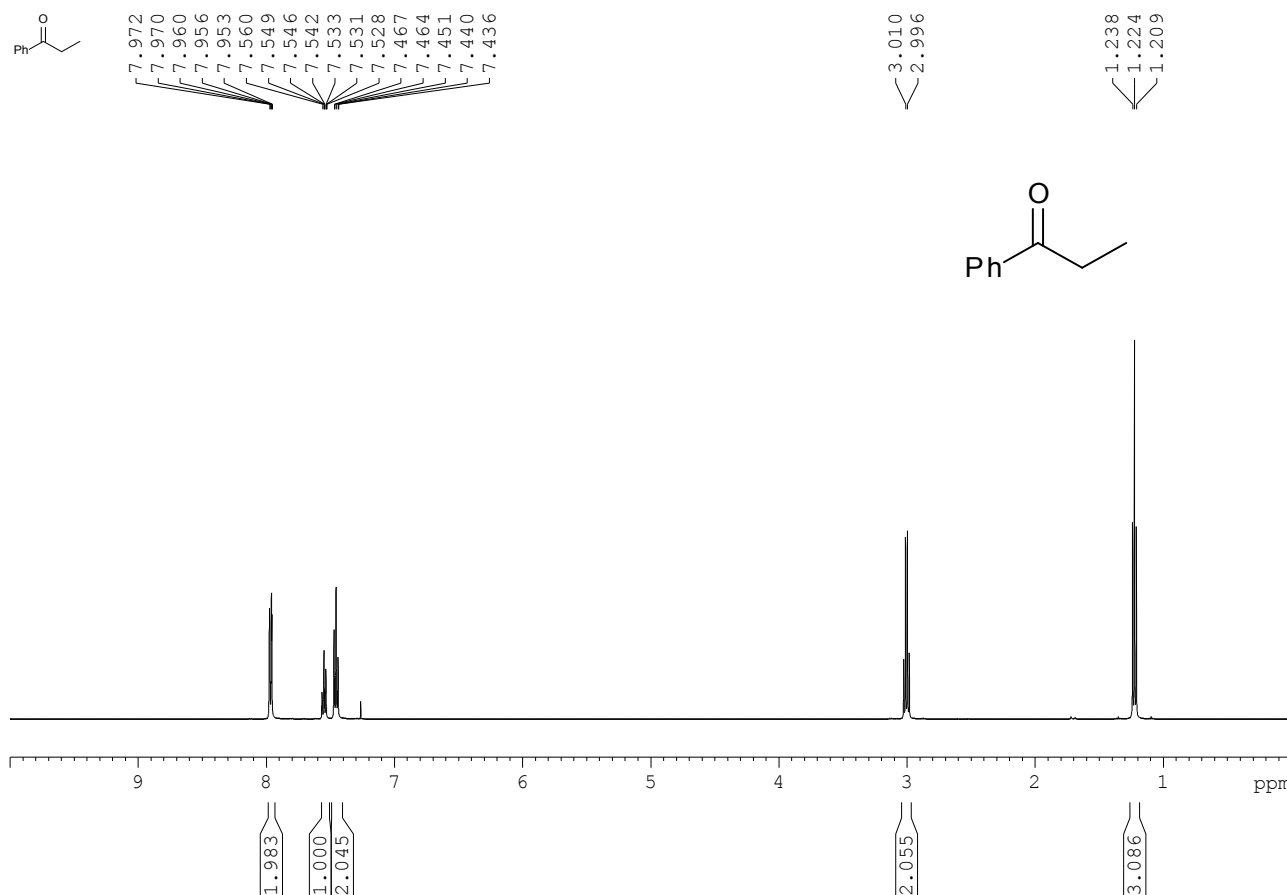
Using the general procedure, *trans*-1,3-diphenyl-2-propen-1-ol (**2**) (210 mg, 1 mmol) was reacted for 1 h to generate the reported compound (204 mg, 97 % yield). Spectroscopic data for the product were in accordance with the literature.⁸



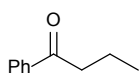
Propiophenone



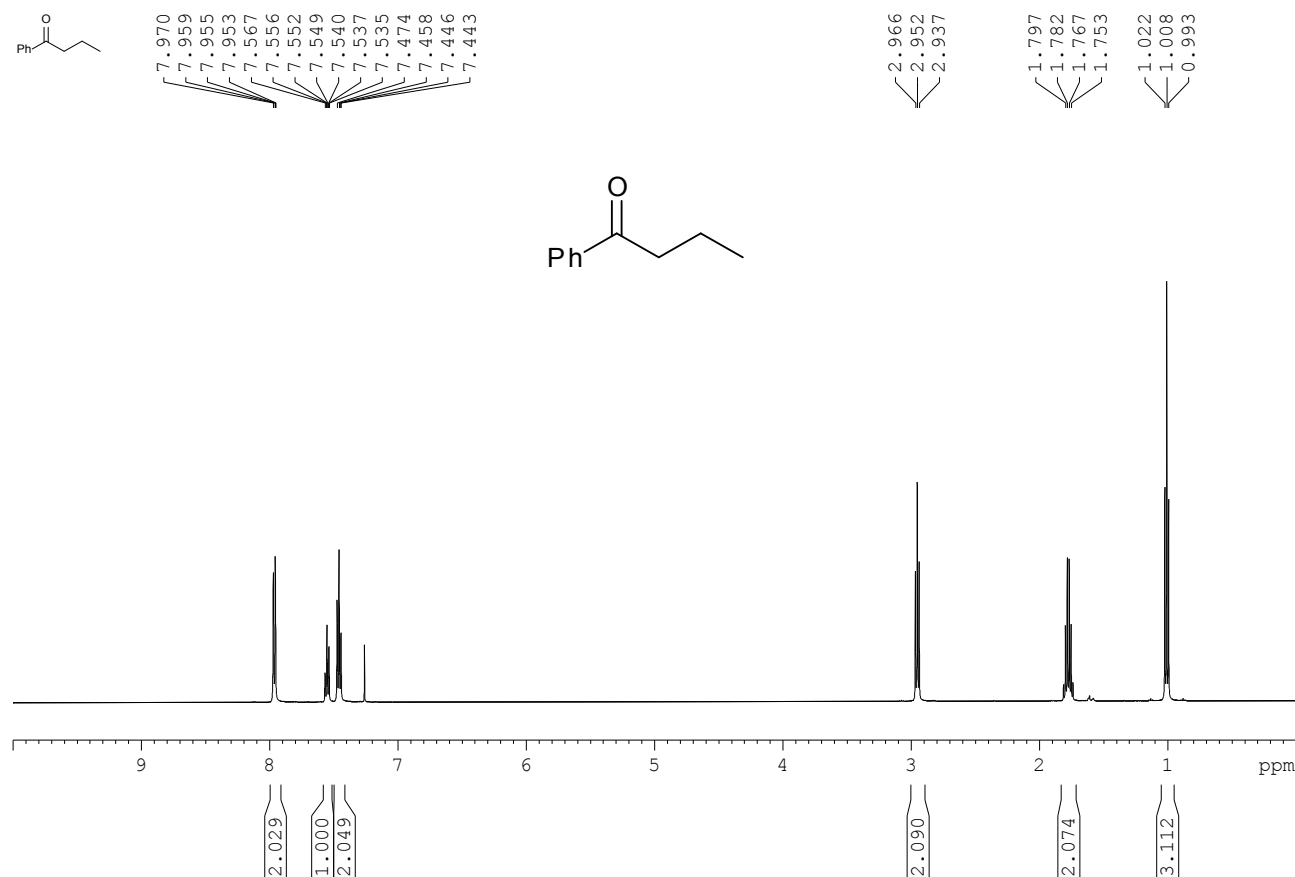
Using the general procedure, 1-phenyl-2-propen-1-ol (**8**) (134 mg, 1 mmol) was reacted for 1 h to generate the reported compound (131 mg, 95 % yield). Spectroscopic data for the product were in accordance with the literature.⁹



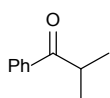
Propyl phenyl ketone



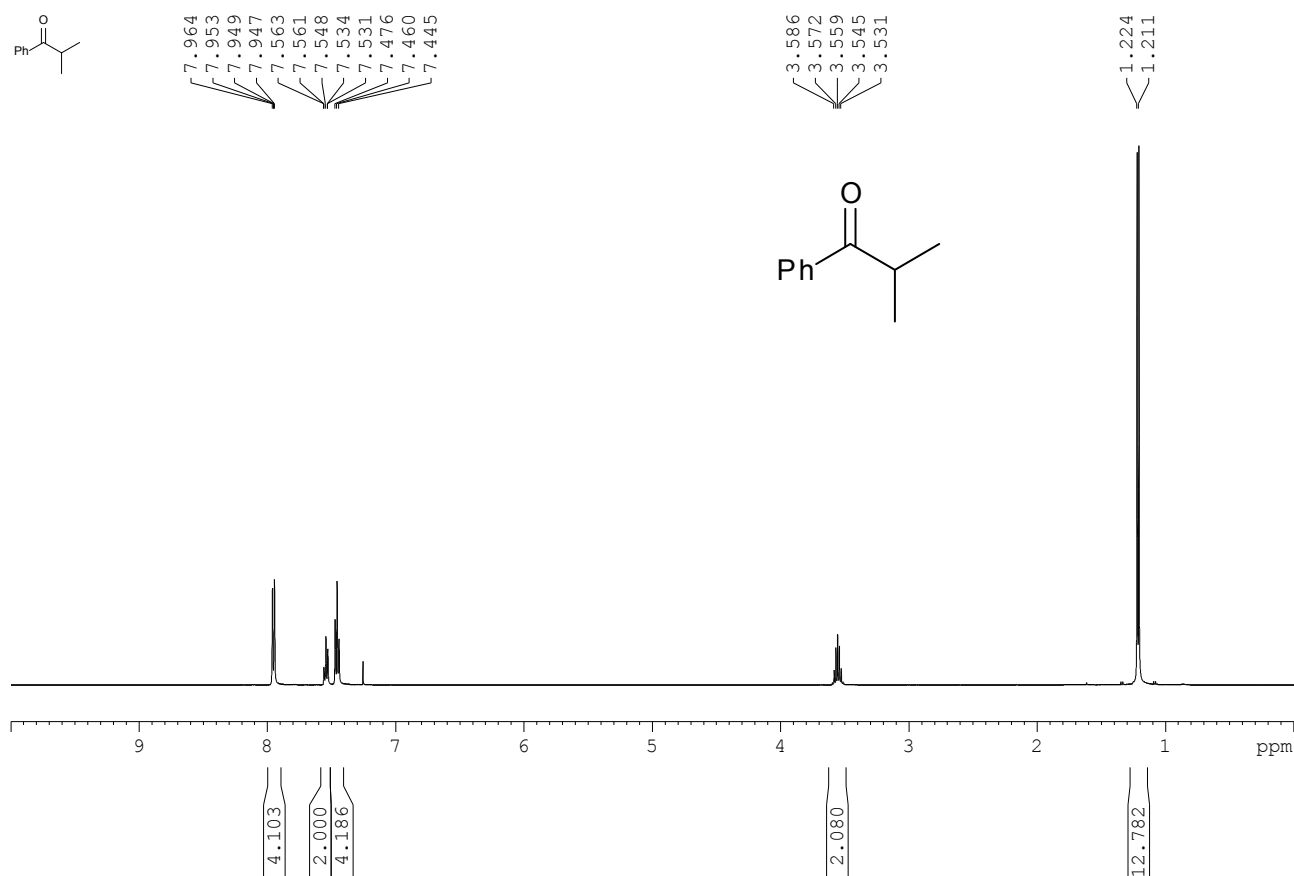
Using the general procedure, trans-1-phenylbut-2-en-1-ol (**9**) (148 mg, 1 mmol) was reacted for 1 h to generate the reported compound (143 mg, 97 % yield). Spectroscopic data for the product were in accordance with the literature.¹⁰



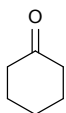
1-phenyl-2-methyl-1-propanone



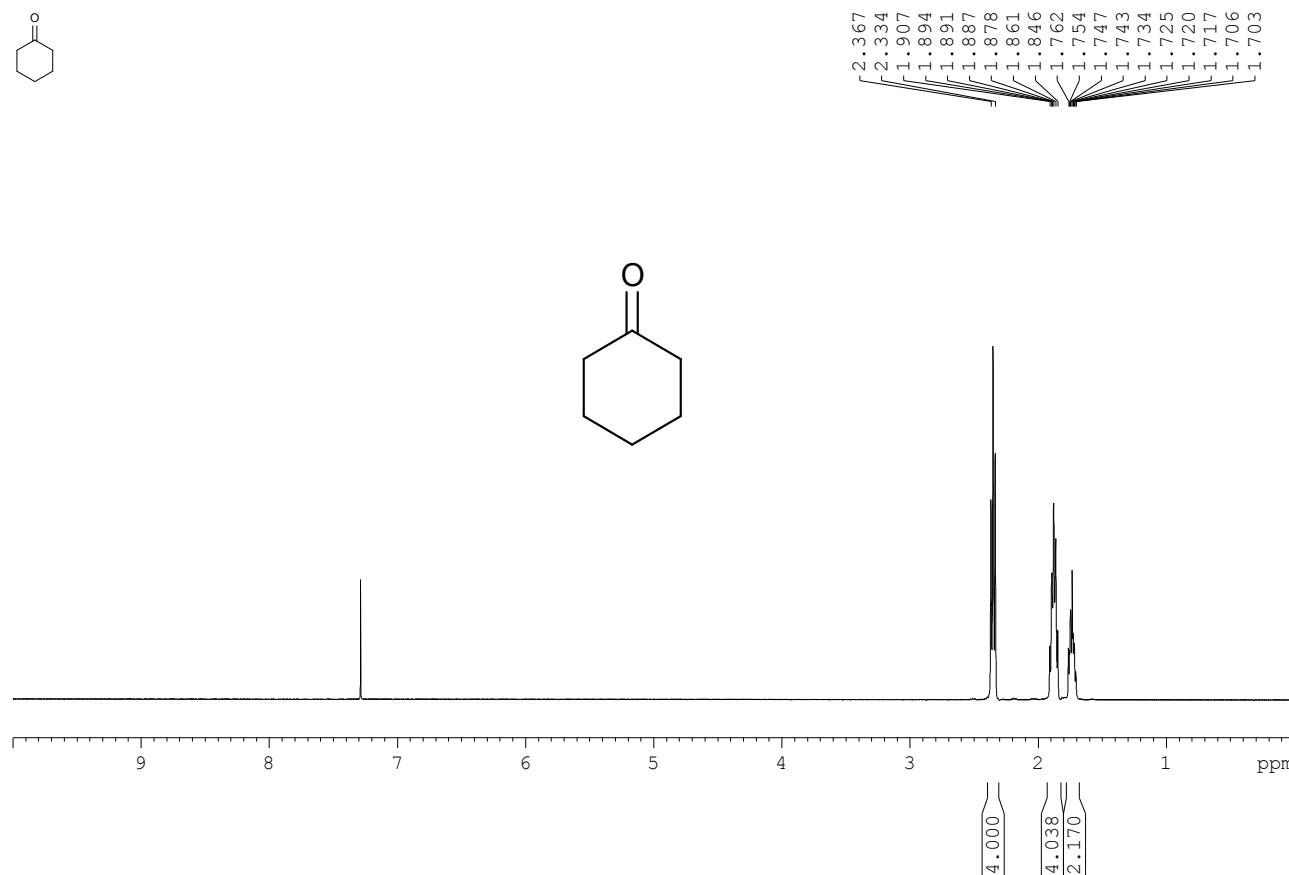
Using the general procedure, 2-methyl-1-phenyl-2-propen-1-ol (**10**) (148 mg, 1 mmol) was reacted for 1 h to generate the reported compound (131 mg, 89 % yield). Spectroscopic data for the product were in accordance with the literature.¹¹



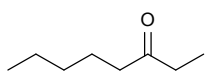
Cyclohexanone



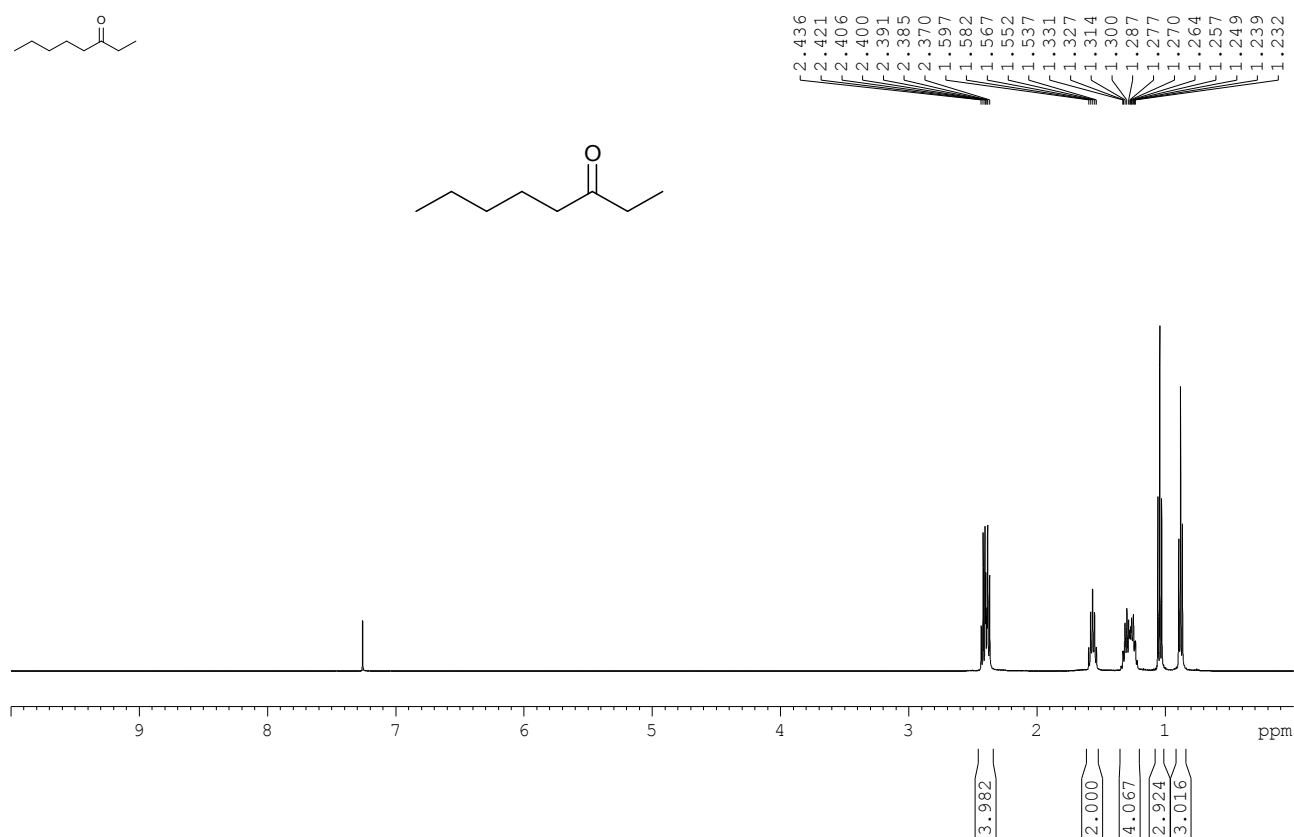
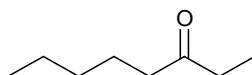
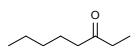
Using the general procedure, 2-cyclohexenol (**11**) (98 mg, 1 mmol) was reacted for 1.5 h to generate the reported compound (80 mg, 81 % yield). Spectroscopic data for the product were in accordance with the literature.¹²



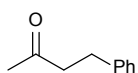
Octan-3-one



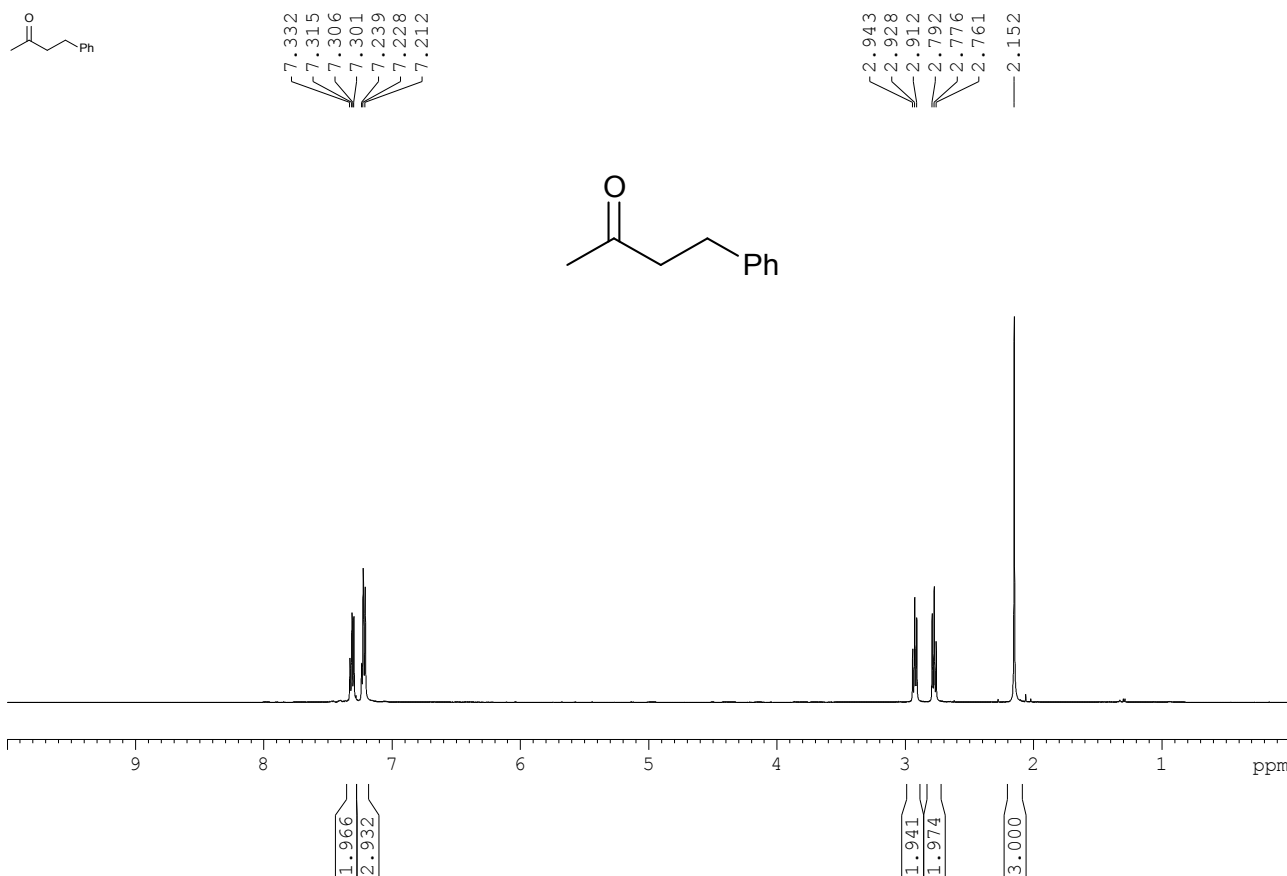
Using the general procedure, 1-octen-3-ol (**12**) (128 mg, 1 mmol) was reacted for 2 h to generate the reported compound (120 mg, 94 % yield). Spectroscopic data for the product were in accordance with the literature.¹³



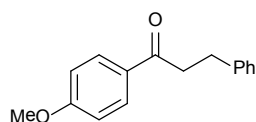
4-Pheny-butan-2-one



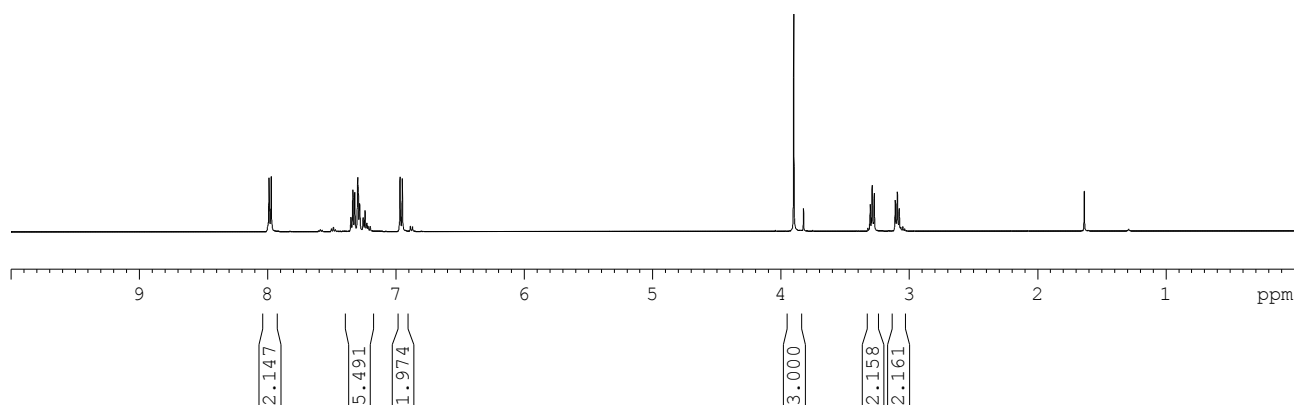
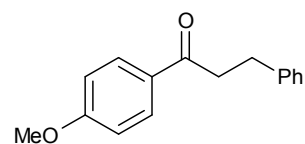
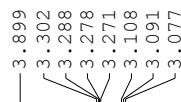
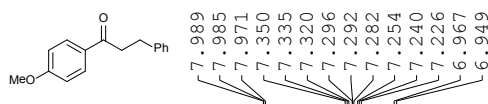
Using the general procedure, 1-methyl-3-phenyl-2-propen-1-ol (**13**) (148 mg, 1 mmol) was reacted for 6 h to generate the reported compound (142 mg, 96 % yield). Spectroscopic data for the product were in accordance with the literature.¹⁴



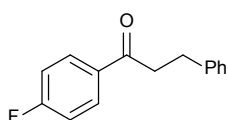
1-(4-methoxyphenyl)-3-phenyl-1-propanone



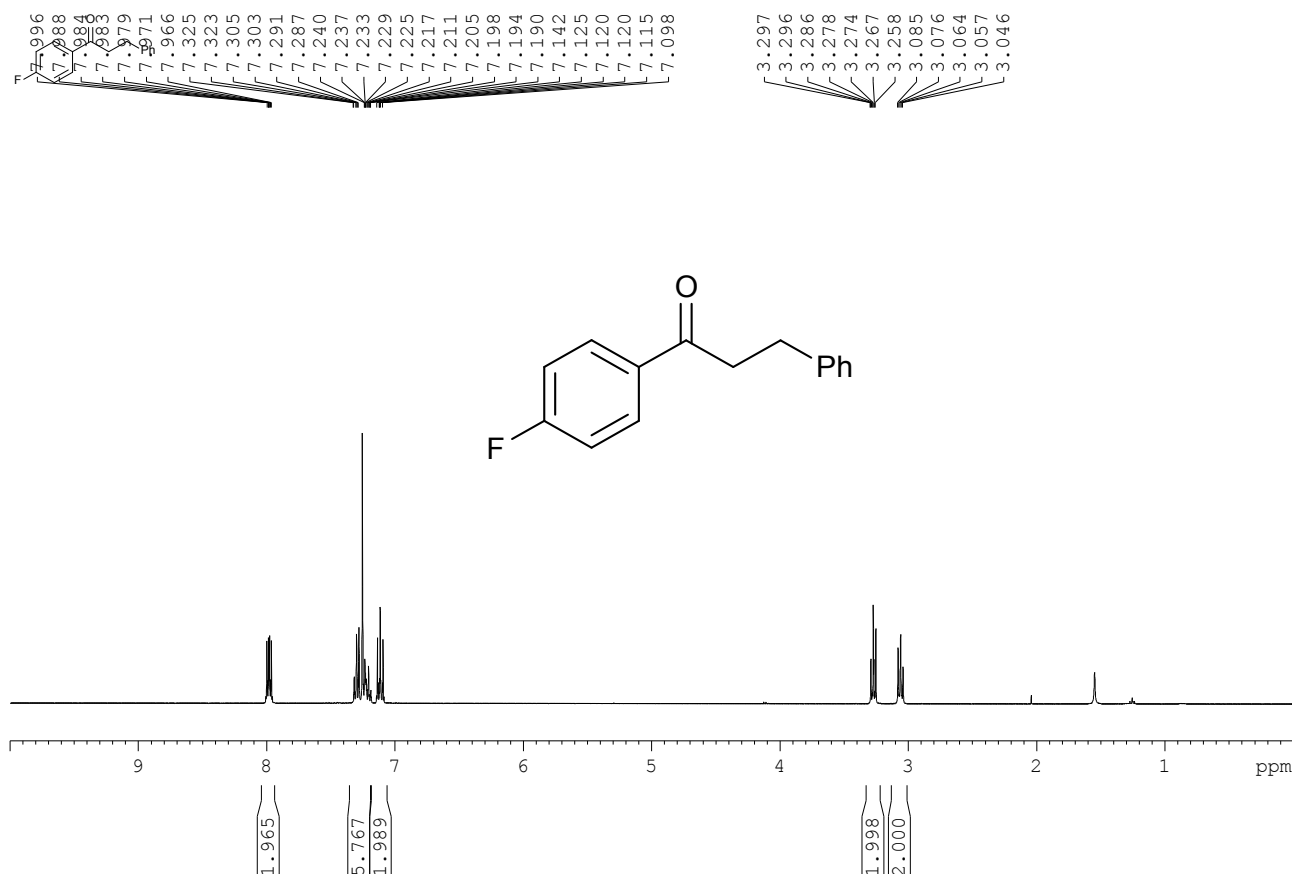
Using the general procedure, 1-(4-methoxyphenyl)-3-phenylprop-2-en-1-ol (**14**) (240 mg, 1 mmol) was reacted for 2.5 h to generate the reported compound (220 mg, 92 % yield). Spectroscopic data for the product were in accordance with the literature.¹⁵



1-(4-fluorophenyl)-3-phenylpropan-1-one



Using the general procedure, *trans*-1-(4-fluorophenyl)-3-phenylprop-2-en-1-ol (**15**) (228 mg, 1 mmol) was reacted for 1 h to generate the reported compound (210 mg, 92 % yield). Spectroscopic data for the product were in accordance with the literature.¹⁶



MECHANISTIC STUDIES:

General procedure for isomerisation in presence of TBACl

In a vial fitted with a screw cap, in the glovebox, *trans*-1,3-diphenyl-2-propen-1-ol (**2**) (0.5 mmol), **1** (0.00125 mmol), NaO^tBu (0.04 mmol) and tetrabutylammonium chloride (the amount is reported below) were charged and dissolved in *isobutyl* methyl ketone (1 mL). The solution was stirred for 1 h. The solvent was removed under vacuum and the crude reaction was analysed by ¹H NMR spectroscopy.

TBACl (mol%)	Conv. %
0	97
10	91
25	61
50	58
100	52

General procedure for isomerisation with variable amount of base

In a vial fitted with a screw cap, in the glovebox, *trans*-1,3-diphenyl-2-propen-1-ol (**2**) (0.5 mmol), **1** (0.00125 mmol) and NaO^tBu (see below) were charged and dissolved in toluene (1 mL). The solution was stirred at given temperature for 1 h. The solvent was removed under vacuum and the crude reaction was analysed by ¹H NMR spectroscopy.

NaO ^t Bu (mol%)	Conv. %
0	0
1	87
2	93
4	>99
8	96
50	decomposition
100	decomposition

ISOMERISATION OF PRIMARY ALLYLIC ALCOHOLS

Method A:

Substrate solution (0.6 mL of a 0.5 mol L⁻¹ solution in toluene-*d*₈) added to solid **14** in an NMR tube equipped with J. Young valve and mixed at room temperature for the specified time. Conversion was determined by integration of the ¹H NMR spectrum.

Method B:

In a vial fitted with a screw cap, in the glovebox, the allylic alcohol (1 mmol), **14** (0.01 mmol) were charged and dissolved in toluene (1 mL). The solution was stirred at room temperature for the determine time. The solvent was removed under vacuum and the crude reaction was analyzed by ¹H NMR in order to determine reaction conversion.

COMPUTATIONAL DETAILS:

All the DFT static calculations were performed at the GGA level with the Gaussian09 set of programs,¹⁹ using the BP86 functional of Becke and Perdew.¹⁹⁻²⁰ The electronic configuration of the molecular systems was described with the standard split-valence basis set with a polarization

function of Ahlrichs and co-workers for H, C, N, O, and Cl (SVP keyword in Gaussian).²¹ For Ru we used the small-core, quasi-relativistic Stuttgart/Dresden effective core potential, with an associated valence basis set contracted (standard SDD keywords in gaussian09).²² The geometry optimizations were performed without symmetry constraints, and the characterization of the located stationary points was performed by analytical frequency calculations. The reported energies have been optimized via single point calculations on the BP86 geometries with triple zeta valence plus polarization (TZVP keyword in Gaussian) using the M06 functional^{19,23} however estimating solvent effects with the polarizable continuous solvation model PCM using DCM as solvent.²⁴

Since in this work we had to compare a dissociative versus an associative/interchange mechanism, careful treatment of the entropic contribution to the free energy was fundamental. In this respect, it is clear that the contribution calculated in the gas phase ($p = 1$ atm) most likely exaggerates the entropic contribution.²⁵ Thus, some kind of correction is needed when mechanisms of different molecularity have to be compared, or calculations will be biased in favor of the dissociative mechanism. Various recipes have been proposed in the literature, like using only a fraction of the gas-phase entropy,^{25b,c} or using a higher pressure that would represent better the liquid state. In the present work we adopted the latter, and all the thermochemical analysis was performed at $p = 1254$ atm, as suggested by Martin et al.^{25a,b}

Table S1. Coordinate data sets, absolute energies (in a.u. calculated at $P = 1$ atm) for DFT optimized complexes

16			$E_g(\text{BP86/SVP}) = -694.021887$ $G_g(\text{BP86/SVP}) = -693.799772$ $E_s(\text{M06/TZVP//BP86/SVP}) = -694.220021$
C	4.228099	-1.862403	
C	4.145528	-1.537575	
C	3.173008	-0.624656	
C	2.269834	-0.037381	
C	2.357529	-0.370148	
C	3.333444	-1.272899	
H	4.991801	-2.573280	
H	4.846401	-1.990496	
H	3.116965	-0.361679	
H	1.652217	0.093984	
H	3.395650	-1.523639	
C	1.181906	0.937581	
O	1.116705	2.109440	
C	2.228480	2.972452	
H	2.346161	3.321004	
H	2.045494	3.854585	
H	3.185068	2.492215	
C	-0.171872	0.263132	
C	-1.266483	0.742115	
C	-2.607437	0.134381	
C	-3.649247	0.828113	
C	-2.920184	-1.118955	
C	-4.947936	0.300116	
H	-3.425989	1.802453	
C	-4.215930	-1.647374	
H	-2.134919	-1.691900	
C	-5.238537	-0.941436	
H	-5.738087	0.861929	
H	-4.432972	-2.623585	
H	-6.255702	-1.360607	
H	-1.151180	1.697090	
H	-0.206369	-0.680596	
H	1.430620	1.216609	

17				E_g(BP86/SVP) = -694.0257434 G_g(BP86/SVP) = -693.8038630 E_s(M06//TZVP//BP86/SVP) = -694.22244
C	-4.673134	-1.524018	-0.031200	
C	-3.440855	-2.179408	0.144767	
C	-2.239167	-1.456851	0.080971	
C	-2.244172	-0.064665	-0.175200	
C	-3.491961	0.584577	-0.344826	
C	-4.692807	-0.138624	-0.273738	
H	-5.616025	-2.090783	0.025936	
H	-3.415874	-3.262306	0.346827	
H	-1.279277	-1.970537	0.248550	
H	-3.505337	1.665577	-0.555232	
H	-5.653047	0.382785	-0.416509	
C	-0.978181	0.711660	-0.293814	
O	-1.022643	2.043446	0.081963	
C	-1.346693	2.305946	1.448700	
H	-0.554741	1.921410	2.131297	
H	-1.409243	3.406451	1.555055	
H	-2.319920	1.856309	1.746444	
C	0.159539	0.220533	-0.855671	
C	1.449504	0.982926	-1.009261	
C	2.662330	0.262993	-0.430167	
C	2.643613	-0.230564	0.893618	
C	3.836436	0.083887	-1.192124	
C	3.766040	-0.872643	1.441851	
H	1.729288	-0.110331	1.498099	
C	4.962505	-0.559306	-0.648135	
H	3.868363	0.457502	-2.229555	
C	4.931679	-1.039764	0.672099	
H	3.730843	-1.247438	2.477710	
H	5.868697	-0.687806	-1.261968	
H	5.812090	-1.545464	1.099820	
H	1.641282	1.178484	-2.088832	
H	1.330984	1.979755	-0.532496	
H	0.125004	-0.801254	-1.268061	

A (and 1)				E _g (BP86/SVP) = -3204.4932517 G _g (BP86/SVP) = -3203.835754 E _s (M06//TZVP//BP86/SVP) = -3205.0421427
Ru	-0.273308	-0.755413	0.098268	
Cl	5656011	-1.146734	-2.310218	
P	-1.102871	1.381728	0.148510	
P	1.999962	-0.199539	-0.215077	
C	-1.933696	-2.190475	0.768000	
C	-0.196798	-1.438272	2.194509	
C	-0.790251	2.070289	2.902844	
C	-3.291149	-2.457494	0.242709	
C	0.551177	3.388618	1.367603	
C	-1.389640	3.976188	-1.024298	
C	-1.087868	2.614391	-1.270230	
C	2.395329	-2.578245	-1.748145	
C	3.333720	0.361627	3.684420	
C	-5.782790	1.611098	0.415177	
C	1.441688	-3.438796	1.697030	
C	2.613019	0.431286	2.479997	
C	2.647222	2.913270	-2.859260	
C	2.209630	1.729027	-2.245827	
C	-5.896398	-3.077748	-0.700428	
C	-3.618635	2.281793	1.319920	
C	-0.786217	-3.101502	0.637124	
C	-3.728919	0.709006	-0.536570	
C	-1.396619	4.438645	-3.416940	
C	-1.530089	4.881276	-2.088345	
C	3.012357	-0.324466	1.353123	
C	0.259310	-2.660373	1.543073	
C	-0.973548	2.175050	-2.605232	
C	3.454620	3.822332	-2.151409	
C	3.119091	-3.444355	-2.587848	
C	-5.024233	2.353372	1.335691	
C	-0.426061	2.386075	1.570215	
C	1.126931	4.065384	2.457995	
C	-1.568990	-1.234287	1.789133	
C	-5.130327	0.792775	-0.524086	
C	2.938722	-1.334581	-1.369495	
C	1.564785	-4.627294	0.979529	
C	-4.410756	-2.402897	1.108707	
C	-0.219894	2.752287	3.990842	
C	4.389132	-3.077590	-3.062428	
C	4.142102	-1.164081	1.469231	
C	-5.699009	-2.708320	0.642152	
C	0.544696	-5.053672	0.082223	
C	4.216943	-0.968998	-1.855038	
C	0.741005	3.756674	3.772978	
C	-1.128187	3.084068	-3.668530	
C	2.575127	1.434677	-0.911826	
C	-2.959089	1.451266	0.387692	
C	3.391996	2.346888	-0.209164	
C	3.825775	3.535100	-0.827079	
C	4.456512	-0.479160	3.790633	
C	4.937496	-1.835813	-2.693361	
C	-0.615088	-4.301998	-0.105568	
C	-4.793571	-3.128984	-1.573103	
C	-3.503287	-2.822783	-1.110854	
C	4.854545	-1.242594	2.680660	
H	0.319230	-0.928553	3.017287	
H	-1.533404	1.284402	3.102300	
H	0.872751	3.646352	0.348432	
H	-1.534149	4.338338	0.005091	
H	1.389339	-2.860303	-1.408572	
H	3.008755	0.966522	4.545909	
H	-6.882763	1.672456	0.427622	
H	2.223432	-3.118860	2.401748	
H	1.724996	1.077385	2.414296	
H	2.351885	3.127678	-3.898339	
H	1.589859	1.013272	-2.808564	
H	-6.906266	-3.324578	-1.065606	
H	-3.042722	2.892758	2.031188	
H	-3.222115	0.066709	-1.274717	
H	-1.515517	5.148138	-4.251698	
H	-1.759165	5.937989	-1.875691	
H	-0.787738	1.108019	-2.809844	
H	3.798111	4.750928	-2.634691	
H	2.674915	-4.408807	-2.881028	
H	-5.525921	3.003687	2.070567	
H	1.885677	4.841867	2.270899	
H	-2.268564	-0.504086	2.216662	
H	-5.713045	0.203890	-1.249278	
H	2.463606	-5.250580	1.108645	
H	-4.263044	-2.133643	2.166559	
H	-0.531203	2.495800	5.016180	
H	4.950031	-3.754673	-3.726765	
H	4.468242	-1.769105	0.610682	
H	-6.554466	-2.664642	1.335381	
H	0.670919	-6.001305	-0.465175	
H	4.654649	0.003034	-1.579305	
H	1.187036	4.293620	4.625138	
H	-1.041272	2.719775	-4.705018	
H	3.705090	2.129043	0.822767	
H	4.467564	4.235063	-0.267834	
H	5.017256	-0.540394	4.737020	
H	5.930156	-1.534827	-3.065207	
H	-1.409347	-4.649111	-0.782622	
H	-4.939804	-3.403003	-2.630569	
H	-2.649294	-2.808184	-1.806699	
H	5.729772	-1.908349	2.752386	

B				$E_g(\text{BP86/SVP}) = -2168.7456344$ $G_g(\text{BP86/SVP}) = -2168.338765$ $E_s(\text{M06//TZVP//BP86/SVP}) = -2169.0530326$
Ru	-0.727182	-1.002299	-0.042156	
Cl	-0.299742	-2.147732	-2.044036	
P	1.314587	0.022907	-0.020165	
C	-2.350339	0.173469	0.733406	
C	-1.319283	-1.559100	1.938923	
C	-2.756425	1.527364	0.288014	
C	2.539973	-2.492662	0.351590	
C	1.252299	2.980452	2.896508	
C	-2.777704	-3.512267	0.931713	
C	1.028146	2.241922	1.722894	
C	1.438470	1.892725	-3.726125	
C	1.143095	1.017611	-2.666965	
C	-3.567311	4.117960	-0.537111	
C	-3.024306	-1.100224	0.379751	
C	1.697191	1.012368	1.508997	
C	-2.383502	-2.162975	1.129240	
C	2.282121	2.998496	-3.521097	
C	3.593531	-3.422718	0.334236	
C	-1.418197	-0.126083	1.805835	
C	2.743930	-1.171410	-0.103099	
C	-3.801283	-3.786390	0.022957	
C	-2.909180	2.573962	1.229687	
C	4.858866	-3.045137	-0.147902	
C	2.582667	0.536755	2.499629	
C	-3.308453	3.857203	0.819660	
C	-4.439524	-2.743973	-0.702680	
C	4.015658	-0.800770	-0.592223	
C	1.699293	1.235502	-1.386334	
C	2.551736	2.346726	-1.187322	
C	2.838287	3.222412	-2.249858	
C	2.137346	2.498586	3.879199	
C	5.066250	-1.734286	-0.613128	
C	-4.060958	-1.409367	-0.538582	
C	-3.418738	3.086519	-1.483156	
C	-3.014871	1.805819	-1.077071	
C	2.797801	1.275124	3.678447	
H	-0.694967	-2.091263	2.669395	
H	1.537354	-2.789090	0.702071	
H	0.729569	3.939029	3.044264	
H	-2.286741	-4.321615	1.494107	
H	0.324836	2.625262	0.965548	
H	1.000044	1.707718	-4.719872	
H	0.486215	0.147460	-2.829718	
H	-3.881590	5.123697	-0.858426	
H	2.505714	3.687381	-4.351486	
H	3.419428	-4.451855	0.686756	
H	-0.840801	0.613042	2.373602	
H	-4.124312	-4.827462	-0.134893	
H	-2.729369	2.369933	2.297123	
H	5.682905	-3.776188	-0.170830	
H	3.114337	-0.415386	2.348585	
H	-3.425586	4.657571	1.567944	
H	-5.248769	-2.995662	-1.406020	
H	4.187109	0.218973	-0.970612	
H	2.994215	2.536690	-0.197348	
H	3.501457	4.085873	-2.079614	
H	2.311041	3.078105	4.799848	
H	6.052606	-1.435802	-1.003157	
H	-4.567661	-0.607283	-1.093833	
H	-3.608325	3.285306	-2.550065	
H	-2.859048	1.012401	-1.824867	
H	3.493631	0.890515	4.441284	

C (R = H)			E _g (BP86/SVP) = -2361.7520274 G _g (BP86/SVP) = -2361.260483 E _s (M06//TZVP//BP86/SVP) = -2362.1524185
Ru	0.650288	0.234652	-0.440863
Cl	1.013194	0.750832	1.929722
P	-1.657000	0.217138	0.009235
C	2.740939	-0.713563	-0.744979
C	0.872569	-1.134259	-2.132790
C	4.071212	-0.247540	-0.294857
C	-1.385359	-1.560916	2.205018
C	-3.202466	-1.003410	-3.658574
C	0.014275	-3.246877	-0.827825
C	-2.488391	-0.330832	-2.653128
C	-2.630799	3.993243	1.359485
C	-2.042303	2.730410	1.183917
C	6.656925	0.583158	0.528783
C	1.983137	-1.853619	-0.194354
C	-2.650329	-0.681450	-1.291183
C	0.865572	-2.134275	-1.076060
C	-3.676865	4.413201	0.517006
C	-1.818111	-2.220093	3.368624
C	2.087173	-0.357670	-1.975563
C	-2.212608	-0.605600	1.580129
C	0.295688	-4.077790	0.255316
C	5.081618	0.037568	-1.246932
C	-3.075338	-1.927030	3.923804
C	-3.529524	-1.738304	-0.966658
C	6.359277	0.451526	-0.838923
C	1.391357	-3.803669	1.122617
C	-3.475128	-0.310597	2.144979
C	-2.502385	1.866998	0.159395
C	-3.554119	2.291982	-0.680559
C	-4.135862	3.561233	-0.501221
C	-4.077141	-2.053372	-3.323874
C	-3.902902	-0.969841	3.309980
C	2.222523	-2.701075	0.921780
C	5.662375	0.307712	1.483512
C	4.381800	-0.099934	1.079862
C	-4.233412	-2.419865	-1.977111
H	0.218440	-1.145604	-3.013506
H	-0.390654	-1.774783	1.790177
H	-3.069201	-0.708269	-4.711756
H	-0.827564	-3.458414	-1.504520
H	-1.790267	0.473266	-2.928453
H	-2.265401	4.655022	2.160816
H	-1.221713	2.403293	1.845369
H	7.660388	0.905412	0.849313
H	-4.134842	5.405460	0.656176
H	-1.157875	-2.958250	3.850684
H	2.465079	0.384153	-2.691389
H	-0.336699	-4.958836	0.446720
H	4.867871	-0.090547	-2.320099
H	-3.408589	-2.438598	4.841027
H	-3.664404	-2.037918	0.083095
H	7.131033	0.664781	-1.595870
H	1.590928	-4.483436	1.966267
H	-4.128343	0.442343	1.676608
H	-3.932251	1.629376	-1.474286
H	-4.957765	3.880629	-1.161919
H	-4.631790	-2.585981	-4.112669
H	-4.886642	-0.727830	3.743090
H	3.074840	-2.511112	1.589555
H	5.879807	0.428584	2.556790
H	3.589575	-0.253374	1.828340
H	-4.911180	-3.244340	-1.703437
C	0.176770	1.853593	-1.796546
C	0.901844	2.362884	-0.672253
H	-0.888998	2.125458	-1.887955
H	0.679471	1.750199	-2.775797
H	0.305243	2.869535	0.107753
C	2.321824	2.884490	-0.721252
H	2.934740	2.285601	-1.443625
O	2.925934	2.963775	0.552654
H	2.563851	2.216905	1.085648
H	2.290452	3.922685	-1.136590

D (R = H)				E _g (BP86/SVP) = -2594.6826195 G _g (BP86/SVP) = -2594.088241 E _s (M06//TZVP//BP86/SVP) = -2595.2089526
Ru	0.075988	0.651760	-0.586715	
Cl	-0.847952	0.346775	1.630581	
P	1.628948	-0.958325	0.024584	
C	-0.695120	2.840523	-0.720792	
C	1.003383	1.968441	-2.103077	
C	-1.966518	3.467852	-0.260338	
C	2.417619	0.377379	2.399161	
C	4.268928	-0.886689	-3.209236	
C	3.023190	2.771338	-0.622467	
C	3.112911	-0.941706	-2.413093	
C	-0.646845	-4.354527	0.548460	
C	-0.119912	-3.054600	0.617108	
C	-4.320571	4.830992	0.552292	
C	0.616180	3.094695	-0.091585	
C	3.201827	-0.938696	-1.000050	
C	1.657471	2.598006	-0.968076	
C	0.031117	-5.354708	-0.171550	
C	2.992890	0.472896	3.677445	
C	-0.419111	2.246451	-2.000770	
C	2.325259	-0.872233	1.751815	
C	3.340357	3.449235	0.560950	
C	-1.953997	4.864561	-0.006659	
C	3.468270	-0.678161	4.330936	
C	4.484283	-0.860356	-0.412002	
C	-3.116852	5.541422	0.395329	
C	2.320082	3.915631	1.431864	
C	2.800953	-2.025729	2.412848	
C	1.084592	-2.736661	-0.055546	
C	1.760389	-3.744077	-0.778666	
C	1.236794	-5.049664	-0.828765	
C	5.540355	-0.807838	-2.611208	
C	3.368137	-1.928521	3.696652	
C	0.965367	3.727757	1.128085	
C	-4.338751	3.447520	0.305101	
C	-3.178467	2.756764	-0.091484	
C	5.641337	-0.791099	-1.210650	
H	1.521869	1.600951	-2.998257	
H	2.021284	1.277224	1.907321	
H	4.173313	-0.897584	-4.307368	
H	3.814858	2.394112	-1.288625	
H	2.124651	-0.981357	-2.893941	
H	-1.611920	-4.558664	1.036924	
H	-0.653874	-2.271973	1.182865	
H	-5.237599	5.355306	0.870524	
H	-0.386926	-6.373127	-0.230551	
H	3.051375	1.456051	4.171412	
H	-1.172625	2.067502	-2.779330	
H	4.397068	3.612197	0.828592	
H	-1.016090	5.428272	-0.143453	
H	3.906986	-0.602429	5.339574	
H	4.582769	-0.847210	0.683501	
H	-3.081044	6.628022	0.582195	
H	2.600613	4.431285	2.364866	
H	2.719926	-3.010223	1.926073	
H	2.698168	-3.510176	-1.306835	
H	1.772120	-5.829730	-1.395260	
H	6.446842	-0.755513	-3.236119	
H	3.726232	-2.839080	4.204566	
H	0.175356	4.075190	1.810568	
H	-5.270442	2.871330	0.428878	
H	-3.261904	1.653187	-0.240523	
H	6.629969	-0.722921	-0.727612	
C	-0.388936	-0.707401	-2.194347	
C	-1.497668	-0.695721	-1.287643	
H	0.236535	-1.617355	-2.257758	
H	-0.498580	-0.199913	-3.174084	
H	-1.570791	-1.520154	-0.557161	
C	-2.901767	-0.222644	-1.684495	
H	-2.808770	0.709947	-2.327579	
O	-3.820957	-0.124673	-0.702538	
H	-3.841444	-1.407019	0.080677	
H	-3.161098	-1.027421	-2.462491	
C	-5.204601	-2.847741	0.339675	
C	-5.236200	-4.297056	0.864630	
H	-6.246956	-4.752890	0.775902	
H	-4.517424	-4.922228	0.293042	
H	-4.931415	-4.318827	1.932719	
C	-5.590582	-2.810270	-1.161346	
H	-5.480852	-1.765100	-1.520364	
H	-4.895533	-3.450937	-1.745128	
H	-6.631852	-3.159293	-1.345558	
C	-6.200101	-1.972961	1.146277	
H	-5.908189	-1.966558	2.217719	
H	-6.151605	-0.928545	0.774776	
H	-7.251452	-2.331628	1.065218	
O	-3.890070	-2.368439	0.519815	

DE (R = H)		
Ru	0.167367	-0.227752 -0.028300
Cl	0.210503	0.341742 -2.367392
P	-2.042942	-0.563854 -0.133680
C	1.739175	1.938973 0.686680
C	0.466316	0.527645 2.066891
C	2.803613	2.398255 -0.218504
C	-2.576297	2.006949 -1.201525
C	-3.223542	-1.263543 3.813121
C	-1.474843	2.240744 2.500651
C	-2.519267	-1.247190 2.596911
C	-2.596067	-3.594298 -2.897424
C	-2.234850	-2.399211 -2.255151
C	4.882446	3.233334 -1.985980
C	0.478541	2.638308 1.025007
C	-3.030571	-0.564631 1.469083
C	-0.277886	1.785925 1.914634
C	-3.318640	-4.584608 -2.204576
C	-3.306443	2.969494 -1.918841
C	1.758668	0.742735 1.447652
C	-3.018637	0.668689 -1.148165
C	-1.930790	3.541679 2.218587
C	4.104449	1.833501 -0.145636
C	-4.480725	2.607556 -2.601965
C	-4.262849	0.113785 1.600064
C	5.122163	2.240203 -1.017758
C	-1.195850	4.381745 1.355146
C	-4.200685	0.311260 -1.834747
C	-2.611231	-2.168213 -0.908874
C	-3.332075	-3.166418 -0.219723
C	-3.680416	-4.369158 -0.864568
C	-4.448354	-0.582172 3.931670
C	-4.925928	1.274894 -2.558879
C	-0.000733	3.941585 0.755309
C	3.594356	3.786616 -2.091985
C	2.567898	3.367932 -1.230172
C	-4.962432	0.107705 2.820721
H	0.285556	-0.172743 2.893477
H	-1.648128	2.298559 -0.687833
H	-2.804197	-1.804499 4.677135
H	-2.035359	1.590829 3.190412
H	-1.549642	-1.759229 2.520004
H	-2.299172	-3.757675 -3.946219
H	-1.646918	-1.630321 -2.787014
H	5.685347	3.553634 -2.670819
H	-3.593434	-5.525728 -2.708511
H	-2.942174	4.008658 -1.950236
H	2.573208	0.008386 1.440309
H	-2.859316	3.909514 2.684591
H	4.329758	1.028733 0.567951
H	-5.045761	3.362222 -3.173594
H	-4.677830	0.664949 0.743234
H	6.101848	1.742327 -0.945159
H	-1.553852	5.405605 1.156094
H	-4.558070	-0.729994 -1.810642
H	-3.633805	-3.005110 0.826834
H	-4.243079	-5.139674 -0.311950
H	-4.995831	-0.584232 4.888331
H	-5.842161	0.977818 -3.095507
H	0.573767	4.631664 0.121495
H	3.374993	4.535919 -2.871145
H	1.552931	3.759761 -1.383044
H	-5.916852	0.653563 2.901562
C	0.415515	-2.164623 0.838451
C	0.751767	-2.210620 -0.558469
H	-0.484502	-2.711161 1.176741
H	1.249845	-2.155358 1.562755
H	0.050475	-2.691783 -1.264813
C	2.211836	-2.151425 -0.981879
H	2.602877	-3.222853 -0.927733
O	2.887713	-1.266667 -0.174254
H	4.397402	-1.172728 -0.136038
C	5.915239	-2.148110 0.767174
C	7.390538	-1.839135 1.091393
H	7.867740	-2.655821 1.675557
H	7.962999	-1.694261 0.150758
H	7.458997	-0.897648 1.675946
C	5.827245	-3.445516 -0.076863
H	4.767125	-3.665692 -0.322725
H	6.373690	-3.306848 -1.033540
H	6.253813	-4.327644 0.451307
C	5.103092	-2.322658 2.073787
H	5.215122	-1.422099 2.714561
H	4.029454	-2.417972 1.808491
H	5.421125	-3.212876 2.661016
O	5.426481	-1.050029 0.024801
H	2.247441	-1.893248 -2.077847

$E_g(\text{BP86/SVP}) = -2594.6751251$
 $G_g(\text{BP86/SVP}) = -2594.079076$
 $E_s(\text{M06//TZVP//BP86/SVP}) = -2595.1954611$

E (R = H)				E _g (BP86/SVP) = -2594.6892024 G _g (BP86/SVP) = -2594.09277 E _s (M06//TZVP//BP86/SVP) = -2595.213858
Ru	0.170067	0.142030	-1.201204	
Cl	1.423085	1.232453	0.647464	
P	-1.749084	0.533440	0.122713	
C	1.077877	-2.179254	-0.744204	
C	-0.810697	-1.799859	-2.049065	
C	2.491438	-2.323475	-0.347936	
C	-0.774758	-0.598947	2.530714	
C	-5.065732	-0.874722	-1.970973	
C	-2.418724	-3.337894	-0.637795	
C	-3.825488	-0.316084	-1.618604	
C	-1.647012	4.675771	0.491812	
C	-1.329793	3.307970	0.510827	
C	5.216212	-2.678553	0.415925	
C	-0.059139	-2.882137	-0.102959	
C	-3.403275	-0.268088	-0.269542	
C	-1.221287	-2.678295	-0.925112	
C	-2.894154	5.113801	0.007965	
C	-0.706255	-0.795494	3.920971	
C	0.626533	-1.772441	-2.053922	
C	-1.679643	0.332300	1.984236	
C	-2.484702	-4.200087	0.486652	
C	3.496287	-2.602557	-1.310718	
C	-1.532071	-0.053574	4.782701	
C	-4.250534	-0.822089	0.713600	
C	4.835128	-2.784252	-0.934536	
C	-1.354298	-4.393632	1.295261	
C	-2.504360	1.078860	2.856340	
C	-2.263436	2.345244	0.054223	
C	-3.512046	2.793743	-0.428660	
C	-3.822443	4.167801	-0.455239	
C	-5.905426	-1.414640	-0.979670	
C	-2.431320	0.886402	4.247141	
C	-0.130638	-3.743207	1.003986	
C	4.240075	-2.375729	1.381267	
C	2.898442	-2.207497	1.006226	
C	-5.488440	-1.390612	0.361589	
H	-1.430458	-1.650704	-2.944106	
H	-0.117784	-1.161436	1.853114	
H	-5.373006	-0.895166	-3.029559	
H	-3.304618	-3.194434	-1.277224	
H	-3.165417	0.082865	-2.403008	
H	-0.905017	5.406699	0.853099	
H	-0.340837	2.967741	0.865483	
H	6.270002	-2.809764	0.711251	
H	-3.138870	6.188704	-0.009728	
H	0.007735	-1.527537	4.331230	
H	1.273472	-1.516920	-2.904384	
H	-3.427913	-4.720218	0.720902	
H	3.212570	-2.687847	-2.370753	
H	-1.470252	-0.201015	5.873660	
H	-3.938295	-0.822339	1.767962	
H	5.591050	-3.007031	-1.706211	
H	-1.411739	-5.072561	2.162813	
H	-3.205521	1.822111	2.445077	
H	-4.261868	2.069698	-0.780560	
H	-4.803905	4.494399	-0.837509	
H	-6.875899	-1.859708	-1.254006	
H	-3.077437	1.479054	4.915907	
H	0.760394	-3.935389	1.622363	
H	4.529716	-2.245270	2.436043	
H	2.152636	-1.934471	1.767328	
H	-6.128077	-1.824658	1.147620	
C	-0.655173	1.106539	-2.946027	
C	0.196763	2.021054	-2.253355	
H	-1.740415	1.311422	-2.974035	
H	-0.266421	0.577722	-3.837619	
H	-0.213766	2.909340	-1.744129	
C	1.688455	1.896643	-2.535009	
H	1.963621	2.218693	-3.579107	
O	1.936644	0.526073	-2.319786	
H	3.638110	0.999862	1.228975	
C	5.279550	1.894112	0.628314	
C	6.717829	1.963173	1.170790	
H	7.374095	2.560185	0.502930	
H	6.724829	2.425255	2.180735	
H	7.138771	0.940093	1.260063	
C	4.672008	3.312942	0.539882	
H	3.616856	3.248548	0.201349	
H	4.682313	3.794369	1.540793	
H	5.230039	3.961311	-0.170804	
C	5.250114	1.205457	-0.752041	
H	5.701250	0.194293	-0.679715	
H	4.205768	1.075426	-1.110121	
H	5.811810	1.789578	-1.514012	
O	4.552962	1.116493	1.585000	
H	2.261311	2.553772	-1.828771	

EF (R = H)			E _g (BP86/SVP) = -2594.6695876 G _g (BP86/SVP) = -2594.6695876 E _s (M06//TZVP//BP86/SVP) = -2595.1925239
Ru	-1.143617	1.382984	0.093752
Cl	2.782922	-0.202298	1.304863
P	-1.767217	-0.822815	0.149852
C	0.334592	2.787854	-1.076521
C	-1.392661	1.679141	-2.214974
C	1.090994	3.802644	-0.317282
C	0.552167	-2.109588	-0.725873
C	-5.940177	-1.239665	0.307644
C	0.162514	-0.043200	-3.445587
C	-4.583859	-1.219106	0.685065
C	-0.134507	-2.002617	3.768023
C	-0.457325	-1.278109	2.605428
C	2.536957	5.772268	1.129550
C	0.903798	1.597308	-1.749778
C	-3.564927	-1.052550	-0.281524
C	-0.140988	0.994439	-2.548311
C	-0.859689	-3.153454	4.118112
C	1.313285	-3.097418	-1.375059
C	-1.035912	2.885422	-1.501602
C	-0.849699	-2.062114	-0.901063
C	1.491942	-0.499315	-3.528492
C	0.832341	5.184025	-0.506767
C	0.684438	-4.043863	-2.203185
C	-3.950227	-0.893401	-1.635410
C	1.544453	6.159010	0.209835
C	2.503487	0.047134	-2.707681
C	-1.478575	-3.018607	-1.729292
C	-1.511183	-1.718523	1.773245
C	-2.209057	-2.902976	2.105132
C	-1.896204	-3.606273	3.280597
C	-6.305199	-1.103969	-1.041325
C	-0.710032	-4.001713	-2.379707
C	2.220506	1.090740	-1.811334
C	2.797694	4.404321	1.329224
C	2.083098	3.422279	0.624064
C	-5.301502	-0.931479	-2.013308
H	-2.342758	1.538400	-2.749231
H	1.086606	-1.390413	-0.070186
H	-6.715485	-1.366390	1.080946
H	-0.626151	-0.497141	-4.067366
H	-4.321636	-1.343134	1.746792
H	0.709753	-1.661140	4.387439
H	0.156123	-0.402521	2.323558
H	3.102111	6.535632	1.690094
H	-0.605050	-3.713296	5.033254
H	2.407509	-3.089761	-1.226529
H	-1.694249	3.748252	-1.335933
H	1.741531	-1.317705	-4.222912
H	0.074561	5.493750	-1.245317
H	1.282273	-4.817437	-2.713595
H	-3.175135	-0.731868	-2.399671
H	1.331087	7.227908	0.040313
H	3.517846	-0.380602	-2.725509
H	-2.571562	-3.019336	-1.858283
H	-2.988420	-3.295200	1.432793
H	-2.453830	-4.523573	3.533006
H	-7.366919	-1.125854	-1.336077
H	-1.212559	-4.744133	-3.022503
H	3.009905	1.487398	-1.159294
H	3.561180	4.086472	2.058056
H	2.274043	2.352647	0.831272
H	-5.572959	-0.817862	-3.075570
C	-2.958494	2.327660	0.653385
C	-2.551793	1.459015	1.719696
H	-3.862388	2.075683	0.067222
H	-2.771487	3.414439	0.748386
H	-3.179759	0.591943	1.990040
C	-1.471272	1.904017	2.696217
H	-1.709429	2.888464	3.186791
O	-0.325248	1.980653	1.884850
H	3.832034	-1.348224	-0.094973
H	-1.352037	1.156705	3.521235
C	5.508046	-2.348805	0.166896
C	4.979334	-3.119360	1.398272
H	5.800763	-3.418794	2.086466
H	4.262516	-2.469636	1.943879
H	4.440993	-4.035696	1.074996
C	6.283731	-1.092187	0.624733
H	6.666520	-0.538029	-0.258642
H	5.589838	-0.425021	1.179004
H	7.145030	-1.348944	1.280284
C	6.397515	-3.250965	-0.704545
H	5.828152	-4.141666	-1.044921
H	6.736382	-2.698185	-1.606055
H	7.292128	-3.598182	-0.144838
O	4.410877	-1.952665	-0.661466

F (R = H)				E _g (BP86/SVP) = -1900.9769884 G _g (BP86/SVP) = -1901.2725485 E _s (M06//TZVP//BP86/SVP) = -1901.2725485
Ru	0.837055	0.329334	-0.309448	
P	-1.528591	0.217790	-0.062308	
C	2.871869	-0.485187	-0.759857	
C	0.972982	-1.135479	-2.019108	
C	4.165978	0.127698	-0.397945	
C	-1.116531	-0.992841	2.454931	
C	-2.776457	-1.246013	-3.755634	
C	0.231436	-3.072629	-0.383308	
C	-2.178239	-0.489399	-2.734056	
C	-3.557710	3.656655	1.147042	
C	-2.831624	2.453556	1.131452	
C	6.668426	1.265171	0.305439	
C	2.194652	-1.568236	-0.046222	
C	-2.355411	-0.834213	-1.372054	
C	1.031882	-1.975151	-0.824223	
C	-4.076807	4.189152	-0.045735	
C	-1.507394	-1.564183	3.681161	
C	2.115552	-0.279180	-1.996391	
C	-2.093541	-0.545341	1.540618	
C	0.579406	-3.735347	0.788999	
C	5.183462	0.299030	-1.368837	
C	-2.867973	-1.693707	4.003074	
C	-3.118678	-1.982471	-1.067465	
C	6.421723	0.862350	-1.019443	
C	1.710464	-3.326812	1.558042	
C	-3.464513	-0.660716	1.878859	
C	-2.607359	1.756706	-0.080450	
C	-3.138605	2.300345	-1.271473	
C	-3.866563	3.503660	-1.253739	
C	-3.542852	-2.381929	-3.438004	
C	-3.847770	-1.237073	3.100534	
C	2.508663	-2.258103	1.162918	
C	5.659553	1.114645	1.274961	
C	4.417877	0.556168	0.931507	
C	-3.702914	-2.750534	-2.092520	
H	0.266847	-1.256495	-2.847882	
H	-0.050868	-0.840315	2.218936	
H	-2.632054	-0.951860	-4.807683	
H	-0.625407	-3.403990	-0.988852	
H	-1.539344	0.367679	-3.000114	
H	-3.720204	4.178543	2.103718	
H	-2.443372	2.048508	2.078340	
H	7.642150	1.701631	0.579736	
H	-4.646918	5.131605	-0.032519	
H	-0.735875	-1.900795	4.391746	
H	2.408291	0.407246	-2.801447	
H	-0.021398	-4.593364	1.129287	
H	5.005810	-0.034650	-2.404031	
H	-3.170287	-2.140061	4.964242	
H	-3.254022	-2.290808	-0.020690	
H	7.204148	0.978937	-1.786792	
H	1.961767	-3.879533	2.477376	
H	-4.238243	-0.287266	1.188900	
H	-3.002390	1.778811	-2.229419	
H	-4.276053	3.902399	-2.195788	
H	-4.004644	-2.981812	-4.238168	
H	-4.916943	-1.323187	3.353176	
H	3.393911	-1.965574	1.746400	
H	5.836639	1.449360	2.310069	
H	3.597696	0.499443	1.666754	
H	-4.288870	-3.646187	-1.830484	
C	1.606266	2.326020	-0.824956	
C	0.520891	2.496361	0.056194	
H	1.487384	2.598297	-1.886932	
H	2.640289	2.346910	-0.439832	
H	-0.424466	2.920119	-0.318900	
C	0.750802	2.313649	1.551041	
H	1.492049	3.051030	1.960654	
O	1.199169	0.982098	1.650817	
H	-0.206198	2.481340	2.111864	

FG (R = H)				E _g (BP86/SVP) = -1900.9745107 G _g (BP86/SVP) = -1900.493341 E _s (M06//TZVP//BP86/SVP) = -1901.2728849
Ru	-0.865622	-0.237342	-0.149060	
P	1.520081	-0.138480	-0.119856	
C	-3.002041	0.444184	-0.635303	
C	-1.176554	1.280950	-1.850496	
C	-4.299882	-0.214224	-0.363903	
C	1.655850	-0.095502	2.721187	
C	2.562190	3.280062	-2.306729	
C	-0.586354	3.208395	-0.128115	
C	2.069192	2.016833	-1.938467	
C	3.316383	-3.612122	-1.568070	
C	2.611366	-2.679447	-0.787362	
C	-6.835070	-1.413931	0.111701	
C	-2.417990	1.534950	0.136334	
C	2.207599	1.532735	-0.614857	
C	-1.280502	2.054653	-0.609341	
C	3.945583	-3.220633	-2.761732	
C	2.296043	-0.180612	3.970123	
C	-2.251412	0.358247	-1.890466	
C	2.364645	-0.363757	1.532209	
C	-1.020712	3.819781	1.040862	
C	-5.194810	-0.479302	-1.429908	
C	3.652225	-0.539616	4.045236	
C	2.837874	2.369646	0.333652	
C	-6.445909	-1.072523	-1.195235	
C	-2.139771	3.312385	1.769625	
C	3.731154	-0.716099	1.615097	
C	2.516630	-1.323304	-1.191605	
C	3.175876	-0.937218	-2.381391	
C	3.877632	-1.875777	-3.159272	
C	3.188181	4.100602	-1.351438	
C	4.367632	-0.806651	2.864048	
C	-2.831649	2.188357	1.340651	
C	-5.956950	-1.160565	1.180978	
C	-4.703873	-0.573263	0.947078	
C	3.317537	3.640883	-0.030632	
H	-0.474712	1.474069	-2.667278	
H	0.588222	0.171100	2.656708	
H	2.449316	3.626412	-3.346601	
H	0.253364	3.626436	-0.700939	
H	1.562540	1.403850	-2.697515	
H	3.374930	-4.658264	-1.226699	
H	2.150716	-3.023589	0.154465	
H	-7.816525	-1.878458	0.296621	
H	4.496322	-3.955085	-3.370956	
H	1.725858	0.026880	4.889728	
H	-2.488728	-0.311801	-2.726679	
H	-0.504297	4.721448	1.405987	
H	-4.912642	-0.193560	-2.455490	
H	4.152166	-0.616386	5.024074	
H	2.955365	2.029610	1.372608	
H	-7.125353	-1.262544	-2.041563	
H	-2.469303	3.836253	2.681151	
H	4.304112	-0.923363	0.698239	
H	3.177020	0.110817	-2.707179	
H	4.384302	-1.541832	-4.079149	
H	3.570377	5.093626	-1.636338	
H	5.430845	-1.091570	2.913537	
H	-3.717093	1.831688	1.886437	
H	-6.246040	-1.434015	2.208510	
H	-4.010192	-0.414455	1.787020	
H	3.800805	4.274079	0.730569	
C	-1.903489	-2.116756	-0.119390	
C	-0.522914	-2.421091	0.060348	
H	-2.380729	-2.336637	-1.087425	
H	-2.585004	-2.207203	0.746590	
H	0.065766	-2.845345	-0.769050	
C	-0.116374	-2.810076	1.436304	
H	-0.826086	-0.366390	1.437168	
O	0.904025	-3.413067	1.750467	
H	-0.875375	-2.522165	2.225853	

G (R = H)				E _g (BP86/SVP) = -1901.002071 G _g (BP86/SVP) = -1900.528101 E _s (M06//TZVP//BP86/SVP) = -1901.3022414
Ru	0.681385	0.241168	-0.421233	
P	-1.576622	0.209917	0.040095	
C	2.806752	-0.621092	-0.662061	
C	1.037288	-1.212617	-2.124768	
C	4.124663	-0.121135	-0.204250	
C	-1.197917	-1.335456	2.394441	
C	-3.049094	-0.999143	-3.642410	
C	0.092310	-3.164838	-0.630334	
C	-2.347116	-0.351108	-2.612635	
C	-2.723428	3.914554	1.487915	
C	-2.123447	2.657189	1.314482	
C	6.694288	0.739851	0.637657	
C	2.033791	-1.697845	-0.047993	
C	-2.578829	-0.685809	-1.256959	
C	0.949197	-2.062647	-0.953778	
C	-3.662271	4.385687	0.551837	
C	-1.594835	-1.936713	3.602826	
C	2.193371	-0.374823	-1.952184	
C	-2.116772	-0.582481	1.636646	
C	0.346605	-3.897992	0.519050	
C	5.198230	-0.029038	-1.124101	
C	-2.912420	-1.789256	4.067141	
C	-3.508064	-1.706547	-0.960669	
C	6.468353	0.400952	-0.707995	
C	1.425102	-3.554621	1.397223	
C	-3.440583	-0.430747	2.114181	
C	-2.456489	1.847930	0.202025	
C	-3.402706	2.325863	-0.729374	
C	-4.000249	3.588567	-0.554042	
C	-3.975373	-2.013407	-3.336450	
C	-3.834847	-1.033178	3.320259	
C	2.248676	-2.467392	1.140072	
C	5.636231	0.657109	1.559777	
C	4.363628	0.237145	1.144166	
C	-4.196314	-2.367944	-1.995441	
H	0.406703	-1.287083	-3.018825	
H	-0.161173	-1.437465	2.038924	
H	-2.863600	-0.717185	-4.691357	
H	-0.725268	-3.442290	-1.313129	
H	-1.593789	0.414646	-2.856335	
H	-2.454009	4.530629	2.360511	
H	-1.396928	2.292815	2.058970	
H	7.690268	1.078149	0.964829	
H	-4.131058	5.373306	0.687196	
H	-0.863590	-2.518601	4.186070	
H	2.582221	0.334394	-2.695138	
H	-0.287891	-4.764344	0.764123	
H	5.036145	-0.320215	-2.174278	
H	-3.221016	-2.255489	5.016560	
H	-3.694541	-1.998172	0.083646	
H	7.289862	0.463630	-1.439683	
H	1.604347	-4.172877	2.291221	
H	-4.166089	0.173743	1.546735	
H	-3.687946	1.707794	-1.594501	
H	-4.739698	3.945864	-1.288622	
H	-4.518185	-2.530225	-4.143828	
H	-4.866854	-0.902943	3.683652	
H	3.089868	-2.223011	1.806113	
H	5.796101	0.945666	2.610671	
H	3.526792	0.228999	1.859008	
H	-4.911730	-3.168029	-1.746020	
C	0.343899	2.041725	-1.526712	
C	0.952984	2.392156	-0.266220	
H	-0.694896	2.367891	-1.707223	
H	0.969761	2.069944	-2.437897	
H	0.345722	2.868789	0.520086	
C	2.394025	2.690664	-0.154424	
H	0.708441	0.556856	1.151919	
O	2.933143	3.193613	0.824907	
H	3.003455	2.414394	-1.071229	

GH (R = H)				E _g (BP86/SVP) = -1900.9728078 G _g (BP86/SVP) = -1900.497242 E _s (M06//TZVP//BP86/SVP) = -1901.2725485
Ru	0.868477	0.326962	-0.252599	
P	-1.487750	0.123060	-0.053532	
C	2.951929	-0.459155	-0.631242	
C	1.170129	-1.244678	-1.960464	
C	4.258135	0.147613	-0.289022	
C	-1.147031	-1.101903	2.482722	
C	-2.527528	-1.550812	-3.724602	
C	0.368832	-3.092992	-0.253901	
C	-1.990971	-0.738605	-2.711703	
C	-3.879688	3.405749	0.892105	
C	-3.037239	2.284450	0.974688	
C	6.807156	1.238105	0.342145	
C	2.273187	-1.516019	0.110948	
C	-2.227306	-1.022761	-1.345145	
C	1.155172	-1.983532	-0.699891	
C	-4.320476	3.872433	-0.355386	
C	-1.571009	-1.675104	3.696117	
C	2.273878	-0.363411	-1.931975	
C	-2.088851	-0.627577	1.547262	
C	0.699214	-3.717103	0.940839	
C	5.246844	0.317935	-1.288761	
C	-2.940618	-1.781160	3.987324	
C	-2.988777	-2.167850	-1.024277	
C	6.505198	0.858895	-0.977210	
C	1.801301	-3.264856	1.732727	
C	-3.468585	-0.736253	1.849567	
C	-2.627968	1.600889	-0.192018	
C	-3.068102	2.087178	-1.444341	
C	-3.906376	3.211370	-1.524566	
C	-3.290977	-2.684149	-3.391215	
C	-3.889405	-1.309898	3.060473	
C	2.577055	-2.181966	1.341184	
C	5.833678	1.080368	1.345627	
C	4.572857	0.548528	1.033934	
C	-3.510730	-2.992567	-2.039040	
H	0.492898	-1.415112	-2.804668	
H	-0.073637	-1.003026	2.253057	
H	-2.338712	-1.301249	-4.781162	
H	-0.458056	-3.463898	-0.877524	
H	-1.354563	0.118070	-2.984836	
H	-4.177637	3.924642	1.816491	
H	-2.695191	1.946105	1.963055	
H	7.794594	1.660220	0.587251	
H	-4.979528	4.752844	-0.418919	
H	-0.821269	-2.035661	4.418186	
H	2.589141	0.288089	-2.757542	
H	0.114049	-4.585433	1.282313	
H	5.031691	-0.000252	-2.321168	
H	-3.272656	-2.225060	4.939614	
H	-3.172825	-2.430730	0.027388	
H	7.259122	0.976722	-1.772118	
H	2.047121	-3.799265	2.664247	
H	-4.220897	-0.356384	1.140407	
H	-2.778381	1.579535	-2.374733	
H	-4.243330	3.566057	-2.511857	
H	-3.705232	-3.327660	-4.183471	
H	-4.965770	-1.381907	3.285007	
H	3.445788	-1.866052	1.937562	
H	6.053821	1.387718	2.380643	
H	3.801836	0.467282	1.815929	
H	-4.095957	-3.884638	-1.763423	
C	1.887409	2.206734	-0.466363	
C	0.513470	2.529732	-0.255297	
H	2.320331	2.324133	-1.472606	
H	2.607027	2.386483	0.353855	
H	-0.126150	2.873638	-1.085597	
C	0.206453	3.123783	1.075381	
H	0.889186	0.636491	1.312048	
O	-0.690546	3.917349	1.315923	
H	0.939280	2.808827	1.882809	

H (R = H)			E _g (BP86/SVP) = -1900.9999686 G _g (BP86/SVP) = -1900.524572 E _s (M06//TZVP//BP86/SVP) = -1901.2974656
Ru	0.827433	-0.232854	
P	-1.480299	-0.145426	
C	2.964668	0.329687	
C	1.150653	0.471007	
C	4.215571	-0.148873	0.025161
C	-1.314785	2.291833	
C	-2.631705	-0.937518	
C	0.363592	2.872960	
C	-2.090763	-1.034989	
C	-2.989550	-2.606178	-3.108082
C	-2.286375	-1.624563	-2.391592
C	6.640649	-1.069704	-1.143078
C	2.273409	1.594308	0.423241
C	-2.294981	0.003462	1.537764
C	1.151006	1.679699	1.359556
C	-3.905002	-3.444849	-2.446095
C	-1.840353	3.364151	-2.378223
C	2.278992	-0.303460	1.767318
C	-2.169720	1.317406	-1.080610
C	0.701211	3.949808	0.626095
C	5.177095	-0.851677	0.793997
C	-3.225891	3.476143	-2.576728
C	-3.022290	1.147591	1.934587
C	6.372314	-1.308803	0.215896
C	1.802826	3.873483	-0.286438
C	-3.564885	1.433936	-1.292672
C	-2.481263	-1.469736	-0.998258
C	-3.411245	-2.306401	-0.344666
C	-4.116172	-3.287520	-1.066193
C	-3.360811	0.203155	4.158304
C	-4.088708	2.507426	-2.030183
C	2.571644	2.724335	-0.407980
C	5.695903	-0.375785	-1.920786
C	4.496328	0.073373	-1.347398
C	-3.546816	1.246783	3.237318
H	0.470295	0.246882	2.999306
H	-0.227331	2.200026	-1.486254
H	-2.470533	-1.759995	4.489385
H	-0.470889	2.933544	2.146774
H	-1.493472	-1.923708	2.219863
H	-2.824211	-2.713380	-4.192118
H	-1.587564	-0.958373	-2.923477
H	7.579414	-1.426030	-1.595747
H	-4.456459	-4.215763	-3.007310
H	-1.156832	4.113322	-2.808575
H	2.568235	-1.259739	2.221738
H	0.119291	4.882683	0.687133
H	4.992396	-1.023095	1.866141
H	-3.636160	4.313824	-3.163321
H	-3.179844	1.974636	1.226320
H	7.104139	-1.850313	0.836500
H	2.051861	4.756180	-0.897105
H	-4.247475	0.669746	-0.887841
H	-3.591063	-2.196649	0.735313
H	-4.838446	-3.932149	-0.540150
H	-3.775841	0.280124	5.175928
H	-5.176524	2.582063	-2.188835
H	3.434558	2.695616	-1.089618
H	5.889075	-0.193188	-2.990144
H	3.747141	0.579563	-1.975237
H	-4.106932	2.149844	3.529161
C	1.218136	-1.788267	-1.429901
C	1.271469	-2.365482	-0.117922
H	2.167598	-1.651294	-1.974875
H	0.357968	-2.025694	-2.077909
H	2.255520	-2.560343	0.342893
C	0.150651	-3.079261	0.507136
H	0.719029	0.305135	-1.466469
O	0.179566	-3.599030	1.626947
H	-0.784844	-3.119166	-0.121712

HI (R = H)			E _g (BP86/SVP) = -1900.9941771 G _g (BP86/SVP) = -1900.519964 E _s (M06//TZVP//BP86/SVP) = -1901.2932347
Ru	0.824058	-0.206840	0.042413
P	-1.498302	-0.146724	-0.099676
C	2.925821	0.345645	0.671678
C	1.077532	0.541012	2.132018
C	4.174374	-0.169233	0.067041
C	-1.329547	2.289672	-1.566552
C	-2.542349	-1.170461	3.776414
C	0.385044	2.964952	1.378468
C	-2.029273	-1.183400	2.468419
C	-3.073713	-2.445611	-3.173717
C	-2.376845	-1.485630	-2.422341
C	6.588183	-1.168813	-1.062700
C	2.280443	1.639194	0.423896
C	-2.280869	-0.099345	1.589309
C	1.148974	1.761586	1.337798
C	-3.920616	-3.367537	-2.531674
C	-1.843470	3.383516	-2.288795
C	2.199694	-0.269815	1.770304
C	-2.199593	1.349124	-0.979362
C	0.754140	4.025971	0.558165
C	5.090218	-0.921507	0.844871
C	-3.230987	3.550931	-2.425303
C	-3.022889	1.004180	2.064433
C	6.279324	-1.416880	0.286121
C	1.863577	3.914531	-0.332275
C	-3.596879	1.518381	-1.132555
C	-2.507078	-1.435422	-1.013365
C	-3.369737	-2.355738	-0.379840
C	-4.069927	-3.313834	-1.135825
C	-3.287918	-0.069890	4.238863
C	-4.108177	2.615595	-1.843620
C	2.614954	2.745218	-0.417448
C	5.689796	-0.426042	-1.849735
C	4.496775	0.062952	-1.294960
C	-3.518284	1.018770	3.382334
H	0.371520	0.342683	2.947187
H	-0.241363	2.150787	-1.460721
H	-2.345007	-2.025942	4.442028
H	-0.460275	3.052684	2.078280
H	-1.413130	-2.038625	2.143976
H	-2.959188	-2.468925	-4.269385
H	-1.738032	-0.751818	-2.941078
H	7.522796	-1.554476	-1.499626
H	-4.467706	-4.121034	-3.120107
H	-1.150443	4.106644	-2.747459
H	2.449068	-1.234327	2.232061
H	0.187474	4.969428	0.597148
H	4.873764	-1.102973	1.909204
H	-3.632846	4.406788	-2.991165
H	-3.213429	1.865810	1.407133
H	6.974926	-1.996124	0.914257
H	2.139018	4.779366	-0.956930
H	-4.290855	0.776914	-0.705032
H	-3.500373	-2.330102	0.712404
H	-4.739716	-4.023083	-0.623670
H	-3.680084	-0.058713	5.268327
H	-5.197864	2.735198	-1.955314
H	3.488729	2.691028	-1.083525
H	5.915401	-0.232903	-2.910911
H	3.787860	0.614369	-1.931546
H	-4.089822	1.891429	3.737523
C	1.190743	-1.589522	-1.639959
C	1.321223	-2.254584	-0.351194
H	2.121820	-1.461613	-2.222039
H	0.331550	-1.882486	-2.271191
H	2.334880	-2.463221	0.037383
C	0.246212	-3.059832	0.240936
H	0.849402	-0.101258	-1.605171
O	0.322395	-3.664643	1.315598
H	-0.704490	-3.085343	-0.366939

I (R = H)				E _g (BP86/SVP) = -1900.9968893 G _g (BP86/SVP) = -1900.519737 E _s (M06//TZVP//BP86/SVP) = -1901.3000428
Ru	0.821991	-0.167066	0.023224	
P	-1.517924	-0.140813	-0.078583	
C	2.906959	0.344695	0.667637	
C	1.018992	0.583645	2.060748	
C	4.155522	-0.198147	0.087545	
C	-1.391996	2.333632	-1.469870	
C	-2.432268	-1.347592	3.772074	
C	0.448916	3.049419	1.342862	
C	-1.942579	-1.284885	2.456581	
C	-3.142048	-2.342973	-3.200960	
C	-2.448760	-1.395124	-2.431082	
C	6.566643	-1.257544	-0.993422	
C	2.312835	1.668664	0.419157	
C	-2.263590	-0.181191	1.625934	
C	1.174118	1.827801	1.311862	
C	-3.937947	-3.318379	-2.572723	
C	-1.918461	3.444354	-2.156325	
C	2.135915	-0.264057	1.738013	
C	-2.251138	1.375794	-0.893602	
C	0.861730	4.101901	0.525576	
C	5.031512	-0.981561	0.880343	
C	-3.308404	3.611206	-2.267191	
C	-3.048532	0.866065	2.155128	
C	6.219185	-1.506135	0.345887	
C	1.974472	3.953206	-0.348741	
C	-3.650885	1.544006	-1.022975	
C	-2.531194	-1.409804	-1.017617	
C	-3.343481	-2.383624	-0.397554	
C	-4.040217	-3.329694	-1.171598	
C	-3.222856	-0.303949	4.288799	
C	-4.174724	2.658510	-1.697351	
C	2.692026	2.757634	-0.419871	
C	5.707716	-0.484888	-1.795676	
C	4.516361	0.034093	-1.264825	
C	-3.520753	0.804883	3.480165	
H	0.285689	0.402479	2.856129	
H	-0.301582	2.193832	-1.382214	
H	-2.180792	-2.216513	4.401011	
H	-0.406324	3.162401	2.026862	
H	-1.289283	-2.093053	2.086096	
H	-3.065297	-2.314760	-4.299850	
H	-1.850607	-0.619853	-2.938076	
H	7.500399	-1.665918	-1.411147	
H	-4.482028	-4.062721	-3.175423	
H	-1.234003	4.180619	-2.606748	
H	2.346985	-1.234247	2.207180	
H	0.324054	5.062426	0.557906	
H	4.783504	-1.165895	1.937199	
H	-3.720848	4.480241	-2.804630	
H	-3.290430	1.742874	1.535714	
H	6.883048	-2.109407	0.985677	
H	2.284693	4.805550	-0.974343	
H	-4.336727	0.787613	-0.608765	
H	-3.435953	-2.409812	0.698613	
H	-4.669932	-4.081479	-0.669343	
H	-3.596714	-0.351743	5.324012	
H	-5.266160	2.778117	-1.790505	
H	3.571251	2.675100	-1.075681	
H	5.963671	-0.290904	-2.849824	
H	3.838416	0.608835	-1.914567	
H	-4.126830	1.634250	3.879093	
C	1.145205	-1.497694	-1.840790	
C	1.331139	-2.145934	-0.515008	
H	2.059533	-1.465918	-2.466169	
H	0.274773	-1.866503	-2.418808	
H	2.366328	-2.372705	-0.197137	
C	0.307948	-3.016617	0.073703	
H	0.899802	-0.288182	-1.774024	
O	0.438738	-3.655023	1.124302	
H	-0.661446	-3.059704	-0.504763	

IJ (R = H)				E _g (BP86/SVP) = -1900.9708327 G _g (BP86/SVP) = -1900.496157 E _s (M06//TZVP//BP86/SVP) = -1901.2757718
Ru	0.772856	0.009888	-0.940996	
P	-1.372288	0.250024	0.177906	
C	2.813910	-0.655045	-0.584984	
C	1.342481	-1.646080	-2.131592	
C	3.930235	0.126228	-0.010340	
C	-0.286196	-0.119579	2.765097	
C	-3.239842	-2.192436	-2.585529	
C	0.268921	-3.375341	-0.459066	
C	-2.497756	-1.171532	-1.967490	
C	-2.927406	4.062975	0.716467	
C	-2.168631	2.886587	0.819236	
C	6.102602	1.598878	1.079391	
C	2.007845	-1.679920	0.115664	
C	-2.420764	-1.104114	-0.553469	
C	1.133369	-2.319311	-0.855806	
C	-4.013952	4.128656	-0.175459	
C	-0.328939	-0.226103	4.167532	
C	2.479108	-0.756210	-1.992166	
C	-1.472384	0.026681	2.021153	
C	0.329846	-3.839325	0.854038	
C	5.137372	0.286795	-0.734284	
C	-1.562580	-0.188342	4.837802	
C	-3.071567	-2.089670	0.218835	
C	6.209752	1.016409	-0.195511	
C	1.238229	-3.262951	1.790541	
C	-2.711088	0.081268	2.704320	
C	-2.482733	1.752510	0.032441	
C	-3.580584	1.823829	-0.851712	
C	-4.337970	3.005653	-0.954052	
C	-3.891887	-3.169282	-1.809826	
C	-2.753730	-0.034080	4.103036	
C	2.063184	-2.194921	1.445489	
C	4.908620	1.450302	1.809482	
C	3.834446	0.726888	1.270186	
C	-3.800397	-3.1117225	-0.408961	
H	0.836612	-1.887677	-3.076331	
H	0.670677	-0.143673	2.221491	
H	-3.298510	-2.227468	-3.685285	
H	-0.410933	-3.836302	-1.192081	
H	-1.959923	-0.433394	-2.590101	
H	-2.668018	4.934594	1.338610	
H	-1.327076	2.846561	1.530227	
H	6.944198	2.170394	1.501725	
H	-4.607577	5.052741	-0.259516	
H	0.607671	-0.335242	4.737344	
H	2.948059	-0.196840	-2.811077	
H	-0.313473	-4.675306	1.169336	
H	5.238599	-0.184402	-1.724554	
H	-1.598938	-0.269052	5.936044	
H	-3.004442	-2.069469	1.316582	
H	7.139950	1.125500	-0.775886	
H	1.291969	-3.679153	2.809295	
H	-3.645417	0.232215	2.140863	
H	-3.852488	0.953969	-1.468253	
H	-5.190750	3.042807	-1.650770	
H	-4.465886	-3.973165	-2.298017	
H	-3.723219	0.008354	4.624874	
H	2.780758	-1.781531	2.170613	
H	4.809476	1.912825	2.804655	
H	2.888778	0.651043	1.828293	
H	-4.299495	-3.882508	0.207195	
C	1.339570	3.103934	-0.775299	
C	1.194052	1.967369	-1.774376	
H	1.535471	4.071361	-1.294634	
H	0.420407	3.238516	-0.168090	
H	2.067411	1.840176	-2.440866	
C	-0.096227	1.754703	-2.411450	
H	2.186090	2.930094	-0.079572	
O	-0.324659	1.016311	-3.409268	
H	-0.957528	2.298916	-1.928843	

J (R = H)			E _g (BP86/SVP) = -1900.9989622 G _g (BP86/SVP) = -1900.519114 E _s (M06//TZVP//BP86/SVP) = -1901.2959314
Ru	0.760293	-0.132889	
P	-1.565047	-0.253157	
C	2.875715	0.191990	
C	0.917748	0.540957	2.118517
C	4.133384	-0.437469	0.392614
C	-1.820944	2.293442	-1.187977
C	-2.254064	-1.491387	3.925892
C	0.486848	3.010033	1.330955
C	-1.768976	-1.360131	2.614492
C	-3.327343	-2.701369	-2.875349
C	-2.792763	-1.598950	-2.187039
C	6.572054	-1.693766	-0.408322
C	2.368017	1.541148	0.557594
C	-2.281678	-0.365855	1.744886
C	1.166002	1.757494	1.356690
C	-3.458507	-3.943398	-2.230296
C	-2.503917	3.376859	-1.771978
C	1.972316	-0.381855	1.831791
C	-2.526446	1.156962	-0.742611
C	0.999986	4.043274	0.552437
C	4.715183	-1.483701	1.157357
C	-3.900236	3.334079	-1.917893
C	-3.260349	0.520351	2.244349
C	5.910621	-2.100975	0.764494
C	2.181533	3.846562	-0.221512
C	-3.933669	1.119643	-0.898772
C	-2.386201	-1.712231	-0.835342
C	-2.514452	-2.967991	-0.203656
C	-3.048418	-4.070946	-0.893109
C	-3.239827	-0.610230	4.407535
C	-4.614016	2.202073	-1.480500
C	2.857678	2.628599	-0.234054
C	6.015736	-0.660716	-1.180533
C	4.817126	-0.042933	-0.788073
C	-3.730935	0.400630	3.566134
H	0.127447	0.410775	2.866211
H	-0.725939	2.317429	-1.070386
H	-1.847720	-2.278987	4.580687
H	-0.415023	3.153462	1.946438
H	-0.955251	-2.017704	2.267270
H	-3.643288	-2.585011	-3.924547
H	-2.701950	-0.634778	-2.711521
H	7.512128	-2.177827	-0.716533
H	-3.876752	-4.808380	-2.769121
H	-1.937298	4.256356	-2.117011
H	2.089672	-1.368173	2.297478
H	0.498140	5.023374	0.538112
H	4.228594	-1.808652	2.089046
H	-4.435823	4.180200	-2.377617
H	-3.659827	1.320539	1.604043
H	6.333618	-2.907195	1.385196
H	2.579897	4.686365	-0.813551
H	-4.500747	0.232620	-0.574316
H	-2.204934	-3.097493	0.842620
H	-3.141145	-5.038980	-0.375344
H	-3.613125	-0.705297	5.439559
H	-5.708887	2.159699	-1.597869
H	3.788973	2.529238	-0.808180
H	6.516215	-0.330723	-2.105124
H	4.402074	0.751521	-1.423274
H	-4.489956	1.108374	3.936690
C	1.038236	0.835634	-3.180093
C	1.453930	-0.150398	-2.117954
H	1.572433	0.638060	-4.137553
H	-0.051781	0.791154	-3.382370
H	2.536614	-0.241740	-1.926097
C	0.663186	-1.293202	-1.804130
H	1.283260	1.877604	-2.884280
O	1.006598	-2.086572	-0.811432
H	-0.284954	-1.492135	-2.353931

JK (R = H)				E _g (BP86/SVP) = -2093.9614749 G _g (BP86/SVP) = -2093.408439 E _s (M06//TZVP//BP86/SVP) = -2094.3521469
Ru	0.499451	0.775128	-0.156211	
P	-1.591187	-0.205658	0.102289	
C	2.485722	0.815515	0.934970	
C	0.455914	1.509787	1.870537	
C	3.691897	0.018889	0.618836	
C	-2.929103	2.242587	0.651485	
C	-0.644750	-2.978103	3.056855	
C	0.517784	3.959124	0.842732	
C	-0.660585	-2.208842	1.881476	
C	-3.271905	-1.743980	-3.377184	
C	-2.807368	-0.889018	-2.364487	
C	6.062486	-1.430517	0.066237	
C	2.239977	2.173956	0.477671	
C	-1.644097	-1.210509	1.683179	
C	0.951924	2.601098	1.035509	
C	-3.182123	-3.138553	-3.220360	
C	-4.042919	3.072396	0.873850	
C	1.440534	0.457587	1.872006	
C	-3.097169	0.882196	0.321730	
C	1.314487	4.816799	0.106269	
C	4.357935	-0.695695	1.643997	
C	-5.343042	2.551594	0.762835	
C	-2.590650	-0.985081	2.706784	
C	5.534124	-1.413043	1.369145	
C	2.564699	4.384560	-0.464342	
C	-4.410468	0.366460	0.213027	
C	-2.246368	-1.409064	-1.173529	
C	-2.165466	-2.809694	-1.025812	
C	-2.630879	-3.665351	-2.040856	
C	-1.592289	-2.745259	4.070387	
C	-5.523286	1.196221	0.430614	
C	3.029175	3.091608	-0.285910	
C	5.401666	-0.732238	-0.961858	
C	4.224576	-0.016210	-0.694009	
C	-2.558717	-1.742100	3.893395	
H	-0.437821	1.541301	2.508060	
H	-1.909904	2.651447	0.711846	
H	0.118294	-3.763243	3.180746	
H	-0.414875	4.315813	1.307308	
H	0.099762	-2.382266	1.106005	
H	-3.709044	-1.315012	-4.292060	
H	-2.902715	0.199758	-2.497436	
H	6.984577	-1.993499	-0.149492	
H	-3.545287	-3.811038	-4.013778	
H	-3.892412	4.134370	1.126300	
H	1.389569	-0.470660	2.452963	
H	1.000054	5.863103	-0.036430	
H	3.960309	-0.665754	2.670933	
H	-6.216881	3.201258	0.930692	
H	-3.362931	-0.211269	2.584735	
H	6.043892	-1.957769	2.179963	
H	3.169832	5.108844	-1.031863	
H	-4.565608	-0.693297	-0.043175	
H	-1.742142	-3.247893	-0.111283	
H	-2.561400	-4.756126	-1.901531	
H	-1.573666	-3.342117	4.996204	
H	-6.539450	0.779752	0.340218	
H	3.999122	2.776269	-0.698289	
H	5.798893	-0.757626	-1.989291	
H	3.669966	0.472416	-1.512625	
H	-3.301798	-1.543867	4.682591	
C	-1.133727	2.755501	-2.262908	
C	0.167346	2.022002	-2.013905	
H	-1.100420	3.291319	-3.239822	
H	-2.010906	2.077513	-2.287478	
H	1.050981	2.683468	-1.959014	
C	0.418124	0.752462	-2.615548	
H	-1.327121	3.518223	-1.483506	
O	1.578875	0.236210	-2.816236	
H	-0.479935	0.159855	-2.934027	
C	1.526234	-4.994850	-0.095735	
C	1.431245	-4.012782	-1.011949	
H	1.106127	-5.998298	-0.272778	
H	2.046452	-4.834599	0.865506	
H	0.904409	-4.196237	-1.966919	
C	2.024168	-2.634341	-0.862252	
H	2.406714	-2.492953	0.175314	
O	1.075847	-1.616264	-1.185707	
H	1.398125	-1.068907	-1.987483	
H	2.910819	-2.543238	-1.532908	

K (R = H)				E _g (BP86/SVP) = -2093.9757865 G _g (BP86/SVP) = -2093.421649 E _s (M06//TZVP//BP86/SVP) = -2094.3601276
Ru	0.604460	0.289625	-0.064365	
P	-1.681220	-0.128058	0.024515	
C	2.756002	0.501742	0.793604	
C	0.769320	0.754337	2.043677	
C	4.030157	-0.065580	0.308184	
C	-2.488550	2.538858	-0.453497	
C	-1.986705	-1.733366	3.855229	
C	0.487884	3.330646	1.586604	
C	-1.582209	-1.431685	2.544290	
C	-3.042878	-2.675504	-2.994847	
C	-2.585490	-1.557224	-2.279163	
C	6.505359	-1.173707	-0.571612	
C	2.327507	1.886403	0.692217	
C	-2.288594	-0.482470	1.765712	
C	1.090494	2.045179	1.446843	
C	-3.264518	-3.897396	-2.337495	
C	-3.375624	3.573907	-0.799627	
C	1.812281	-0.168629	1.686732	
C	-2.898966	1.189558	-0.508076	
C	1.115657	4.434914	1.019527	
C	4.754237	-0.983866	1.114479	
C	-4.684034	3.272655	-1.214955	
C	-3.395676	0.171946	2.347126	
C	5.972331	-1.530030	0.680176	
C	2.342709	4.283960	0.300286	
C	-4.221982	0.896463	-0.913818	
C	-2.345034	-1.631164	-0.887781	
C	-2.583057	-2.862531	-0.236748	
C	-3.035602	-3.984378	-0.954358	
C	-3.092276	-1.074142	4.423847	
C	-5.104312	1.931439	-1.270334	
C	2.944166	3.042135	0.122030	
C	5.804540	-0.262621	-1.382361	
C	4.586101	0.283880	-0.950369	
C	-3.789204	-0.117912	3.667718	
H	-0.028918	0.580181	2.774707	
H	-1.458890	2.774410	-0.141448	
H	-1.427211	-2.481231	4.439995	
H	-0.435895	3.441356	2.176278	
H	-0.693988	-1.928579	2.119998	
H	-3.221524	-2.587298	-4.078219	
H	-2.433628	-0.609274	-2.814012	
H	7.460432	-1.603018	-0.913085	
H	-3.620454	-4.775435	-2.899704	
H	-3.036563	4.621237	-0.752553	
H	1.917231	-1.191913	2.069272	
H	0.678303	5.438825	1.135551	
H	4.361174	-1.252834	2.107665	
H	-5.376962	4.081821	-1.496276	
H	-3.958869	0.919205	1.768626	
H	6.514751	-2.235457	1.330258	
H	2.829513	5.181526	-0.114392	
H	-4.567336	-0.148131	-0.952267	
H	-2.436536	-2.952575	0.848927	
H	-3.218752	-4.930897	-0.420446	
H	-3.403693	-1.301650	5.455783	
H	-6.129677	1.686495	-1.591319	
H	3.902626	2.956848	-0.410588	
H	6.205840	0.019282	-2.369083	
H	4.037709	0.969216	-1.614285	
H	-4.651437	0.411173	4.104723	
C	0.550788	2.634821	-2.329520	
C	0.908208	1.165910	-2.159527	
H	1.063026	3.059718	-3.223383	
H	-0.540113	2.762269	-2.489497	
H	1.990547	0.941159	-2.233587	
C	0.095390	0.250037	-2.898772	
H	0.841845	3.266262	-1.468844	
O	0.381350	-0.944974	-3.235239	
H	-0.912413	0.650909	-3.202397	
C	1.978730	-4.053826	1.452211	
C	1.250762	-3.586717	0.420086	
H	1.563135	-4.776738	2.172822	
H	3.028118	-3.744621	1.601054	
H	0.204342	-3.915398	0.280527	
C	1.771138	-2.662444	-0.648457	
C	2.754184	-2.227636	-0.362012	
O	0.818945	-1.644288	-0.969548	
H	0.751477	-1.479228	-2.029644	
H	1.933983	-3.250127	-1.583263	

KL (R = H)				E _g (BP86/SVP) = -2093.966625 G _g (BP86/SVP) = -2093.413794 E _s (M06//TZVP//BP86/SVP) = -2094.3528148
Ru	-0.668236	0.039383	0.231960	
P	1.695751	0.160860	0.004575	
C	-2.721201	-0.389490	1.035831	
C	-0.747265	-0.269508	2.339304	
C	-4.060755	-0.045461	0.511080	
C	1.789484	-2.381815	-1.216474	
C	2.924191	0.788381	3.919069	
C	-0.030406	-2.785314	2.029409	
C	2.334893	0.921646	2.651241	
C	2.734524	3.368676	-2.419028	
C	2.099469	2.241436	-1.870565	
C	-6.662175	0.655552	-0.420211	
C	-2.016120	-1.685311	0.963702	
C	2.540311	-0.059980	1.651446	
C	-0.838762	-1.626080	1.825097	
C	3.822106	3.967425	-1.759790	
C	2.358927	-3.425691	-1.966385	
C	-1.929919	0.448920	1.910399	
C	2.487649	-1.169181	-1.032182	
C	-0.388778	-3.976611	1.410008	
C	-4.901787	0.822305	1.256611	
C	3.627161	-3.263380	-2.551200	
C	3.342841	-1.179283	1.955484	
C	-6.180731	1.171018	0.796001	
C	-1.542377	-4.042093	0.568553	
C	3.761790	-1.012264	-1.622826	
C	2.547846	1.691479	-0.647424	
C	3.647829	2.294633	0.005591	
C	4.277736	3.424938	-0.546542	
C	3.717967	-0.335992	4.215194	
C	4.325275	-2.054489	-2.379187	
C	-2.345117	-2.929602	0.337144	
C	-5.846602	-0.211473	-1.168808	
C	-4.565143	-0.556489	-0.712256	
C	3.922611	-1.317619	3.231719	
H	-0.004876	0.087062	3.063457	
H	0.790393	-2.495750	-0.766555	
H	2.760540	1.566699	4.681733	
H	0.841909	-2.730002	2.698715	
H	1.709293	1.801983	2.428451	
H	2.366392	3.782111	-3.371647	
H	1.247423	1.802893	-2.409354	
H	-7.666273	0.927053	-0.782350	
H	4.314930	4.853617	-2.191059	
H	1.802356	-4.366758	-2.101462	
H	-2.172804	1.477544	2.206954	
H	0.212613	-4.884263	1.574120	
H	-4.551767	1.210292	2.225968	
H	4.070348	-4.077537	-3.146865	
H	3.521517	-1.949779	1.189930	
H	-6.810751	1.844803	1.398746	
H	-1.811916	-5.004735	0.104925	
H	4.314856	-0.068370	-1.497382	
H	4.026871	1.879503	0.951022	
H	5.134757	3.878428	-0.022751	
H	4.176395	-0.443655	5.211059	
H	5.316733	-1.918351	-2.840386	
H	-3.250533	-3.018222	-0.280202	
H	-6.206419	-0.617075	-2.127921	
H	-3.934666	-1.206542	-1.335256	
H	4.545690	-2.199298	3.452317	
C	-1.402646	-2.332341	-3.089804	
C	-1.351649	-0.875218	-2.720092	
H	-2.449312	-2.690405	-3.225544	
H	-0.861941	-2.523199	-4.040672	
H	-1.901776	-0.544720	-1.814186	
C	-0.782913	0.072979	-3.518596	
H	-0.950625	-2.985768	-2.312693	
O	-0.708998	1.393799	-3.290065	
H	-0.320866	-0.221722	-4.483081	
C	-1.964430	4.263091	1.639358	
C	-1.230295	3.755254	0.631018	
H	-1.542304	4.982336	2.360231	
H	-3.028214	3.994397	1.768235	
H	-0.169111	4.044614	0.514325	
C	-1.744689	2.815661	-0.433966	
H	-2.741274	2.400586	-0.143787	
O	-0.805241	1.807391	-0.762010	
H	-0.834076	1.570320	-2.277477	
H	-1.916595	3.414380	-1.365396	

L (R = H)				E _g (BP86/SVP) = -1901.2491499 G _g (BP86/SVP) = -2093.421048 E _s (M06//TZVP//BP86/SVP) = -2094.3560212
Ru	0.595975	0.070724	-0.548150	
P	-1.716777	0.194096	-0.041248	
C	2.576115	-0.631552	-1.275561	
C	0.602287	-0.607755	-2.576061	
C	3.922810	-0.294638	-0.762253	
C	-1.540053	-2.047746	1.671516	
C	-3.361448	0.087525	-3.849570	
C	-0.290157	-2.967611	-1.801395	
C	-2.632404	0.447820	-2.704183	
C	-2.472937	3.699050	2.025033	
C	-1.931870	2.480145	1.584717	
C	6.526870	0.354316	0.166625	
C	1.772494	-1.827219	-0.951905	
C	-2.747988	-0.303137	-1.509475	
C	0.599737	-1.846243	-1.822221	
C	-3.566824	4.275885	1.355519	
C	-1.981514	-2.933339	2.670650	
C	1.853674	0.081947	-2.296691	
C	-2.327642	-0.936403	1.304741	
C	-0.005155	-4.039018	-0.967215	
C	4.927018	0.147896	-1.659303	
C	-3.208774	-2.710997	3.318756	
C	-3.602925	-1.425435	-1.492567	
C	6.213988	0.470851	-1.199073	
C	1.147977	-4.024572	-0.116249	
C	-3.560653	-0.717293	1.960601	
C	-2.484278	1.814490	0.465128	
C	-3.587364	2.396701	-0.198813	
C	-4.122675	3.620362	0.244052	
C	-4.206309	-1.038168	-3.825205	
C	-3.996365	-1.600958	2.962355	
C	2.023210	-2.946160	-0.092855	
C	5.538725	-0.080766	1.068554	
C	4.250143	-0.400223	0.612770	
C	-4.322799	-1.792062	-2.645707	
H	-0.131297	-0.327140	-3.341734	
H	-0.573619	-2.210294	1.168075	
H	-3.266407	0.687996	-4.768601	
H	-1.162241	-2.985145	-2.472568	
H	-1.964774	1.324645	-2.733580	
H	-2.027224	4.201233	2.898363	
H	-1.073080	2.055378	2.124183	
H	7.536263	0.606703	0.528403	
H	-3.986865	5.234210	1.700864	
H	-1.356420	-3.796979	2.947975	
H	2.180334	1.016936	-2.771770	
H	-0.667541	-4.918628	-0.959865	
H	4.694903	0.219273	-2.733894	
H	-3.550355	-3.399647	4.108130	
H	-3.708852	-2.020090	-0.572502	
H	6.980157	0.809580	-1.914875	
H	1.350146	-4.897863	0.524493	
H	-4.180362	0.152793	1.692071	
H	-4.042710	1.892308	-1.064276	
H	-4.985126	4.058204	-0.284068	
H	-4.772853	-1.324882	-4.725422	
H	-4.956257	-1.417783	3.471426	
H	2.925362	-2.965651	0.536855	
H	5.766781	-0.157069	2.143640	
H	3.472442	-0.686290	1.338368	
H	-4.983440	-2.673489	-2.616233	
C	1.820137	-1.652111	4.240064	
C	1.480269	-0.499551	3.333722	
H	2.710456	-2.221728	3.888033	
H	2.039183	-1.305463	5.272281	
H	1.237627	-0.729279	2.277109	
C	1.422763	0.789014	3.749802	
H	0.986244	-2.387274	4.307964	
O	1.113964	1.892169	3.024832	
H	1.633830	1.050097	4.805000	
C	2.354563	3.967136	-2.144414	
C	1.561683	3.643878	-1.105164	
H	2.039568	4.696368	-2.908738	
H	3.361836	3.527991	-2.257368	
H	0.558913	4.099751	-1.006270	
C	1.942723	2.700204	0.008313	
H	2.879335	2.150418	-0.248503	
O	0.871956	1.821349	0.341196	
H	0.993752	1.682689	2.047951	
H	2.161393	3.301107	0.925976	

LF (R = H)				E _g (BP86/SVP) = -1900.9459039 G _g (BP86/SVP) = -1900.470205 E _s (M06//TZVP//BP86/SVP) = -1901.2491499
Ru	0.734514	0.060942	-0.287682	
P	-1.585020	0.201508	-0.061413	
C	2.815208	-0.667279	-0.700800	
C	0.937622	-1.248409	-2.063204	
C	4.145217	-0.138283	-0.342840	
C	-1.344462	-0.986540	2.497699	
C	-3.045410	-1.227314	-3.667762	
C	0.017383	-3.140904	-0.475232	
C	-2.367635	-0.492525	-2.680611	
C	-2.545302	4.102941	0.900756	
C	-1.997255	2.810662	0.876544	
C	6.741313	0.851097	0.293002	
C	2.040140	-1.700756	-0.016544	
C	-2.555901	-0.780020	-1.306806	
C	0.894218	-2.066695	-0.874270	
C	-3.468715	4.502240	-0.083761	
C	-1.811215	-1.417967	3.752857	
C	2.075255	-0.379997	-1.927986	
C	-2.229580	-0.375425	1.585689	
C	0.277356	-3.823952	0.695039	
C	5.062096	0.229501	-1.361797	
C	-3.159467	-1.242402	4.107032	
C	-3.420746	-1.836937	-0.949250	
C	6.338686	0.723070	-1.047901	
C	1.403928	-3.480791	1.525572	
C	-3.581969	-0.184875	1.953778	
C	-2.373378	1.892969	-0.135028	
C	-3.303726	2.297521	-1.116306	
C	-3.845238	3.596828	-1.089471	
C	-3.906825	-2.277613	-3.300017	
C	-4.044983	-0.622505	3.205441	
C	2.264137	-2.451666	1.194268	
C	5.847012	0.486230	1.316425	
C	4.566536	0.004837	1.005334	
C	-4.086740	-2.582179	-1.940505	
H	0.251835	-1.304611	-2.916358	
H	-0.282665	-1.095410	2.226418	
H	-2.894009	-0.982766	-4.731471	
H	-0.823121	-3.424375	-1.126750	
H	-1.673393	0.310698	-2.977385	
H	-2.247971	4.805046	1.696312	
H	-1.266054	2.493601	1.638715	
H	7.744506	1.233105	0.539654	
H	-3.896748	5.517251	-0.063468	
H	-1.109579	-1.886527	4.461349	
H	2.371315	0.377383	-2.667691	
H	-0.377478	-4.654785	1.001560	
H	4.773708	0.106028	-2.417613	
H	-3.521594	-1.578936	5.091917	
H	-3.572008	-2.086285	0.111786	
H	7.029679	0.999368	-1.860719	
H	1.586295	-4.065169	2.441529	
H	-4.276638	0.317470	1.261325	
H	-3.624118	1.596371	-1.901618	
H	-4.573685	3.896909	-1.860011	
H	-4.432155	-2.859903	-4.073662	
H	-5.100818	-0.470773	3.482053	
H	3.141820	-2.237056	1.820318	
H	6.144797	0.591785	2.372108	
H	3.862926	-0.228155	1.818192	
H	-4.753494	-3.407399	-1.642769	
C	2.317545	2.996410	-1.071678	
C	1.418899	2.880692	-0.066526	
H	2.042804	3.444977	-2.041137	
H	3.355734	2.641040	-0.954818	
H	0.390857	3.263167	-0.211125	
C	1.683756	2.226298	1.278149	
H	2.763279	1.927605	1.331991	
O	0.793890	1.152741	1.477147	
H	1.524972	2.976774	2.096462	

C (R = Me)				E _g (BP86/SVP) = -2401.0400328 G _g (BP86/SVP) = -2400.523787 E _s (M06//TZVP//BP86/SVP) = -2401.4512855
Ru	0.608092	0.141924	-0.390676	
Cl	0.956645	0.420174	2.021802	
P	-1.702194	0.203625	0.036564	
C	2.647005	-0.896468	-0.765032	
C	0.778231	-1.067083	-2.204691	
C	3.996483	-0.558790	-0.262166	
C	-1.540776	-1.795435	2.046236	
C	-3.298678	-0.569400	-3.734812	
C	-0.224482	-3.238842	-1.121106	
C	-2.550713	-0.035052	-2.672265	
C	-2.503461	3.878311	1.738734	
C	-1.976233	2.609873	1.447412	
C	6.619588	0.019867	0.653736	
C	1.812560	-2.034150	-0.332986	
C	-2.733123	-0.506416	-1.349329	
C	0.694519	-2.160322	-1.249006	
C	-3.515002	4.430061	0.930835	
C	-2.014202	-2.541672	3.139226	
C	2.034302	-0.385395	-1.961330	
C	-2.310264	-0.737759	1.520136	
C	-0.008741	-4.188820	-0.124343	
C	5.030986	-0.233757	-1.174738	
C	-3.254329	-2.233986	3.724078	
C	-3.670650	-1.539529	-1.126246	
C	6.327257	0.055543	-0.720952	
C	1.086858	-4.066579	0.777494	
C	-3.555430	-0.428596	2.115088	
C	-2.464572	1.873138	0.340512	
C	-3.482270	2.429603	-0.463991	
C	-4.002134	3.704009	-0.168676	
C	-4.228763	-1.598607	-3.500655	
C	-4.023288	-1.174385	3.210590	
C	1.983229	-3.000376	0.696192	
C	5.601191	-0.295701	1.570253	
C	4.302256	-0.578869	1.121321	
C	-4.407945	-2.082968	-2.194770	
H	0.143703	-0.956535	-3.092307	
H	-0.557401	-2.024066	1.612863	
H	-3.148582	-0.180978	-4.754954	
H	-1.065757	-3.332346	-1.824583	
H	-1.814902	0.756474	-2.878089	
H	-2.117020	4.440496	2.603727	
H	-1.182691	2.178584	2.080839	
H	7.637696	0.243431	1.010079	
H	-3.924653	5.426547	1.160846	
H	-1.398352	-3.360518	3.543479	
H	2.466503	0.396967	-2.598615	
H	-0.693212	-5.046181	-0.028461	
H	4.820478	-0.233102	-2.256086	
H	-3.619243	-2.813885	4.586979	
H	-3.828178	-1.927476	-0.109138	
H	7.117381	0.301598	-1.448438	
H	1.233485	-4.837039	1.551173	
H	-4.163119	0.403302	1.725900	
H	-3.881534	1.865486	-1.320806	
H	-4.798100	4.126736	-0.802536	
H	-4.809629	-2.021920	-4.335439	
H	-4.992549	-0.920059	3.668604	
H	2.834281	-2.928004	1.388169	
H	5.815458	-0.304404	2.650885	
H	3.496137	-0.764315	1.847270	
H	-5.130831	-2.890991	-1.998378	
C	0.239866	1.903587	-1.587164	
C	0.986619	2.266554	-0.421191	
H	-0.810471	2.236339	-1.656877	
H	0.743088	1.858983	-2.570591	
H	0.417152	2.737289	0.401772	
C	2.438603	2.719678	-0.424412	
H	3.007483	2.123630	-1.185213	
C	2.544947	4.200954	-0.823480	
H	1.943034	4.832136	-0.137092	
H	3.602556	4.528740	-0.751863	
H	2.192765	4.365598	-1.862853	
O	3.029001	2.576777	0.857719	
H	2.590312	1.809957	1.297622	

D (R = Me)			E_g(BP86/SVP) = -2633.9617502 G_g(BP86/SVP) = -2633.342478 E_s(M06//TZVP//BP86/SVP) = -2634.4999825
Ru	-0.189780	-0.493655	
Cl	0.524652	0.125097	
P	-2.107731	0.728528	
C	1.057893	-2.405352	
C	-0.852090	-1.973467	
C	2.471133	-2.697631	
C	-2.628613	-0.734646	
C	-4.328788	0.265999	
C	-2.558712	-3.214679	
C	-3.313821	0.562905	
C	-0.833054	4.578439	
C	-0.969104	3.181319	
C	5.176671	-3.272230	
C	-0.123777	-2.949354	
C	-3.520699	0.383055	
C	-1.291521	-2.716972	
C	-1.726819	5.405637	
C	-3.267249	-0.983492	
C	0.595782	-1.911237	
C	-2.920483	0.436895	
C	-2.648814	-3.939786	
C	3.069134	-3.900260	
C	-4.193863	-0.063087	
C	-4.766583	-0.123500	
C	4.410737	-4.189418	
C	-1.507385	-4.148148	
C	-3.847482	1.362375	
C	-2.010402	2.593399	
C	-2.904798	3.428265	
C	-2.762254	4.827511	
C	-5.566635	-0.237179	
C	-4.481739	1.113123	
C	-0.252060	-3.646823	
C	4.591465	-2.078182	
C	3.242180	-1.802302	
C	-5.777967	-0.434982	
H	-1.481582	-1.738418	
H	-1.881226	-1.442874	
H	-4.146738	0.422045	
H	-3.445954	-3.050196	
H	-2.342056	0.932641	
H	-0.011084	5.020494	
H	-0.265656	2.531570	
H	6.237138	-3.486377	
H	-1.611702	6.501351	
H	-3.022479	-1.900859	
H	1.252872	-1.568743	
H	-3.622467	-4.348833	
H	2.474358	-4.607809	
H	-4.684877	-0.256675	
H	-4.950377	-0.280539	
H	4.863556	-5.128777	
H	-1.615134	-4.716363	
H	-4.070752	2.291463	
H	-3.718112	2.987187	
H	-3.465929	5.467495	
H	-6.360448	-0.477554	
H	-5.197787	1.847655	
H	0.634411	-3.803845	
H	5.174510	-1.307299	
H	2.778474	-0.875687	
H	-6.740203	-0.834731	
C	0.078292	1.060098	
C	1.243942	1.058509	
H	-0.637139	1.898979	
H	0.151500	0.662866	
H	1.261527	1.765255	
C	2.719119	0.835592	
H	3.068332	-0.173958	
O	3.448848	1.871468	
H	4.337722	1.433261	
C	6.069565	2.158635	
C	7.129333	1.827786	
H	7.961674	2.565675	
H	6.659854	1.818215	
H	7.556374	0.818738	
C	5.472379	3.566577	
H	4.672261	3.760883	
H	5.012859	3.596216	
H	6.235389	4.375224	
C	6.699106	2.119551	
H	7.147858	1.119658	
H	5.885826	2.270345	
H	7.486341	2.893718	
O	5.054167	1.183110	
C	2.829135	0.797551	
H	2.245844	-0.020922	
H	2.492969	1.767453	
H	3.896208	0.658697	

DE (R = Me)			E_g(BP86/SVP) = -2633.9413082 G_g(BP86/SVP) = -2633.321772 E_s(M06//TZVP//BP86/SVP) = -2634.4825789
Ru	-0.025054	-0.338950	
Cl	0.998612	0.867186	
P	-2.031781	0.482434	
C	1.499610	-2.278109	
C	-0.616690	-2.237189	
C	2.959958	-2.279757	
C	-1.650827	-0.481659	
C	-4.860249	-1.354583	
C	-1.886127	-3.429319	
C	-3.747724	-0.642751	
C	-1.724242	4.596245	
C	-1.494296	3.235207	
C	5.758957	-2.408718	
C	0.514257	-2.794098	
C	-3.565451	-0.420941	
C	-0.777668	-2.847943	
C	-2.899098	5.006449	
C	-1.885399	-0.537970	
C	0.805572	-2.045917	
C	-2.314929	0.474230	
C	-1.714270	-3.963216	
C	3.823283	-2.869361	
C	-2.773003	0.366717	
C	-4.524566	-0.955516	
C	5.206306	-2.937941	
C	-0.455049	-3.902480	
C	-3.205057	1.381645	
C	-2.449604	2.263876	
C	-3.627491	2.681681	
C	-3.848342	4.046292	
C	-5.807933	-1.880184	
C	-3.431936	1.328674	
C	0.657382	-3.316331	
C	4.914177	-1.806111	
C	3.528963	-1.751232	
C	-5.631567	-1.679996	
H	-1.385628	-2.258535	
H	-0.933742	-1.175623	
H	-4.981408	-1.506671	
H	-2.863246	-3.480176	
H	-3.005149	-0.257327	
H	-0.972947	5.341364	
H	-0.572193	2.907166	
H	6.847335	-2.452880	
H	-3.073000	6.074629	
H	-1.353968	-1.288738	
H	1.281757	-1.760503	
H	-2.567175	-4.435660	
H	3.393013	-3.287119	
H	-2.945272	0.328192	
H	-4.403736	-0.810035	
H	5.860240	-3.404290	
H	-0.342858	-4.332352	
H	-3.722457	2.141366	
H	-4.381766	1.938761	
H	-4.771325	4.358098	
H	-6.675311	-2.447538	
H	-4.123809	2.048502	
H	1.637291	-3.292550	
H	5.329145	-1.335318	
H	2.879188	-1.230324	
H	-6.361392	-2.091255	
C	-0.628017	0.659527	
C	0.576805	1.259530	
H	-1.567099	1.245259	
H	-0.562580	-0.008368	
H	0.522222	2.197204	
C	1.951786	0.967810	
H	1.750346	0.291714	
O	2.707608	0.379430	
H	3.315740	1.180899	
C	4.791549	2.453489	
C	6.009250	2.869068	
H	6.592450	3.669032	
H	5.682824	3.238216	
H	6.676244	1.996322	
C	3.834258	3.652532	
H	2.938515	3.334686	
H	3.495299	4.028414	
H	4.319597	4.488147	
C	5.228906	1.900908	
H	5.949733	1.067887	
H	4.353733	1.498663	
H	5.721127	2.686839	
O	4.137734	1.430371	
C	2.567004	2.260547	
H	3.572646	2.032635	
H	1.938767	2.695369	
H	2.697862	3.023994	

E (R = Me)			$E_g(\text{BP86/SVP}) = -2633.9755471$ $G_g(\text{BP86/SVP}) = -2633.35116$ $E_s(\text{M06//TZVP//BP86/SVP}) = -2634.5085947$
Ru	-0.123916	-0.178610	
Cl	1.521738	1.229567	
P	-1.666329	0.518809	
C	0.899260	-2.402622	
C	-1.223258	-2.226301	
C	2.366190	-2.442629	
C	-0.123005	-0.134157	
C	-5.362186	-1.201775	
C	-2.490327	-3.445434	
C	-4.083463	-0.626545	
C	-1.582945	4.641308	
C	-1.238618	3.301814	
C	5.210779	-2.557044	
C	-0.076475	-2.951293	
C	-3.345250	-0.301708	
C	-1.384038	-2.870283	
C	-2.913992	4.996120	
C	0.297861	-0.034192	
C	0.181717	-2.242191	
C	-1.137582	0.708238	
C	-2.330026	-4.097643	
C	3.197307	-2.667351	
C	-0.285953	0.914781	
C	-3.913107	-0.604433	
C	4.592118	-2.730452	
C	-1.048639	-4.170608	
C	-1.719134	1.662406	
C	-2.226423	2.286367	
C	-3.559281	2.652392	
C	-3.898489	3.995834	
C	-5.921875	-1.487241	
C	-1.296487	1.763452	
C	0.082223	-3.605577	
C	4.409125	-2.302331	
C	3.012360	-2.248427	
C	-5.187417	-1.193671	
H	-2.010370	-2.245873	
H	0.344645	-0.861017	
H	-5.919522	-1.438851	
H	-3.486762	-3.399128	
H	-3.641545	-0.437125	
H	-0.797518	5.414291	
H	-0.189751	3.022277	
H	6.308513	-2.600572	
H	-3.181091	6.047887	
H	1.102129	-0.691278	
H	0.633214	-2.175068	
H	-3.190063	-4.550166	
H	2.735433	-2.790608	
H	0.053444	1.001190	
H	-3.350867	-0.387776	
H	5.206216	-2.910233	
H	-0.920004	-4.688548	
H	-2.504101	2.338421	
H	-4.351286	1.889132	
H	-4.946117	4.257095	
H	-6.921558	-1.945922	
H	-1.755096	2.516459	
H	1.078407	-3.715668	
H	4.870987	-2.111460	
H	2.410834	-2.005106	
H	-5.604900	-1.428735	
C	-1.430640	0.502236	
C	-0.367019	1.437368	
H	-2.454897	0.809613	
H	-1.383220	-0.216198	
H	-0.546790	2.442296	
C	0.925447	1.110103	
H	0.688159	0.971336	
O	1.303311	-0.117140	
H	3.225648	0.840003	
C	4.862371	1.907884	
C	6.026121	1.874135	
H	6.795242	2.636208	
H	5.650381	2.068449	
H	6.505417	0.873150	
C	4.175189	3.292294	
H	3.314674	3.298525	
H	3.789457	3.509988	
H	4.873334	4.105931	
C	5.358371	1.577736	
H	5.852949	0.584891	
H	4.496024	1.530689	
H	6.075673	2.339528	
O	3.946034	0.903451	
C	2.014204	2.189362	
H	2.938814	1.828660	
H	1.686097	3.122451	
H	2.252635	2.413691	

EF (R = Me)			$E_g(\text{BP86/SVP}) = -2633.9516485$ $G_g(\text{BP86/SVP}) = -2633.331116$ $E_s(\text{M06//TZVP//BP86/SVP}) = -2634.4855443$
Ru	1.134892	0.698984	
Cl	-3.376673	-0.083962	
P	1.019325	-1.338728	
C	1.936919	2.665488	0.117382
C	3.297121	0.871941	-0.479552
C	1.096844	3.871896	0.023188
C	-0.514101	-0.008519	1.846188
C	4.771002	-3.123694	-0.166180
C	3.996515	0.238477	1.975758
C	3.600188	-2.420537	-0.497277
C	-1.961817	-3.537999	-1.962511
C	-1.256308	-2.577582	-1.218338
C	-0.537840	6.202105	-0.173728
C	2.406446	2.017610	1.372308
C	2.556086	-2.259137	0.442658
C	3.287673	0.946128	1.002039
C	-1.291401	-4.620001	-2.561275
C	-1.388976	0.082853	2.942023
C	2.712854	2.107999	-0.960549
C	-0.057635	-1.263154	1.401386
C	3.815748	0.572343	3.342038
C	1.286016	4.820899	-1.015569
C	-1.810065	-1.079065	3.604688
C	2.728781	-2.798121	1.734949
C	0.485325	5.968379	-1.110000
C	2.943720	1.606886	3.708635
C	-0.513692	-2.434800	2.051212
C	0.146219	-2.694240	-1.063446
C	0.817025	-3.783373	-1.662843
C	0.100598	-4.739497	-2.408018
C	4.925001	-3.669776	1.121267
C	-1.375188	-2.340001	3.154524
C	2.237236	2.343395	2.726088
C	-0.752245	5.266556	0.854418
C	0.051674	4.122059	0.951617
C	3.902094	-3.499022	2.069185
H	4.064358	0.313646	-1.033882
H	-0.204163	0.899244	1.306233
H	5.569657	-3.239708	-0.917072
H	4.694411	-0.563427	1.687914
H	3.495947	-1.973606	-1.498249
H	-3.052088	-3.414695	-2.066605
H	-1.834655	-1.734176	-0.775026
H	-1.172751	7.099319	-0.252747
H	-1.851079	-5.370116	-3.144547
H	-1.764871	1.068001	3.257618
H	2.910155	2.582423	-1.932924
H	4.368222	0.015822	4.116653
H	2.084966	4.659109	-1.755163
H	-2.507135	-1.007725	4.455029
H	1.947512	-2.656845	2.495739
H	0.659768	6.686751	-1.928049
H	2.812709	1.863871	4.772646
H	-0.216563	-3.426990	1.675807
H	1.903435	-3.908269	-1.539736
H	0.639992	-5.586191	-2.864321
H	5.843944	-4.217704	1.386024
H	-1.729960	-3.257677	3.651418
H	1.593914	3.182220	3.031243
H	-1.568548	5.418725	1.578859
H	-0.162833	3.381819	1.735969
H	4.018394	-3.905435	3.087190
C	1.794215	-0.116572	-3.140168
C	0.363339	-0.111093	-3.088373
H	2.326364	-1.085578	-3.141582
H	2.329428	0.682211	-3.690783
H	-0.210966	-1.050599	-3.045180
C	-0.370922	1.201137	-3.389711
H	0.050776	1.702942	-4.302713
C	-1.887080	1.083249	-3.520934
H	-2.335270	0.731900	-2.562737
H	-2.325205	2.074201	-3.760568
H	-2.150094	0.379224	-4.339962
O	-0.018234	1.970096	-2.230990
H	-5.078320	0.614666	0.750316
C	-6.782639	-0.326366	0.939706
C	-6.132840	-1.610547	1.508484
H	-6.741628	-2.519893	1.304920
H	-5.127801	-1.729695	1.050381
H	-6.001686	-1.511998	2.607406
C	-6.986821	-0.472349	-0.587316
H	-7.456009	0.448689	-0.994650
H	-5.992201	-0.594347	-1.067258
H	-7.631054	-1.342413	-0.845918
C	-8.121842	-0.039169	1.641443
H	-7.958811	0.097468	2.731713
H	-8.565979	0.898922	1.245837
H	-8.848025	-0.866828	1.492049
O	-5.950679	0.795781	1.211907

F (R = Me)			E _g (BP86/SVP) = -1940.2664827 G _g (BP86/SVP) = -1939.761011 E _s (M06//TZVP//BP86/SVP) = -1940.5729196
Ru	0.793561	0.121245	
P	-1.569727	0.154427	
C	2.798252	-0.841080	
C	0.856157	-1.704521	-1.726212
C	4.115450	-0.200786	-0.491931
C	-1.183646	-0.421758	2.602696
C	-2.861726	-1.990970	-3.457318
C	0.090398	-3.180183	0.326258
C	-2.247349	-1.058979	-2.604551
C	-3.555297	3.795689	0.343255
C	-2.856068	2.599066	0.576638
C	6.657741	1.010392	-0.133217
C	2.104720	-1.705820	0.277208
C	-2.427974	-1.123096	-1.201322
C	0.915057	-2.244372	-0.369168
C	-4.016333	4.109375	-0.946714
C	-1.587986	-0.697392	3.923220
C	2.021573	-0.901755	-1.917937
C	-2.151274	-0.234476	1.592715
C	0.440263	-3.560032	1.617669
C	5.097373	-0.256259	-1.512324
C	-2.951675	-0.788611	4.245318
C	-3.205782	-2.177863	-0.675811
C	6.354614	0.343557	-1.334054
C	1.598684	-3.022187	2.254757
C	-3.526139	-0.301430	1.928497
C	-2.603970	1.687154	-0.476682
C	-3.072686	2.015375	-1.768866
C	-3.772760	3.212721	-2.000551
C	-3.645847	-3.028788	-2.921574
C	-3.922236	-0.584580	3.245444
C	2.422215	-2.105277	1.609777
C	5.686063	1.084524	0.881875
C	4.425144	0.491448	0.707885
C	-3.804836	-3.123679	-1.529801
H	0.130771	-1.995129	-2.493425
H	-0.116617	-0.291115	2.354391
H	-2.714752	-1.913218	-4.546589
H	-0.788073	-3.612429	-0.175826
H	-1.587930	-0.286651	-3.031780
H	-3.741891	4.485529	1.181885
H	-2.512008	2.369544	1.596347
H	7.646062	1.476312	0.008187
H	-4.566011	5.046417	-1.128942
H	-0.824330	-0.832956	4.705632
H	2.315061	-0.427579	-2.863460
H	-0.179603	-4.292810	2.157793
H	4.876361	-0.795283	-2.447748
H	-3.263936	-1.005919	5.279607
H	-3.340513	-2.274876	0.411217
H	7.107167	0.282291	-2.136848
H	1.851240	-3.352776	3.274905
H	-4.293316	-0.116647	1.159458
H	-2.908810	1.328470	-2.610858
H	-4.134334	3.440246	-3.016226
H	-4.120728	-3.766674	-3.587454
H	-4.994322	-0.637500	3.494934
H	3.328310	-1.717486	2.097680
H	5.907284	1.624491	1.816937
H	3.635333	0.609718	1.467559
H	-4.401842	-3.942209	-1.096415
C	1.616590	1.921928	-1.354267
C	0.549755	2.323610	-0.526259
H	1.489586	1.966998	-2.449106
H	2.657717	1.973525	-0.994042
H	-0.379503	2.698998	-0.984190
C	0.767935	2.474113	0.979846
O	1.226419	1.190350	1.351352
H	-0.232239	2.685405	1.448537
C	1.722042	3.595547	1.408489
H	1.312299	4.595032	1.145670
H	1.867772	3.560938	2.508755
H	2.715021	3.479732	0.927375

FG (R = Me)				E _g (BP86/SVP) = -1940.2617823 G _g (BP86/SVP) = -1939.757457 E _s (M06//TZVP//BP86/SVP) = -1940.5716619
Ru	-0.829258	-0.104873	-0.157879	
P	1.548245	-0.054205	-0.196334	
C	-2.973974	0.639886	-0.640887	
C	-1.091328	1.596481	-1.653427	
C	-4.284530	-0.035827	-0.514152	
C	1.808318	-0.495603	2.605055	
C	2.638419	3.680551	-1.777850	
C	-0.558182	3.278906	0.326763	
C	2.134429	2.376639	-1.634190	
C	3.174069	-3.264143	-2.301918	
C	2.529990	-2.462810	-1.343196	
C	-6.844379	-1.265400	-0.319946	
C	-2.411103	1.605704	0.295403	
C	2.255877	1.671888	-0.411927	
C	-1.238621	2.204564	-0.327867	
C	3.783726	-2.687205	-3.428627	
C	2.500320	-0.805273	3.789473	
C	-2.177132	0.708073	-1.864727	
C	2.454778	-0.574099	1.354609	
C	-1.041171	3.744392	1.542323	
C	-5.111914	-0.189576	-1.654875	
C	3.847155	-1.201787	3.736514	
C	2.881960	2.332799	0.669950	
C	-6.374211	-0.796769	-1.559112	
C	-2.197046	3.163022	2.149691	
C	3.812695	-0.963794	1.310551	
C	2.476353	-1.053994	-1.496574	
C	3.120816	-0.483460	-2.618635	
C	3.761579	-1.291163	-3.575592	
C	3.260308	4.322258	-0.692463	
C	4.500920	-1.279123	2.493746	
C	-2.874353	2.108868	1.553515	
C	-6.035244	-1.124207	0.821754	
C	-4.771116	-0.521851	0.726245	
C	3.373297	3.643390	0.531812	
H	-0.357822	1.889947	-2.409880	
H	0.748824	-0.193317	2.637122	
H	2.537850	4.198731	-2.745021	
H	0.309946	3.754859	-0.150678	
H	1.634447	1.908479	-2.493347	
H	3.201797	-4.355763	-2.153312	
H	2.088784	-2.951339	-0.456818	
H	-7.835086	-1.740789	-0.244277	
H	4.286041	-3.318982	-4.178636	
H	1.979070	-0.741702	4.758109	
H	-2.388784	0.162320	-2.792822	
H	-0.536064	4.586467	2.041128	
H	-4.767774	0.194749	-2.627744	
H	4.387922	-1.453885	4.662808	
H	2.987346	1.821805	1.637670	
H	-6.998978	-0.897859	-2.461037	
H	-2.566601	3.573996	3.102890	
H	4.338240	-1.023753	0.345258	
H	3.160104	0.605123	-2.750115	
H	4.257244	-0.815225	-4.437162	
H	3.651885	5.346039	-0.801511	
H	5.556672	-1.590252	2.442612	
H	-3.786591	1.700787	2.012004	
H	-6.388073	-1.495927	1.797211	
H	-4.135338	-0.447868	1.621499	
H	3.853170	4.133384	1.394101	
C	-1.914090	-1.959931	-0.271539	
C	-0.547531	-2.328830	-0.120963	
H	-2.383785	-2.059301	-1.263689	
H	-2.617860	-2.102805	0.565409	
H	0.014264	-2.641040	-1.015963	
C	-0.059568	-2.992836	1.133293	
H	-0.716438	-0.355924	1.403651	
O	1.015622	-3.598314	1.149739	
C	-0.950883	-3.020234	2.371042	
H	-1.719188	-3.813541	2.243797	
H	-0.330919	-3.279274	3.249507	
H	-1.477396	-2.061160	2.541364	

G (R= Me)				E _g (BP86/SVP) = -1940.2892669 G _g (BP86/SVP) = -1939.78968 E _s (M06//TZVP//BP86/SVP) = -1940.6021595
Ru	0.617548	0.140571	-0.388332	
P	-1.647154	0.202413	0.036312	
C	2.702898	-0.802973	-0.652270	
C	0.916406	-1.268181	-2.139041	
C	4.040140	-0.382071	-0.172521	
C	-1.379175	-1.437478	2.340523	
C	-3.133426	-0.771684	-3.711281	
C	-0.124007	-3.221829	-0.711873	
C	-2.411194	-0.205790	-2.647557	
C	-2.666489	3.882107	1.642213	
C	-2.127259	2.603799	1.425853	
C	6.642038	0.327021	0.711391	
C	1.878680	-1.862536	-0.074638	
C	-2.674884	-0.586408	-1.309908	
C	0.784234	-2.150537	-0.995991	
C	-3.537162	4.452418	0.695607	
C	-1.821631	-2.059770	3.522123	
C	2.109758	-0.492791	-1.937428	
C	-2.253029	-0.624899	1.591677	
C	0.088781	-4.000341	0.415801	
C	5.129153	-0.337646	-1.078003	
C	-3.140553	-1.873656	3.968281	
C	-3.657425	-1.571084	-1.068261	
C	6.415712	0.016993	-0.641436	
C	1.175116	-3.731983	1.310118	
C	-3.578348	-0.434603	2.051056	
C	-2.452283	1.873411	0.257507	
C	-3.329369	2.451824	-0.684747	
C	-3.867744	3.733832	-0.465073	
C	-4.113389	-1.749618	-3.459231	
C	-4.018521	-1.058161	3.230197	
C	2.049337	-2.676162	1.091281	
C	5.569611	0.287501	1.620355	
C	4.281005	-0.058205	1.184446	
C	-4.366453	-2.151003	-2.137273	
H	0.291328	-1.289296	-3.039474	
H	-0.341282	-1.567223	1.998018	
H	-2.922067	-0.453901	-4.745022	
H	-0.950046	-3.438770	-1.406412	
H	-1.617693	0.530313	-2.852126	
H	-2.403472	4.435515	2.557705	
H	-1.458311	2.160001	2.181205	
H	7.650927	0.605331	1.055387	
H	-3.959146	5.455670	0.865797	
H	-1.124713	-2.688037	4.099280	
H	2.534877	0.210521	-2.665704	
H	-0.585914	-4.843809	0.631507	
H	4.963937	-0.606039	-2.133815	
H	-3.484572	-2.356066	4.897257	
H	-3.870188	-1.898622	-0.039752	
H	7.248848	0.043189	-1.362186	
H	1.319320	-4.383439	2.186756	
H	-4.267653	0.217837	1.491501	
H	-3.609533	1.897446	-1.593613	
H	-4.555012	4.168830	-1.208393	
H	-4.672938	-2.201753	-4.293542	
H	-5.050841	-0.897364	3.580297	
H	2.894840	-2.489251	1.770423	
H	5.731678	0.550769	2.677500	
H	3.436991	-0.033489	1.889960	
H	-5.124044	-2.923751	-1.929507	
C	0.408463	2.030872	-1.384817	
C	0.965681	2.258946	-0.073926	
H	-0.615922	2.392952	-1.581423	
H	1.061986	2.089139	-2.272431	
H	0.292013	2.645024	0.707818	
C	2.379489	2.635436	0.237757	
H	0.640847	0.368607	1.197625	
O	2.726575	2.839271	1.402172	
C	3.359486	2.871172	-0.908737	
H	3.268852	2.128114	-1.723780	
H	3.144293	3.868357	-1.352738	
H	4.393320	2.872174	-0.516609	

GH (R = Me)				E _g (BP86/SVP) = -1940.2594374 G _g (BP86/SVP) = -1939.759826 E _s (M06//TZVP//BP86/SVP) = -1940.5726477
Ru	0.843093	0.176874	-0.323232	
P	-1.513198	0.060827	-0.105402	
C	2.902319	-0.714443	-0.601305	
C	1.084332	-1.640759	-1.787056	
C	4.222762	-0.089826	-0.365480	
C	-1.202934	-0.931049	2.542452	
C	-2.560402	-1.840809	-3.657007	
C	0.263280	-3.202736	0.174450	
C	-2.027396	-0.963502	-2.697977	
C	-3.796175	3.450644	0.675892	
C	-2.952370	2.335489	0.799909	
C	6.788483	1.064581	0.062647	
C	2.202249	-1.628249	0.294673	
C	-2.266499	-1.159749	-1.316023	
C	1.064850	-2.183623	-0.431181	
C	-4.334677	3.796983	-0.573115	
C	-1.647903	-1.384867	3.798446	
C	2.211304	-0.798213	-1.896883	
C	-2.129214	-0.558604	1.547480	
C	0.597630	-3.660917	1.440842	
C	5.189708	-0.052190	-1.400243	
C	-3.022207	-1.474372	4.072159	
C	-3.024808	-2.284110	-0.923187	
C	6.454832	0.520635	-1.189702	
C	1.717324	-3.123206	2.150699	
C	-3.513824	-0.644391	1.834351	
C	-2.643164	1.535118	-0.322963	
C	-3.183232	1.897297	-1.577019	
C	-4.020132	3.019357	-1.700098	
C	-3.320369	-2.953445	-3.252323	
C	-3.955537	-1.102567	3.086029	
C	2.507474	-2.121134	1.604293	
C	5.838688	1.037731	1.100377	
C	4.570843	0.474819	0.888032	
C	-3.541346	-3.175186	-1.883691	
H	0.390856	-1.913204	-2.589786	
H	-0.125677	-0.849768	2.325887	
H	-2.370362	-1.659578	-4.727197	
H	-0.578709	-3.638349	-0.384079	
H	-1.391774	-0.124815	-3.024631	
H	-4.018397	4.061485	1.564772	
H	-2.532730	2.088614	1.786424	
H	7.781184	1.512070	0.228671	
H	-4.993938	4.674153	-0.670292	
H	-0.910528	-1.666776	4.566842	
H	2.529070	-0.280963	-2.811355	
H	0.001434	-4.461400	1.906340	
H	4.951288	-0.497036	-2.379225	
H	-3.369982	-1.826733	5.056611	
H	-3.211032	-2.478870	0.143045	
H	7.189443	0.534232	-2.010908	
H	1.966026	-3.527919	3.144770	
H	-4.253472	-0.334749	1.079072	
H	-2.975815	1.292603	-2.470953	
H	-4.436081	3.278559	-2.686965	
H	-3.730240	-3.648549	-4.002168	
H	-5.035677	-1.160064	3.296241	
H	3.390838	-1.745826	2.141775	
H	6.083097	1.472520	2.083002	
H	3.819814	0.495807	1.692845	
H	-4.123076	-4.050402	-1.552206	
C	1.878815	1.976459	-0.922866	
C	0.549009	2.389476	-0.630214	
H	2.194592	1.906574	-1.976597	
H	2.696947	2.237843	-0.230281	
H	-0.158106	2.565224	-1.457967	
C	0.283207	3.319031	0.520855	
H	0.878572	0.715934	1.172603	
O	-0.674431	4.089207	0.477710	
C	1.276329	3.408734	1.679187	
H	1.794513	2.454457	1.891239	
H	2.040640	4.176297	1.429395	
H	0.737129	3.759646	2.580010	

H (R = Me)				E _g (BP86/SVP) = -1940.284728 G _g (BP86/SVP) = -1939.783917 E _s (M06//TZVP//BP86/SVP) = -1940.5941161
Ru	0.830328	-0.100707	0.066240	
P	-1.450988	0.003971	-0.090382	
C	2.997831	0.454499	0.659282	
C	1.180568	0.773736	2.140458	
C	4.237972	-0.109159	0.084769	
C	-1.280707	2.319299	-1.767009	
C	-2.591993	-0.449646	3.870059	
C	0.461628	3.121859	1.190669	
C	-2.035385	-0.644150	2.594289	
C	-2.990859	-2.631996	-2.888414	
C	-2.277183	-1.612165	-2.238527	
C	6.643574	-1.189822	-0.984989	
C	2.338987	1.708388	0.309047	
C	-2.283002	0.289711	1.556973	
C	1.215706	1.905507	1.226448	
C	-3.869746	-3.454240	-2.158192	
C	-1.799938	3.334305	-2.592752	
C	2.293340	-0.058501	1.819668	
C	-2.139166	1.380186	-1.161443	
C	0.830286	4.114871	0.296043	
C	5.180784	-0.763054	0.917763	
C	-3.182645	3.423161	-2.820880	
C	-3.066361	1.430609	1.839184	
C	6.365840	-1.299055	0.388878	
C	1.930902	3.928001	-0.601819	
C	-3.531027	1.471561	-1.404855	
C	-2.430998	-1.396072	-0.847603	
C	-3.312437	-2.225530	-0.123352	
C	-4.025523	-3.248204	-0.777516	
C	-3.376985	0.686310	4.141644	
C	-4.048660	2.487638	-2.224122	
C	2.668936	2.752397	-0.617282	
C	5.717565	-0.546756	-1.826185	
C	4.527297	-0.019708	-1.301236	
C	-3.604887	1.627950	3.124999	
H	0.494230	0.644458	2.985416	
H	-0.195233	2.243432	-1.599015	
H	-2.399420	-1.192050	4.661275	
H	-0.374119	3.266843	1.892479	
H	-1.392718	-1.523652	2.411763	
H	-2.864709	-2.781385	-3.972799	
H	-1.606630	-0.959813	-2.821632	
H	7.574927	-1.607275	-1.399184	
H	-4.433151	-4.252495	-2.667073	
H	-1.113472	4.056659	-3.062568	
H	2.563159	-0.973773	2.362109	
H	0.273218	5.064500	0.271745	
H	4.990205	-0.830238	2.000516	
H	-3.587928	4.216206	-3.469762	
H	-3.257139	2.178647	1.055327	
H	7.083429	-1.798748	1.059345	
H	2.204505	4.745350	-1.288298	
H	-4.216389	0.732929	-0.959170	
H	-3.454287	-2.072189	0.956837	
H	-4.713832	-3.884328	-0.198209	
H	-3.803434	0.839898	5.145912	
H	-5.134063	2.543456	-2.405706	
H	3.531895	2.641285	-1.290397	
H	5.917456	-0.466330	-2.906842	
H	3.790409	0.442947	-1.975670	
H	-4.208408	2.527450	3.327999	
C	1.298258	-1.770817	-1.226320	
C	1.083453	-2.253926	0.109656	
H	2.330086	-1.685800	-1.612145	
H	0.555085	-2.004817	-2.006344	
H	1.984138	-2.404748	0.735232	
C	0.035612	-3.234958	0.561356	
H	0.677750	0.293941	-1.469978	
O	-0.331483	-3.284742	1.737636	
C	-0.442446	-4.265675	-0.449670	
H	-0.917339	-3.778753	-1.325583	
H	0.431504	-4.832494	-0.838130	
H	-1.159015	-4.958998	0.028518	

HI (R = Me)			E _g (BP86/SVP) = -1940.2775714 G _g (BP86/SVP) = -1939.778381 E _s (M06//TZVP//BP86/SVP) = -1940.5882826
Ru	0.829179	-0.062322	
P	-1.467650	0.003588	
C	2.950563	0.495541	
C	1.100190	0.870993	
C	4.182929	-0.109487	0.126216
C	-1.316340	2.297821	-1.735215
C	-2.478523	-0.651529	3.898663
C	0.468808	3.228313	1.112765
C	-1.950645	-0.765901	2.601444
C	-3.086901	-2.559014	-2.895241
C	-2.381842	-1.534664	-2.242040
C	6.563411	-1.289118	-0.902233
C	2.336189	1.775009	0.301349
C	-2.264556	0.202794	1.614897
C	1.204977	2.010357	1.192306
C	-3.880541	-3.454316	-2.153864
C	-1.832875	3.320425	-2.553420
C	2.207683	0.006049	1.823404
C	-2.183511	1.397088	-1.084171
C	0.863659	4.197849	0.195685
C	5.065488	-0.834295	0.967248
C	-3.220179	3.455318	-2.725155
C	-3.080559	1.299092	1.968153
C	6.236849	-1.418321	0.459178
C	1.973246	3.976902	-0.672674
C	-3.580000	1.530724	-1.274898
C	-2.454831	-1.387014	-0.835137
C	-3.254041	-2.289400	-0.101588
C	-3.960906	-3.314266	-0.758487
C	-3.298416	0.440311	4.241389
C	-4.094177	2.557163	-2.083486
C	2.699004	2.788089	-0.639080
C	5.698804	-0.574339	-1.751529
C	4.524031	0.003090	-1.246960
C	-3.589043	1.417789	3.276020
H	0.390921	0.770202	2.926420
H	-0.228085	2.181771	-1.603212
H	-2.234120	-1.418598	4.651030
H	-0.377076	3.402115	1.795545
H	-1.272748	-1.603659	2.358952
H	-3.022697	-2.653066	-3.991282
H	-1.787007	-0.822612	-2.837580
H	7.484890	-1.743265	-1.299493
H	-4.437295	-4.255828	-2.664853
H	-1.142121	4.013250	-3.059855
H	2.438307	-0.909900	2.382953
H	0.317060	5.152333	0.140101
H	4.838441	-0.920477	2.041359
H	-3.624103	4.255658	-3.365919
H	-3.319224	2.074427	1.224667
H	6.906242	-1.971820	1.137205
H	2.270048	4.770259	-1.377374
H	-4.271282	0.816332	-0.799367
H	-3.337865	-2.191506	0.990950
H	-4.584247	-4.005407	-0.168717
H	-3.701355	0.532491	5.262716
H	-5.183325	2.650033	-2.223007
H	3.574393	2.652431	-1.291147
H	5.939240	-0.472003	-2.822346
H	3.843630	0.532455	-1.931340
H	-4.217954	2.284244	3.537248
C	1.215417	-1.587493	-1.467686
C	1.155240	-2.149335	-0.117588
H	2.209898	-1.529576	-1.950314
H	0.427456	-1.894243	-2.179822
H	2.135312	-2.326160	0.371006
C	0.198598	-3.213680	0.350660
H	0.883308	-0.134944	-1.568741
O	-0.068854	-3.348576	1.546588
C	-0.322610	-4.205162	-0.680876
H	-0.921567	-3.695830	-1.463708
H	0.534431	-4.689225	-1.197973
H	-0.943346	-4.973240	-0.182993

I (R = Me)			E _g (BP86/SVP) = -1940.2799383 G _g (BP86/SVP) = -1939.77938 E _s (M06//TZVP//BP86/SVP) = -1940.5952083
Ru	0.820733	-0.010657	
P	-1.491281	-0.015894	
C	2.916808	0.539454	
C	1.016722	0.961282	1.995516
C	4.150201	-0.096757	0.152524
C	-1.442545	2.329085	-1.638211
C	-2.361238	-0.872450	3.917506
C	0.499549	3.343305	1.008179
C	-1.880171	-0.920222	2.598265
C	-3.114278	-2.504790	-2.931196
C	-2.417554	-1.492004	-2.251953
C	6.523416	-1.353569	-0.803418
C	2.345151	1.836904	0.260270
C	-2.238910	0.089560	1.670070
C	1.203172	2.114874	1.118684
C	-3.880343	-3.440688	-2.210939
C	-2.002745	3.367170	-2.406837
C	2.125285	0.067599	1.785338
C	-2.272549	1.399006	-0.979505
C	0.934170	4.292280	0.081476
C	4.975219	-0.862790	1.015719
C	-3.397331	3.488132	-2.520014
C	-3.048620	1.161237	2.103891
C	6.142142	-1.484395	0.543571
C	2.050084	4.028954	-0.759785
C	-3.676821	1.518235	-1.113028
C	-2.472347	-1.395024	-0.839983
C	-3.244705	-2.336920	-0.127878
C	-3.942439	-3.351369	-0.810583
C	-3.178265	0.193383	4.339782
C	-4.234543	2.560581	-1.870879
C	2.748732	2.821427	-0.689418
C	5.717975	-0.598521	-1.674748
C	4.546643	0.017114	-1.206133
C	-3.510817	1.213000	3.433132
H	0.277534	0.883792	2.801988
H	-0.348189	2.225551	-1.548823
H	-2.081045	-1.669833	4.624421
H	-0.357943	3.544975	1.668740
H	-1.199256	-1.733856	2.293882
H	-3.065033	-2.558789	-4.030733
H	-1.841486	-0.750265	-2.829843
H	7.441588	-1.837334	-1.172328
H	-4.429737	-4.234053	-2.742167
H	-1.340845	4.083165	-2.919451
H	2.318052	-0.840429	2.371312
H	0.411267	5.258221	0.001611
H	4.705069	-0.954194	2.079215
H	-3.835983	4.301034	-3.120881
H	-3.315060	1.970401	1.407394
H	6.764760	-2.070100	1.238885
H	2.379142	4.800210	-1.474706
H	-4.339684	0.780301	-0.632929
H	-3.314439	-2.278951	0.968533
H	-4.544070	-4.074526	-0.236836
H	-3.544558	0.233661	5.378122
H	-5.329361	2.643453	-1.965035
H	3.632560	2.656460	-1.322726
H	6.000015	-0.493481	-2.734928
H	3.912905	0.577406	-1.910252
H	-4.135521	2.060637	3.758235
C	1.243656	-1.525561	-1.651765
C	1.225896	-2.047097	-0.250760
H	2.240823	-1.514400	-2.136040
H	0.479996	-1.955575	-2.328976
H	2.232930	-2.202878	0.190048
C	0.354111	-3.179595	0.214067
H	0.937500	-0.339138	-1.725471
O	0.192724	-3.394036	1.418237
C	-0.222910	-4.134774	-0.824688
H	-0.780861	-4.942258	-0.315212
H	-0.896776	-3.612389	-1.533757
H	0.602081	-4.573532	-1.427615

IJ (R = Me)				E _g (BP86/SVP) = -1940.2558538 G _g (BP86/SVP) = -1939.756311 E _s (M06//TZVP//BP86/SVP) = -1940.5733957
Ru	0.774332	0.236117	-0.872413	
P	-1.321968	-0.003669	0.299618	
C	2.848708	-0.404789	-0.800852	
C	1.385707	-0.831795	-2.590468	
C	3.936773	0.181457	0.013083	
C	-0.118859	-1.234891	2.552219	
C	-3.288392	-1.641585	-2.954551	
C	0.463789	-3.124675	-1.672672	
C	-2.538770	-0.805064	-2.110432	
C	-2.921405	3.399248	2.057906	
C	-2.135524	2.276561	1.752054	
C	6.054384	1.294813	1.549839	
C	2.146820	-1.680670	-0.538751	
C	-2.379061	-1.132303	-0.740920	
C	1.262976	-1.950777	-1.658576	
C	-4.047365	3.708451	1.271827	
C	-0.093835	-1.807539	3.837219	
C	2.480042	0.008921	-2.142898	
C	-1.329492	-0.785761	1.990417	
C	0.594439	-4.044910	-0.631984	
C	5.096788	0.702367	-0.612142	
C	-1.282945	-1.936235	4.573574	
C	-2.954674	-2.323120	-0.248342	
C	6.141359	1.254385	0.147554	
C	1.507425	-3.812277	0.436019	
C	-2.522739	-0.909847	2.742310	
C	-2.462448	1.438099	0.659338	
C	-3.594540	1.754748	-0.120961	
C	-4.378866	2.883122	0.184469	
C	-3.866539	-2.823869	-2.455478	
C	-2.497730	-1.485670	4.023041	
C	2.272187	-2.646963	0.499640	
C	4.907471	0.783335	2.185822	
C	3.860757	0.237820	1.427697	
C	-3.691577	-3.163420	-1.103726	
H	0.868542	-0.750355	-3.556722	
H	0.804420	-1.130111	1.961621	
H	-3.412881	-1.369081	-4.015042	
H	-0.222771	-3.313905	-2.512312	
H	-2.060837	0.103332	-2.513637	
H	-2.654629	4.034255	2.918058	
H	-1.265441	2.036631	2.385095	
H	6.874370	1.726052	2.145699	
H	-4.665532	4.588666	1.509893	
H	0.861759	-2.152107	4.263916	
H	2.907771	0.854205	-2.698380	
H	0.000463	-4.971942	-0.644267	
H	5.185105	0.653547	-1.708785	
H	-1.265561	-2.381947	5.581109	
H	-2.820281	-2.608795	0.805327	
H	7.034619	1.650460	-0.361802	
H	1.616006	-4.573845	1.224889	
H	-3.475941	-0.543733	2.328788	
H	-3.876244	1.114806	-0.970474	
H	-5.261187	3.112357	-0.434486	
H	-4.446919	-3.482137	-3.121763	
H	-3.432976	-1.577601	4.598379	
H	2.994257	-2.493142	1.316336	
H	4.823321	0.819914	3.283927	
H	2.949004	-0.120580	1.929299	
H	-4.130603	-4.092375	-0.705250	
C	1.245008	3.143721	0.246169	
C	0.855667	2.369324	-1.017511	
H	1.434327	4.224061	0.041160	
H	0.461804	3.097781	1.030958	
H	1.657615	2.502844	-1.781795	
C	-0.401877	2.768707	-1.726084	
H	2.178086	2.731396	0.681938	
O	-0.911420	1.996735	-2.558432	
C	-1.049823	4.114941	-1.447190	
H	-0.306236	4.936649	-1.523278	
H	-1.885092	4.287991	-2.151469	
H	-1.441079	4.135544	-0.407542	

J (R = Me)				E _g (BP86/SVP) = -1940.2839261 G _g (BP86/SVP) = -1939.78171 E _s (M06//TZVP//BP86/SVP) = -1940.5944105
Ru	-0.734968	0.010056	-0.006896	
P	1.564447	0.264091	0.039910	
C	-2.833012	-0.347878	0.944308	
C	-0.779286	-0.802889	2.014355	
C	-4.100480	0.337924	0.626601	
C	2.019554	-1.761428	-1.869960	
C	3.044914	0.582664	3.956535	
C	-0.439191	-3.196984	0.970063	
C	2.521217	0.900523	2.690231	
C	3.651581	3.671013	-1.294802	
C	3.281346	2.328680	-1.097683	
C	-6.553473	1.699794	0.084566	
C	-2.380783	-1.674862	0.524728	
C	2.359657	-0.098341	1.704807	
C	-1.107588	-1.955801	1.181370	
C	2.929225	4.705821	-0.675575	
C	2.777864	-2.641232	-2.665016	
C	-1.842682	0.149799	1.888825	
C	2.650664	-0.832019	-1.019463	
C	-1.030480	-4.157722	0.154668	
C	-4.610267	1.328267	1.508512	
C	4.180891	-2.607022	-2.608339	
C	2.745035	-1.422670	2.020213	
C	-5.813152	1.996884	1.243244	
C	-2.288501	-3.901662	-0.465746	
C	4.064701	-0.829329	-0.942671	
C	2.178896	2.000327	-0.277632	
C	1.438750	3.051365	0.315610	
C	1.819958	4.391005	0.128448	
C	3.416645	-0.738013	4.261927	
C	4.822416	-1.704590	-1.738879	
C	-2.958671	-2.691697	-0.299804	
C	-6.068072	0.725402	-0.803246	
C	-4.862983	0.055331	-0.537870	
C	3.266511	-1.739536	3.286743	
H	0.066110	-0.739666	2.709164	
H	0.919109	-1.798466	-1.875289	
H	3.167564	1.379424	4.707770	
H	0.514945	-3.394878	1.481492	
H	2.247030	1.943076	2.469320	
H	4.512045	3.907341	-1.941485	
H	3.850816	1.537658	-1.606872	
H	-7.499717	2.223695	-0.123463	
H	3.221956	5.756583	-0.830953	
H	2.267142	-3.361330	-3.324303	
H	-1.915607	1.089374	2.450216	
H	-0.533403	-5.127268	-0.004698	
H	-4.060993	1.565735	2.431949	
H	4.777975	-3.293720	-3.229640	
H	2.647202	-2.216125	1.262974	
H	-6.179694	2.755471	1.953501	
H	-2.750489	-4.689317	-1.082994	
H	4.579410	-0.154029	-0.241015	
H	0.533768	2.811948	0.894293	
H	1.230278	5.194129	0.598629	
H	3.827843	-0.985008	5.253564	
H	5.922356	-1.688577	-1.673364	
H	-3.944148	-2.545379	-0.762919	
H	-6.630627	0.483668	-1.719427	
H	-4.505282	-0.688448	-1.263492	
H	3.563057	-2.777365	3.508990	
C	-1.210085	-0.977343	-3.238303	
C	-1.509999	-0.013082	-2.117229	
H	-1.858255	-0.763044	-4.119729	
H	-0.159699	-0.929121	-3.585799	
H	-2.568147	0.010931	-1.805961	
C	-0.814180	1.221774	-1.908624	
H	-1.423348	-2.024452	-2.934108	
O	-1.171218	1.925488	-0.853708	
C	0.209635	1.772555	-2.881502	
H	0.964091	1.019167	-3.182512	
H	-0.323371	2.088162	-3.805469	
H	0.722285	2.651913	-2.454387	

JK (R = Me)				E_g(BP86/SVP) = -2172.5299008 G_g(BP86/SVP) = -2171.926004 E_s(M06//TZVP//BP86/SVP) = -2172.9503329
Ru	0.364994	0.834755	-0.052607	
P	-1.653851	-0.269452	0.187808	
C	2.324129	1.024877	1.124423	
C	0.209579	1.584053	1.948939	
C	3.601756	0.312124	0.903611	
C	-3.133649	2.127732	0.534198	
C	-0.664082	-2.752325	3.370320	
C	0.141986	4.016911	0.886760	
C	-0.681199	-2.065101	2.145214	
C	-3.197797	-2.203992	-3.159704	
C	-2.774251	-1.237304	-2.233359	
C	6.103309	-0.980361	0.555678	
C	2.000675	2.354379	0.624853	
C	-1.722212	-1.157549	1.838282	
C	0.666338	2.700217	1.124093	
C	-3.073927	-3.572619	-2.861014	
C	-4.290329	2.916282	0.669771	
C	1.268327	0.606581	2.016138	
C	-3.227436	0.745090	0.277931	
C	0.897222	4.914121	0.151803	
C	4.205829	-0.399316	1.969638	
C	-5.560966	2.330060	0.543710	
C	-2.730302	-0.936960	2.801947	
C	5.444686	-1.037931	1.796959	
C	2.193880	4.561531	-0.363695	
C	-4.511120	0.162898	0.154818	
C	-2.220523	-1.615355	-0.988283	
C	-2.111428	-2.992195	-0.695014	
C	-2.532715	-3.960957	-1.624183	
C	-1.671465	-2.522969	4.325605	
C	-5.667489	0.951123	0.284672	
C	2.747972	3.312200	-0.130689	
C	5.507483	-0.286478	-0.513641	
C	4.267776	0.351231	-0.347271	
C	-2.698357	-1.608830	4.039116	
H	-0.705707	1.567960	2.556003	
H	-2.134401	2.581897	0.605123	
H	0.148707	-3.466724	3.579085	
H	-0.828770	4.313417	1.313743	
H	0.128598	-2.230294	1.416879	
H	-3.631069	-1.883599	-4.120824	
H	-2.894788	-0.170311	-2.476322	
H	7.076795	-1.478374	0.421267	
H	-3.406186	-4.332251	-3.586392	
H	-4.196624	3.996734	0.865157	
H	1.264327	-0.306460	2.621843	
H	0.511541	5.930078	-0.030265	
H	3.708439	-0.427422	2.951787	
H	-6.468860	2.946363	0.642741	
H	-3.549671	-0.233183	2.593614	
H	5.902819	-1.577449	2.641446	
H	2.764089	5.313340	-0.931677	
H	-4.610417	-0.915898	-0.042516	
H	-1.709567	-3.319565	0.274661	
H	-2.443745	-5.029694	-1.370446	
H	-1.652434	-3.051933	5.291892	
H	-6.659952	0.482909	0.183686	
H	3.754060	3.065744	-0.499861	
H	6.007954	-0.250849	-1.494579	
H	3.775499	0.838970	-1.203287	
H	-3.488785	-1.414040	4.781909	
C	-1.328821	2.577037	-2.338617	
C	0.016926	1.975920	-1.962394	
H	-1.296064	3.068172	-3.339463	
H	-2.153831	1.836435	-2.359296	
H	0.763130	2.759145	-1.728930	
C	0.621529	0.949343	-2.794928	
H	-1.621969	3.357237	-1.609605	
O	1.849359	0.636796	-2.667799	
C	2.046337	-4.338090	0.725259	
C	1.591361	-3.676010	-0.354835	
H	1.534863	-5.233910	1.113667	
H	2.957592	-4.009739	1.255320	
H	0.676038	-4.013947	-0.875951	
C	2.281701	-2.495237	-0.991775	
H	3.066144	-2.116801	-0.294143	
O	1.311050	-1.467488	-1.250897	
H	1.710905	-0.807574	-1.896550	
C	2.962374	-2.915066	-2.307894	
H	2.219805	-3.339000	-3.016153	
H	3.442104	-2.038733	-2.791571	
H	3.743834	-3.678808	-2.117400	
C	-0.172096	0.172124	-3.835840	
H	-1.202941	0.537771	-3.990050	
O	0.382190	0.242257	-4.794878	
H	-0.204960	-0.900892	-3.556125	

K (R = Me)			$E_g(\text{BP86/SVP}) = -2172.5520122$ $G_g(\text{BP86/SVP}) = -2171.946108$ $E_s(\text{M06//TZVP//BP86/SVP}) = -2171.946108$
Ru	-0.610733	-0.325896	
P	1.662494	0.119341	
C	-2.731282	-0.717074	
C	-0.724837	-0.948042	2.158402
C	-4.031093	-0.175619	0.488866
C	2.656796	-2.428303	-0.606516
C	2.352198	0.999018	4.127849
C	-0.292473	-3.458091	1.495246
C	1.860980	0.977713	2.812884
C	2.309617	3.610428	-2.087825
C	1.792728	2.389741	-1.617389
C	-6.561482	0.873422	-0.306265
C	-2.222339	-2.062218	0.723071
C	2.392247	0.081763	1.853513
C	-0.972874	-2.204679	1.461690
C	3.358243	4.251037	-1.406014
C	3.516294	-3.346128	-1.233503
C	-1.821050	-0.066307	1.874830
C	2.841919	-1.035355	-0.767931
C	-0.852753	-4.549569	0.838500
C	-4.785782	0.663855	1.351359
C	4.561081	-2.887577	-2.056633
C	3.425060	-0.792936	2.251130
C	-6.030580	1.180613	0.959310
C	-2.089103	-4.416710	0.133052
C	3.896032	-0.585465	-1.594165
C	2.319852	1.783660	-0.454113
C	3.378530	2.435696	0.222008
C	3.891367	3.657713	-0.248777
C	3.375877	0.113763	4.516855
C	4.743124	-1.506344	-2.238948
C	-2.767043	-3.203668	0.057605
C	-5.828716	0.044300	-1.174669
C	-4.583119	-0.471678	-0.784861
C	3.907014	-0.781611	3.575288
H	0.062725	-0.783299	2.902669
H	1.819369	-2.792963	0.009694
H	1.928601	1.708910	4.856536
H	0.636725	-3.559627	2.078506
H	1.047397	1.663280	2.524646
H	1.880385	4.063091	-2.996164
H	0.960263	1.924916	-2.159756
H	-7.538720	1.277725	-0.613955
H	3.759000	5.208972	-1.774652
H	3.359058	-4.427128	-1.088911
H	-1.977768	0.913988	2.341516
H	-0.353027	-5.530271	0.871807
H	-4.396243	0.891448	2.356241
H	5.228361	-3.606374	-2.558540
H	3.868136	-1.489455	1.523766
H	-6.595915	1.822717	1.654069
H	-2.520800	-5.305191	-0.355613
H	4.060616	0.493080	-1.736522
H	3.815982	1.984035	1.124736
H	4.717116	4.145084	0.294479
H	3.756434	0.124510	5.550650
H	5.555430	-1.136511	-2.885352
H	-3.731298	-3.135649	-0.467119
H	-6.226591	-0.196973	-2.173494
H	-4.012439	-1.090655	-1.493841
H	4.711003	-1.477240	3.865409
C	-0.296083	-2.442296	-2.329885
C	-0.849664	-1.044639	-2.093894
H	-0.669244	-2.877250	-3.287910
H	0.809672	-2.448655	-2.376480
H	-1.954632	-1.020282	-2.003088
C	-0.436411	-0.008873	-3.023340
H	-0.591337	-3.141739	-1.525446
O	-1.025467	1.122554	-3.086736
C	-1.452633	3.699749	2.202812
C	-0.977191	3.321736	1.001352
H	-0.823315	4.235729	2.931562
H	-2.498495	3.502097	2.497902
H	0.069671	3.538984	0.719601
C	-1.800875	2.669973	-0.085728
H	-2.730871	2.239485	0.353168
O	-1.027768	1.624448	-0.704287
H	-1.233639	1.495169	-1.742593
C	-2.198688	3.694229	-1.162273
H	-2.782193	3.208123	-1.970492
H	-2.824070	4.489409	-0.709563
H	-1.300947	4.166547	-1.611143
C	0.728320	-0.242273	-3.970139
H	0.503741	-1.088198	-4.654638
H	0.915763	0.669626	-4.567322
H	1.649569	-0.523887	-3.418437

KL (R = Me)			$E_g(\text{BP86/SVP}) = -2172.5411215$ $G_g(\text{BP86/SVP}) = -2171.93841$ $E_s(\text{M06//TZVP//BP86/SVP}) = -2172.9542458$
Ru	0.650194	-0.077456	
P	-1.705381	0.137035	
C	2.673254	-0.769584	
C	0.712106	-0.774491	-2.400249
C	4.025915	-0.412433	-0.596509
C	-1.818502	-2.048149	1.612157
C	-3.061906	-0.373662	-4.060829
C	-0.148886	-3.148573	-1.647594
C	-2.423069	0.107653	-2.905946
C	-2.705341	3.887349	1.311111
C	-2.091507	2.641966	1.092488
C	6.656575	0.288448	0.247373
C	1.895842	-1.989018	-0.777286
C	-2.606468	-0.532412	-1.656297
C	0.722823	-2.017097	-1.645707
C	-3.769794	4.312941	0.497367
C	-2.368698	-2.855969	2.621947
C	1.937120	-0.063787	-2.099905
C	-2.461746	-0.852975	1.220714
C	0.146584	-4.232139	-0.829046
C	4.920911	0.268551	-1.463054
C	-3.558953	-2.470646	3.264590
C	-3.447581	-1.663675	-1.593930
C	6.214842	0.617391	-1.046237
C	1.303331	-4.217808	0.009938
C	-3.658640	-0.472864	1.868423
C	-2.540628	1.795112	0.052235
C	-3.620752	2.224956	-0.753184
C	-4.226813	3.475319	-0.533638
C	-3.887689	-1.511302	-3.989810
C	-4.199848	-1.277141	2.887585
C	2.165469	-3.126306	0.047653
C	5.786217	-0.391644	1.117821
C	4.489890	-0.735682	0.704575
C	-4.077690	-2.152325	-2.754514
H	-0.004883	-0.515769	-3.188135
H	-0.879616	-2.340463	1.115227
H	-2.912888	0.142746	-5.022748
H	-1.018949	-3.165456	-2.321331
H	-1.780057	1.000965	-2.970113
H	-2.339960	4.530550	2.127794
H	-1.261758	2.335232	1.746437
H	7.672543	0.559379	0.575300
H	-4.244537	5.292507	0.668533
H	-1.858125	-3.787626	2.913441
H	2.245470	0.872820	-2.581330
H	-0.505145	-5.119719	-0.836332
H	4.600409	0.505616	-2.489546
H	-3.985723	-3.098814	4.062972
H	-3.616138	-2.170145	-0.631552
H	6.887627	1.142442	-1.743295
H	1.527916	-5.102062	0.628008
H	-4.170151	0.457862	1.578182
H	-4.007055	1.580329	-1.555948
H	-5.067999	3.789550	-1.172537
H	-4.384518	-1.892828	-4.895962
H	-5.130363	-0.966791	3.389680
H	3.075572	-3.161053	0.663322
H	6.116135	-0.649482	2.136992
H	3.816718	-1.235554	1.415487
H	-4.728334	-3.039034	-2.686298
C	1.385495	-1.819392	3.236819
C	1.260475	-0.409972	2.724279
H	1.163985	-2.572232	2.450660
H	2.420709	-2.036010	3.590731
H	1.931544	-0.115993	1.894286
C	0.537795	0.599474	3.308734
H	0.703387	-2.024125	4.085518
O	0.522829	1.862399	2.821875
C	2.010732	3.591752	-2.675435
C	1.286599	3.346334	-1.566984
H	1.569846	4.075187	-3.562658
H	3.083809	3.334245	-2.730766
H	0.215960	3.622443	-1.527018
C	1.819406	2.747475	-0.278552
H	2.789694	2.230469	-0.486157
O	0.869608	1.838482	0.269948
H	0.777726	1.858103	1.823528
C	2.089616	3.866881	0.748286
H	2.463777	3.442222	1.701913
H	2.848286	4.573455	0.354656
H	1.159887	4.433493	0.962409
C	-0.316093	0.474406	4.543473
H	-0.069791	1.300314	5.243421
H	-1.389749	0.585915	4.277341
H	-0.184938	-0.488974	5.068391

L (R = Me)			E_g(BP86/SVP) = -2172.543812 G_g(BP86/SVP) = -2171.944093 E_s(M06//TZVP//BP86/SVP) = -2172.9543404
Ru	-0.495109	-0.681010	
P	1.794287	-0.074846	
C	-2.435775	-1.611664	
C	-0.403665	-2.795408	-0.222874
C	-3.814604	-1.132492	-0.221669
C	1.684162	1.165727	-2.348021
C	3.535175	-3.782512	0.852290
C	0.475857	-2.385118	-2.674750
C	2.745181	-2.625141	0.949602
C	2.386018	2.664409	3.240110
C	1.922822	1.998036	2.093763
C	-6.480920	-0.275797	0.260174
C	-1.638315	-1.457530	-1.698803
C	2.894351	-1.568156	0.019392
C	-0.423478	-2.258162	-1.568486
C	3.396339	2.096451	4.036823
C	2.138970	1.999586	-3.384710
C	-1.670582	-2.461769	0.409844
C	2.413684	1.062870	-1.144416
C	0.161355	-1.762818	-3.874372
C	-4.759926	-1.996036	0.387038
C	3.318127	2.747398	-3.224924
C	3.844554	-1.703409	-1.014782
C	-6.076673	-1.571386	0.627537
C	-1.032124	-0.980749	-4.006538
C	3.600774	1.815693	-0.990283
C	2.473174	0.748359	1.721115
C	3.493926	0.188332	2.521340
C	3.949564	0.857988	3.672160
C	4.475863	-3.910738	-0.186776
C	4.047306	2.654443	-2.025365
C	-1.917892	-0.815829	-2.949070
C	-5.553523	0.592248	-0.344192
C	-4.235095	0.172608	-0.581081
C	4.625082	-2.870639	-1.119110
H	0.362608	-3.467655	0.182247
H	0.755095	0.586522	-2.468140
H	3.412768	-4.591388	1.590521
H	1.380370	-3.004355	-2.574674
H	2.001255	-2.535581	1.758278
H	1.944879	3.636487	3.512717
H	1.129275	2.465015	1.491188
H	-7.513996	0.057779	0.447081
H	3.753752	2.620010	4.938065
H	1.560309	2.071128	-4.319312
H	-1.979633	-2.781758	1.413698
H	0.831343	-1.872411	-7.41316
H	-4.456965	-3.020407	0.655944
H	3.667906	3.408884	-4.033756
H	3.978286	-0.891517	-1.745798
H	-6.794655	-2.261782	1.098766
H	-1.257215	-0.509605	-4.976800
H	4.175136	1.750112	-0.052980
H	3.951602	-0.773514	2.246365
H	4.749257	0.406537	4.281371
H	5.090808	-4.821135	-0.267977
H	4.969860	3.241992	-1.891781
H	-2.848106	-0.242651	-3.078539
H	-5.854488	1.614844	-0.622768
H	-3.507943	0.879854	-1.009050
H	5.359286	-2.961632	-1.935738
C	-2.004732	3.185927	-2.905939
C	-1.573897	2.798997	-1.517567
H	-1.257488	2.872808	-3.670161
H	-2.964230	2.699212	-3.195385
H	-1.408781	1.717065	-1.339163
C	-1.333893	3.628127	-0.466713
H	-2.150003	4.278909	-3.021136
O	-0.941656	3.186042	0.769490
C	-2.352157	-1.765214	3.983506
C	-1.503281	-0.813673	3.551138
H	-2.039695	-2.531970	4.711519
H	-3.399100	-1.803942	3.633840
H	-0.459150	-0.787226	3.916094
C	-1.861922	0.317492	2.607479
H	-2.818090	0.068604	2.084251
O	-0.804132	0.506001	1.659679
H	-0.941738	2.191097	0.848557
C	-2.055136	1.622682	3.402928
H	-2.265517	2.470509	2.721257
H	-2.898106	1.514521	4.115637
H	-1.136547	1.864169	3.976880
C	-1.439406	5.129751	-0.469336
H	-2.175248	5.463893	0.293538
H	-0.462585	5.577536	-0.186010
H	-1.739461	5.534485	-1.452924

LF (R = Me)			E _g (BP86/SVP) = -1940.2283227 G _g (BP86/SVP) = -1939.727675 E _s (M06//TZVP//BP86/SVP) = -1940.5416318
Ru	0.652474	-0.014348	
P	-1.659357	0.181518	
C	2.700653	-0.912920	
C	0.800933	-1.467569	-2.013877
C	4.066181	-0.467430	-0.341300
C	-1.356970	-0.789187	2.578648
C	-3.234096	-1.484453	-3.505084
C	-0.243456	-3.204339	-0.335652
C	-2.513869	-0.697688	-2.591086
C	-2.479662	4.177634	0.561952
C	-1.954767	2.877441	0.628477
C	6.742724	0.329161	0.234244
C	1.837535	-1.835004	0.077554
C	-2.681332	-0.873211	-1.196250
C	0.696665	-2.205190	-0.782456
C	-3.462034	4.499568	-0.393245
C	-1.781760	-1.095304	3.884294
C	2.001840	-0.671440	-1.921507
C	-2.262534	-0.237750	1.649311
C	-0.047362	-3.816880	0.884904
C	4.996957	-0.206018	-1.380602
C	-3.110886	-0.854005	4.270325
C	-3.572971	-1.867626	-0.739814
C	6.312458	0.192035	-1.097536
C	1.074275	-3.471644	1.719910
C	-3.595477	0.018334	2.047376
C	-2.413437	1.876431	-0.261893
C	-3.402282	2.202707	-1.214897
C	-3.919943	3.510317	-1.279203
C	-4.119697	-2.474407	-3.039862
C	-4.017475	-0.295416	3.349722
C	1.993396	-2.510928	1.341403
C	5.833756	0.076784	1.277581
C	4.513811	-0.308178	0.996125
C	-4.282325	-2.665304	-1.657468
H	0.126236	-1.543481	-2.874876
H	-0.311614	-0.956476	2.273835
H	-3.098569	-1.327564	-4.587271
H	-1.076277	-3.496030	-0.992880
H	-1.804666	0.061240	-2.960375
H	-2.117055	4.946885	1.262599
H	-1.174690	2.612501	1.361944
H	7.777691	0.632836	0.457540
H	-3.871480	5.521166	-0.444634
H	-1.063619	-1.517972	4.604922
H	2.359829	0.009519	-2.706171
H	-0.748025	-4.594938	1.226512
H	4.688500	-0.343450	-2.428536
H	-3.441789	-1.091768	5.294183
H	-3.710534	-2.027367	0.340219
H	7.012262	0.384497	-1.926816
H	1.206998	-4.000097	2.677380
H	-4.304646	0.477177	1.339612
H	-3.784679	1.436620	-1.906303
H	-4.693723	3.751478	-2.025864
H	-4.679262	-3.097314	-3.755688
H	-5.057857	-0.093192	3.651332
H	2.867725	-2.301575	1.973466
H	6.151613	0.194832	2.326075
H	3.804746	-0.446411	1.824932
H	-4.969851	-3.441322	-1.284283
C	2.707369	2.803070	-1.610394
C	1.635606	2.494856	-0.847060
H	2.674250	2.714631	-2.708686
H	3.653772	3.154336	-1.168657
H	0.680078	2.207573	-1.357894
C	1.492695	2.571356	0.666073
O	0.799429	1.434423	1.131897
H	0.825467	3.462511	0.850665
C	2.796102	2.847192	1.427069
H	3.557510	2.071428	1.213034
H	3.216279	3.841149	1.163090
H	2.587695	2.841762	2.515921

C (R = Ph)			E _g (BP86/SVP) = -2592.6393264 G _g (BP86/SVP) = -2592.077368 E _s (M06//TZVP//BP86/SVP) = -2593.0930405
Ru	-0.180562	-0.485309	0.306512
Cl	-0.404165	-0.683409	-2.131985
P	1.827933	0.673286	-0.071943
C	-1.470115	-2.351961	0.788601
C	0.113661	-1.406632	2.268992
C	-2.764824	-2.786854	0.219656
C	2.859999	-1.325432	-1.813423
C	3.233934	1.186886	3.816778
C	2.140796	-2.895636	1.509105
C	2.432485	1.188853	2.663021
C	0.862915	4.058916	-2.224340
C	1.002513	2.735160	-1.777513
C	-5.249007	-3.683145	-0.816966
C	-0.152322	-2.961280	0.530706
C	2.936178	0.706145	1.430487
C	0.803428	-2.410681	1.473770
C	1.407671	5.121230	-1.479642
C	3.747977	-1.832978	-2.778033
C	-1.290288	-1.473025	1.912237
C	2.959722	0.016746	-1.393154
C	2.502313	-3.928618	0.646213
C	-3.892325	-2.940694	1.064278
C	4.736874	-1.006043	-3.337406
C	4.256749	0.205926	1.392242
C	-5.121840	-3.381317	0.550232
C	1.566675	-4.468265	-0.282313
C	3.953215	0.846338	-1.962664
C	1.698022	2.458910	-0.575093
C	2.245590	3.528068	0.166168
C	2.097700	4.852889	-0.285850
C	4.546808	0.683456	3.767451
C	4.837008	0.335807	-2.928435
C	0.258515	-3.989937	-0.360756
C	-4.139175	-3.530405	-1.666490
C	-2.910013	-3.083979	-1.158010
C	5.052105	0.190775	2.553393
H	0.537629	-0.892123	3.140303
H	2.072702	-1.971889	-1.401108
H	2.825903	1.576482	4.763244
H	2.858694	-2.480032	2.232458
H	1.401228	1.567122	2.724925
H	0.319979	4.260752	-3.161314
H	0.575162	1.903195	-2.362512
H	-6.213401	-4.030493	-1.220416
H	1.293356	6.159048	-1.830910
H	3.653506	-2.881175	-3.102918
H	-2.103336	-0.948924	2.431487
H	3.525056	-4.335643	0.679103
H	-3.794887	-2.735296	2.142260
H	5.425548	-1.404253	-4.099779
H	4.670069	-0.180810	0.449081
H	-5.985211	-3.496914	1.224878
H	1.882076	-5.288476	-0.946746
H	4.035675	1.900267	-1.654101
H	2.798764	3.331510	1.097309
H	2.530607	5.678707	0.301173
H	5.171950	0.674628	4.674413
H	5.603801	0.993755	-3.367760
H	-0.458794	-4.428141	-1.069325
H	-4.235656	-3.743557	-2.743060
H	-2.062767	-2.905979	-1.837810
H	6.077629	-0.208879	2.502290
C	-0.831441	1.340175	1.256000
C	-1.551848	1.156005	0.033175
H	-0.100050	2.165659	1.300742
H	-1.331683	1.161592	2.224750
H	-1.220857	1.766452	-0.827100
C	-3.039595	0.821233	-0.070669
H	-3.312990	0.111345	0.752294
O	-3.348652	0.268533	-1.335498
H	-2.529152	-0.169798	-1.671424
C	-3.856089	2.099361	0.142268
C	-4.212716	2.518209	1.441538
C	-4.231359	2.899131	-0.956800
C	-4.915868	3.717838	1.642397
H	-3.946739	1.888997	2.307987
C	-4.936794	4.098284	-0.758264
H	-3.976702	2.548513	-1.968441
C	-5.278283	4.514547	0.541126
H	-5.191938	4.028137	2.663336
H	-5.228457	4.711292	-1.626771
H	-5.834631	5.453100	0.695749

D (R = Ph)			E _g (BP86/SVP) = -2825.5667991 G _g (BP86/SVP) = -2824.900214 E _s (M06//TZVP//BP86/SVP) = -2826.147104
Ru	-0.449751	-0.505100	
Cl	0.037534	-0.686909	
P	-2.353592	0.650621	
C	0.769465	-2.325005	
C	-1.070855	-1.422370	-2.293237
C	2.158110	-2.762545	
C	-3.184759	-1.394580	
C	-4.260171	1.369177	
C	-2.880882	-3.010861	
C	-3.321847	1.319104	-2.316541
C	-1.001983	3.978293	2.314205
C	-1.210199	2.669167	1.849761
C	4.814584	-3.590213	-0.289828
C	-0.457005	-2.993173	-0.661744
C	-3.661976	0.759971	-1.060376
C	-1.580795	-2.470022	-1.417731
C	-1.732267	5.051493	1.771758
C	-3.950251	-1.935737	3.115811
C	0.375283	-1.439781	-2.183862
C	-3.334657	-0.040582	1.704162
C	-3.047301	-0.058338	-0.312765
C	2.891963	-3.476194	-1.780671
C	-4.863809	-1.131076	3.818615
C	-4.962761	0.235691	-0.890676
C	4.208934	-3.893387	-1.522900
C	-1.948538	-4.554359	0.443030
C	-4.249961	0.765511	2.417971
C	-2.159915	2.421412	0.828949
C	-2.890637	3.501911	0.287527
C	-2.676268	4.810588	0.758698
C	-5.553101	0.843556	-3.179349
C	-5.010855	0.222936	3.468526
C	-0.663547	-4.025348	0.289957
C	4.096550	-2.878083	0.687446
C	2.771731	-2.480861	0.439915
C	-5.897396	0.273200	-1.943091
H	-1.653285	-0.908250	-3.068872
H	-2.447745	-2.019680	1.545177
H	-3.974026	1.816078	-4.326503
H	-3.732976	-2.621057	-1.802175
H	-2.307000	1.711324	-2.480027
H	-0.252647	4.158114	3.101482
H	-0.635482	1.825871	2.271183
H	5.858012	-3.891922	-0.099355
H	-1.560670	6.077785	2.135362
H	-3.814679	-2.993459	3.392665
H	1.074433	-0.880671	-2.819067
H	-4.046339	-4.500096	-0.166999
H	2.419777	-3.700323	-2.751718
H	-5.454350	-1.555960	4.646985
H	-5.250642	-0.211048	0.072585
H	4.769220	-4.445379	-2.296218
H	-2.115568	-5.374765	1.159991
H	-4.364258	1.829692	2.157776
H	-3.632592	3.323775	-0.506518
H	-3.251651	5.646075	0.327017
H	-6.286468	0.875740	-4.001441
H	-5.715743	0.866034	4.020578
H	0.187896	-4.408718	0.872243
H	4.569610	-2.547294	1.624546
H	2.220876	-1.892193	1.191315
H	-6.904603	-0.147489	-1.788716
C	0.068913	1.364015	-1.355234
C	1.052754	1.084901	-0.350363
H	-0.646511	2.190057	-1.184536
H	0.341235	1.254162	-2.421405
H	0.937760	1.580442	0.629791
C	2.602524	0.871308	-0.566381
H	2.783984	-0.216836	-0.797150
O	3.271951	1.339472	0.516593
H	3.939470	0.376493	1.502308
C	5.414300	0.773226	2.762010
C	6.217258	0.027243	3.844983
H	6.964913	0.688783	4.334752
H	5.529141	-0.367249	4.622683
H	6.753568	-0.837000	3.397619
C	4.660548	1.974761	3.387227
H	4.030920	2.445993	2.604752
H	3.988220	1.616003	4.195622
H	5.351225	2.737659	3.812897
C	6.355702	1.278011	1.639097
H	6.910924	0.421159	1.200769
H	5.729830	1.724679	0.838752
H	7.093101	2.030785	1.999200
O	4.484219	-0.147729	2.226044
C	3.019100	1.636122	-1.851392
C	3.289891	0.986785	-3.072855
C	3.190239	3.037342	-1.788840
C	3.697345	1.713475	-4.210491
H	3.213148	-0.113679	-3.124349
C	3.579011	3.768942	-2.920745
C	3.034646	3.522060	-0.811392
C	3.833980	3.109991	-4.142176
H	3.920668	1.181878	-5.151705
H	3.698445	4.864301	-2.853787
H	4.153014	3.682997	-5.029169

DE (R = Ph)				$E_g(\text{BP86/SVP}) = -2825.5460104$ $G_g(\text{BP86/SVP}) = -2824.879068$ $E_s(\text{M06//TZVP//BP86/SVP}) = -2826.125800$
Ru	-0.259698	-0.091620	-0.745337	
Cl	0.650650	-0.338457	1.518209	
P	-2.207584	0.536059	0.281015	
C	0.931764	-2.045177	-1.824823	
C	-1.019654	-1.010174	-2.609340	
C	2.338332	-2.453341	-1.664323	
C	-2.314111	-1.769674	1.935829	
C	-4.980350	0.872095	-2.826998	
C	-2.687940	-2.813055	-1.678050	
C	-3.833840	0.990057	-2.023455	
C	-1.275820	4.032826	2.288587	
C	-1.270552	2.726633	1.771281	
C	5.020706	-3.361619	-1.415716	
C	-0.230885	-2.795075	-1.318380	
C	-3.780657	0.400541	-0.737162	
C	-1.429426	-2.207258	-1.878857	
C	-2.315659	4.923246	1.963455	
C	-2.716944	-2.521562	3.052272	
C	0.430309	-1.028521	-2.688068	
C	-2.697891	-0.417911	1.810330	
C	-2.762774	-3.998903	-0.926440	
C	3.217623	-2.446727	-2.775675	
C	-3.495858	-1.931764	4.063454	
C	-4.908298	-0.325258	-0.290673	
C	4.539985	-2.896317	-2.654619	
C	-1.595845	-4.567882	-0.363071	
C	-3.479024	0.169912	2.829876	
C	-2.318444	2.290155	0.924933	
C	-3.361064	3.187645	0.605399	
C	-3.356592	4.497897	1.120488	
C	-6.095672	0.146085	-2.370476	
C	-3.874723	-0.582959	3.950366	
C	-0.334134	-3.976710	-0.543251	
C	4.165115	-3.357357	-0.300238	
C	2.839924	-2.912047	-0.423235	
C	-6.051991	-0.453153	-1.100602	
H	-1.683142	-0.447792	-3.279359	
H	-1.684777	-2.235904	1.164224	
H	-4.997313	1.345728	-3.822259	
H	-3.592737	-2.370175	-2.122657	
H	-2.963335	1.545159	-2.402211	
H	-0.453181	4.357936	2.945737	
H	-0.454139	2.028049	2.023025	
H	6.061630	-3.712476	-1.319466	
H	-2.312067	5.950012	2.364496	
H	-2.401855	-3.573853	3.134911	
H	1.052198	-0.363169	-3.300516	
H	-3.737440	-4.490564	-0.775539	
H	2.845751	-2.093126	-3.750526	
H	-3.799808	-2.520686	4.944531	
H	-4.892918	-0.802904	0.699841	
H	5.203888	-2.882412	-3.535196	
H	-1.675710	-5.500382	0.220009	
H	-3.777667	1.227024	2.754218	
H	-4.186270	2.863049	-0.047323	
H	-4.175372	5.188691	0.859446	
H	-6.991583	0.044701	-3.004406	
H	-4.477485	-0.107091	4.741369	
H	0.567706	-4.443911	-0.120912	
H	4.526645	-3.675486	0.690317	
H	2.206161	-2.859962	0.473179	
H	-6.915646	-1.030010	-0.730853	
C	-0.493018	1.807711	-1.751162	
C	0.710165	1.828180	-0.983619	
H	-1.336283	2.453791	-1.442351	
H	-0.404081	1.705764	-2.850234	
H	0.724323	2.316336	0.006075	
C	2.090703	1.611727	-1.624227	
H	1.900510	1.585311	-2.759177	
O	2.592534	0.465483	-1.119635	
H	2.482722	-1.421712	2.350630	
C	4.152959	-0.853490	3.214195	
C	5.195906	-1.561438	4.095910	
H	6.001225	-0.863290	4.406991	
H	4.713254	-1.975220	5.006441	
H	5.657203	-2.404883	3.540804	
C	3.471799	0.288098	4.001353	
H	2.693572	0.767732	3.372151	
H	2.978618	-0.116136	4.910516	
H	4.200799	1.068584	4.309817	
C	4.802591	-0.306604	1.926541	
H	5.340800	-1.116487	1.392540	
H	4.030261	0.088044	1.231426	
H	5.526499	0.507168	2.149763	
O	3.183759	-1.861562	2.892065	
C	2.974124	2.866793	-1.447512	
C	2.577416	4.138526	-1.915512	
C	4.228062	2.737298	-0.821293	
C	3.410431	5.258709	-1.752775	
H	1.598522	4.248590	-2.415943	
C	5.069906	3.853729	-0.662879	
H	4.502458	1.727884	-0.473850	
C	4.664791	5.119361	-1.125000	
H	3.083886	6.247811	-2.118302	
H	6.052201	3.737365	-0.172940	
H	5.322373	5.996234	-0.998862	

E (R = Ph)				E _g (BP86/SVP) = -2825.5782087 G _g (BP86/SVP) = -2824.909171 E _s (M06//TZVP//BP86/SVP) = -2826.1555976
Ru	-0.114462	0.474921	-1.299889	
Cl	1.532128	0.361000	0.559716	
P	-1.771016	0.586472	0.383988	
C	0.178274	-1.949121	-1.994216	
C	-1.610655	-0.643550	-2.722202	
C	1.540176	-2.502753	-1.893485	
C	-0.907866	-1.629829	1.926054	
C	-5.477007	0.963922	-1.497303	
C	-3.495291	-2.264651	-1.866806	
C	-4.112260	1.039733	-1.171294	
C	-0.585426	4.003716	2.433797	
C	-0.635194	2.736027	1.831863	
C	4.175453	-3.598590	-1.725178	
C	-1.075158	-2.607529	-1.542857	
C	-3.597990	0.394523	-0.021838	
C	-2.180194	-1.819000	-2.019301	
C	-1.693454	4.869013	2.368333	
C	-0.787334	-2.415635	3.085983	
C	-0.219019	-0.921069	-2.928869	
C	-1.632311	-0.423292	1.951378	
C	-3.739627	-3.501519	-1.219272	
C	2.498791	-2.289069	-2.921331	
C	-1.397391	-2.004465	4.282546	
C	-4.490579	-0.357745	0.771531	
C	3.789301	-2.830078	-2.840152	
C	-2.666454	-4.270008	-0.744360	
C	-2.232023	-0.007714	3.163437	
C	-1.803207	2.304031	1.157536	
C	-2.909544	3.178931	1.095486	
C	-2.852803	4.452947	1.694045	
C	-6.357757	0.221704	-0.689808	
C	-2.120563	-0.797452	4.320134	
C	-1.328947	-3.833952	-0.906345	
C	3.251258	-3.800036	-0.685672	
C	1.957864	-3.261744	-0.769112	
C	-5.855234	-0.444005	0.440340	
H	-2.208340	0.009814	-3.372711	
H	-0.420033	-1.936641	0.991005	
H	-5.851264	1.482152	-2.395532	
H	-4.336132	-1.663584	-2.248506	
H	-3.431404	1.601371	-1.827342	
H	0.334737	4.318923	2.952261	
H	0.243072	2.068019	1.861310	
H	5.192611	-0.018961	-1.660501	
H	-1.650955	5.865170	2.838859	
H	-0.184058	-3.334834	3.053118	
H	0.425917	-0.457376	-3.686350	
H	-4.775143	-3.857358	-1.092872	
H	2.223249	-1.683030	-3.796350	
H	-1.297830	-2.617351	5.193690	
H	-4.117822	-0.895173	1.655476	
H	4.505710	-2.644840	-3.658092	
H	-2.860954	-5.235987	-0.248703	
H	-2.785695	0.943656	3.204941	
H	-3.833251	2.866414	0.586031	
H	-3.729144	5.119594	1.633923	
H	-7.427586	0.155298	-0.947041	
H	-2.592296	-0.461893	5.258667	
H	-0.501314	-4.473815	-0.565197	
H	3.539454	-4.357477	0.219493	
H	1.277586	-3.394568	0.083444	
H	-6.528359	-1.045388	1.073228	
H	-0.846842	2.304295	-2.182367	
C	0.350032	2.571490	-1.452396	
H	-1.798491	2.715674	-1.802608	
H	-0.794304	2.220029	-3.285007	
H	0.344317	3.156736	-0.518436	
C	1.651374	2.326103	-2.229299	
H	1.612666	2.928568	-3.186615	
O	1.591547	0.952976	-2.500577	
H	2.162475	-1.522479	1.765971	
C	3.437766	-1.685518	3.263426	
C	3.880413	-2.848925	4.166497	
H	4.649694	-2.522114	4.897134	
H	3.010746	-3.252766	4.725676	
H	4.303274	-3.670831	3.552031	
C	2.807033	-0.555767	4.106491	
H	2.444514	0.255922	3.442102	
H	1.935912	-0.942369	4.674887	
H	3.535586	-0.119727	4.824474	
C	4.632441	-1.144919	2.448884	
H	5.072062	-1.954605	1.830655	
H	4.294648	-0.340497	1.762713	
H	5.426809	-0.729913	3.106808	
O	2.457091	-2.241862	2.379658	
C	2.937116	2.795142	-1.542183	
C	3.097831	4.146762	-1.167488	
C	4.012336	1.906669	-1.346912	
C	4.299790	4.600088	-0.596470	
H	2.267318	4.856907	-1.327326	
C	5.219530	2.359200	-0.785714	
H	3.863359	0.854367	-1.633136	
C	5.369328	3.705418	-0.404644	
H	4.403393	5.657721	-0.299236	
H	6.050934	1.649934	-0.635712	
H	6.314761	4.057128	0.041538	

EF (R = Ph)

Ru	0.896846	0.303359	1.349983
Cl	-2.515935	0.102203	-0.758987
P	1.913500	-0.079843	-0.708428
C	-0.265325	-1.579699	2.572253
C	1.989931	-1.621502	1.989047
C	-1.531247	-1.268093	3.266324
C	0.152012	-1.958113	-1.814704
C	5.875018	1.173786	-0.328390
C	1.848832	-3.874803	0.620225
C	4.489782	1.152367	-0.569765
C	-0.066536	2.763437	-2.992764
C	0.271535	1.833474	-1.993244
C	-3.965947	-0.720421	4.622670
C	-0.062492	-2.707568	1.628231
C	3.773107	-0.068542	-0.589066
C	1.340233	-2.787842	1.336361
C	0.863420	3.117820	-3.983879
C	-0.252386	-2.959382	-2.714636
C	1.033638	-1.111939	2.958643
C	1.502122	-1.546057	-1.785561
C	0.959848	-4.875633	0.154687
C	-1.557965	-1.082163	4.672088
C	0.674333	-3.556233	-3.585772
C	4.488215	-1.263450	-0.336640
C	-2.761052	-0.812656	5.343302
C	-0.416549	-4.775036	0.409212
C	2.428971	-2.129072	-2.679265
C	1.554593	1.245714	-1.980042
C	2.475628	1.577040	-3.001495
C	2.134817	2.515898	-3.990198
C	6.574785	-0.022796	-0.096990
C	2.016263	-3.135937	-3.568910
C	-0.940921	-3.690561	1.151927
C	-3.950710	-0.887619	3.225709
C	-2.750034	-1.156364	2.550137
C	5.873143	-1.241691	-0.099260
H	3.079527	-1.542439	2.120459
H	-0.608756	-1.471599	-1.173383
H	6.408978	2.138047	-0.321928
H	2.930756	-3.971268	0.429530
H	3.960666	2.100608	-0.749688
H	-1.075400	3.204598	-2.986601
H	-0.498431	1.528356	-1.260792
H	-4.911807	-0.507336	5.147935
H	0.595236	3.853295	-4.760202
H	-1.310630	-3.263518	-2.729171
H	1.271123	-0.540561	3.867810
H	1.354227	-5.732036	-0.415492
H	-0.621695	-1.173126	5.246626
H	0.350571	-4.343602	-4.286432
H	3.951650	-2.223377	-0.327607
H	-2.758211	-0.678358	6.438059
H	-1.100528	-5.554616	0.035626
H	3.477567	-1.793623	-2.695777
H	3.465864	1.096848	-3.037492
H	2.867157	2.770626	-4.774228
H	7.660938	-0.005805	0.088693
H	2.748981	-3.587155	-4.258627
H	-2.017531	-3.632847	1.373027
H	-4.879531	-0.784797	2.641456
H	-2.739759	-1.197967	1.446811
H	6.406808	-2.188187	0.086027
C	2.450085	1.505823	2.151027
C	1.588610	2.322642	1.335447
H	3.484662	1.296241	1.825681
H	2.334643	1.545853	3.252711
H	1.930290	2.814816	0.408593
C	0.285767	2.796866	2.009753
H	0.504504	3.238234	3.021189
O	-0.408788	1.569075	2.155860
H	-4.530675	-0.656817	-1.013981
C	-5.602632	-0.822993	-2.643483
C	-4.530351	-1.628392	-3.415467
H	-4.620593	-1.505277	-4.517425
H	-3.523453	-1.285607	-3.096161
H	-4.622404	-2.708160	-3.171394
C	-5.481769	0.680120	-2.988723
H	-6.250609	1.258592	-2.433803
H	-4.481935	1.044849	-2.671671
H	-5.608168	0.874472	-4.076743
C	-7.012632	-1.343212	-2.972281
H	-7.098306	-2.414150	-2.691228
H	-7.771745	-0.779077	-2.390385
H	-7.244131	-1.240158	-4.053815
O	-5.435241	-1.013945	-1.241609
C	-0.513338	3.836124	1.234101
C	-0.079522	5.179946	1.217316
C	-1.684396	3.481541	0.533366
C	-0.795714	6.156833	0.505905
H	0.830266	5.464661	1.774827
C	-2.402458	4.464107	-0.173904
H	-2.024513	2.430636	0.525542
C	-1.964819	5.800146	-0.192581
H	-0.444426	7.202401	0.501847
H	-3.313992	4.169188	-0.719003
H	-2.533142	6.565022	-0.747742

$E_g(\text{BP86/SVP}) = -2825.55850035$

$G_g(\text{BP86/SVP}) = -2824.889826$

$E_s(\text{M06//TZVP//BP86/SVP}) = -2826.1362411$

F (R = Ph)			E _g (BP86/SVP) = -2131.8647132 G _g (BP86/SVP) = -2131.314531 E _s (M06//TZVP//BP86/SVP) = -2132.216922
Ru	0.399826	-0.633739	
P	-1.816164	0.232821	
C	1.945153	-2.260936	
C	-0.295845	-2.625874	-1.204828
C	3.412404	-2.121628	-0.611233
C	-1.376286	0.232998	2.612907
C	-4.023845	-2.110099	-2.811495
C	-1.197450	-3.209736	1.206743
C	-3.066510	-1.258862	-2.235546
C	-2.596557	4.310752	-0.659285
C	-2.281286	3.053138	-0.115223
C	6.240488	-1.891283	-0.760423
C	1.156383	-2.581421	0.654779
C	-3.128131	-0.912278	-0.863649
C	-0.221468	-2.813341	0.243162
C	-2.979589	4.426995	-2.006055
C	-1.719059	0.424370	3.965121
C	1.022291	-2.343228	-1.671939
C	-2.326807	0.483148	1.599779
C	-0.810701	-3.372385	2.532659
C	4.136201	-2.710254	-1.678401
C	-3.005705	0.862541	4.316981
C	-4.149583	-1.485988	-0.075711
C	5.533536	-2.595149	-1.751828
C	0.537821	-3.139355	2.937707
C	-3.616087	0.948734	1.959744
C	-2.345226	1.881752	-0.907204
C	-2.731545	2.013721	-2.260631
C	-3.047471	3.271836	-2.803094
C	-5.047331	-2.660632	-2.018800
C	-3.953733	1.129734	3.310518
C	1.512572	-2.744209	2.027426
C	5.534083	-1.292980	0.298773
C	4.136580	-1.400879	0.372563
C	-5.097454	-2.355089	-0.649449
H	-1.177494	-2.821007	-1.824310
H	-0.352118	-0.058767	2.327120
H	-3.959704	-2.356709	-3.883467
H	-2.230204	-3.414746	0.886576
H	-2.231921	-0.886247	-2.850804
H	-2.543090	5.205234	-0.018294
H	-1.996222	2.986428	0.945246
H	7.337072	-1.803209	-0.817083
H	-3.227662	5.412268	-2.431490
H	-0.965412	0.235695	4.746054
H	1.312728	-2.247557	-2.726026
H	-1.550691	-3.693551	3.282296
H	3.594856	-3.282753	-2.448478
H	-3.270976	1.010110	5.376335
H	-4.207764	-1.263459	0.999609
H	6.076087	-3.066223	-2.587377
H	0.814060	-3.290445	3.993486
H	-4.358176	1.185432	1.180435
H	-2.803784	1.129021	-2.908393
H	-3.352912	3.344163	-3.859235
H	-5.793950	-3.335764	-2.466094
H	-4.960118	1.489482	3.579024
H	2.554555	-2.600151	2.347684
H	6.076459	-0.721372	1.068917
H	3.579525	-0.885011	1.169203
H	-5.882326	-2.794956	-0.013349
C	1.731338	0.504221	-1.771644
C	0.815421	1.406129	-1.194540
H	1.642112	0.254690	-2.841494
H	2.735938	0.385769	-1.332454
H	0.040145	1.888253	-1.810686
C	1.101240	1.902167	0.228073
O	1.251224	0.698174	0.939164
H	0.195127	2.470457	0.576632
C	2.278304	2.870547	0.348646
C	3.433526	2.518488	1.071285
C	2.215834	4.144329	-0.258894
C	4.510123	3.418250	1.181131
H	3.462445	1.528068	1.549140
C	3.292585	5.039786	-0.158632
H	1.309853	4.438194	-0.816364
C	4.445986	4.679079	0.564039
H	5.407106	3.131624	1.754469
H	3.231680	6.028402	-0.642540
H	5.289912	5.382789	0.647608

FG (R = Ph)		
Ru	-0.576159	-0.568412 0.311984
P	1.762840	-0.070939 0.267834
C	-2.427992	-1.977647 0.392659
C	-0.261276	-2.786929 0.739932
C	-3.863492	-1.717323 0.646181
C	1.611834	1.612040 -2.013271
C	3.709754	-3.731163 -0.326070
C	0.297725	-3.133656 -1.829534
C	2.993864	-2.663032 0.239914
C	3.061228	1.500794 3.928352
C	2.341079	1.240373 2.750243
C	-6.640961	-1.333901 1.134197
C	-1.816959	-2.176350 -0.917038
C	2.749085	-1.475197 -0.492064
C	-0.474628	-2.698266 -0.707845
C	4.232187	0.783447 4.224374
C	2.073597	2.589172 -2.913593
C	-1.466002	-2.422330 1.396613
C	2.325683	1.336157 -0.827307
C	-0.249407	-3.047639 -3.102546
C	-4.519841	-2.386848 1.709647
C	3.242689	3.316411 -2.629547
C	3.245656	-1.396501 -1.811768
C	-5.890217	-2.198274 1.949954
C	-1.564137	-2.527024 -3.308651
C	3.498911	2.070013 -0.549432
C	2.768331	0.245540 1.838996
C	3.976822	-0.434796 2.125965
C	4.694353	-0.174110 3.307613
C	4.192487	-3.640066 -1.644507
C	3.949816	3.056644 -1.442453
C	-2.343620	-2.093314 -2.246037
C	-6.004527	-0.657582 0.078001
C	-4.634247	-0.843454 -0.161923
C	3.955575	-2.469044 -2.382427
H	0.618799	-3.217330 1.227426
H	0.681383	1.058947 -2.221319
H	3.893020	-4.639492 0.270097
H	1.292692	-3.573975 -1.677653
H	2.640761	-2.751679 1.278286
H	2.703730	2.286384 4.613463
H	1.484786	1.878039 2.492879
H	-7.716290	-1.186101 1.321613
H	4.792637	0.984285 5.151514
H	1.508477	2.786562 -3.838779
H	-1.648162	-2.470120 2.477607
H	0.331772	-3.402184 -3.968369
H	-3.949540	-3.085199 2.341722
H	3.599851	4.088525 -3.329780
H	3.080332	-0.487453 -2.407738
H	-6.376424	-2.737791 2.778552
H	-1.973516	-2.490123 -4.330918
H	4.063183	1.876177 0.375069
H	4.386821	-1.167417 1.418330
H	5.629763	-0.723433 3.501984
H	4.753049	-4.477034 -2.090181
H	4.861433	3.628333 -1.205611
H	-3.370881	-1.740388 -2.415328
H	-6.579304	0.029971 -0.563028
H	-4.144879	-0.281780 -0.971543
H	4.329921	-2.380224 -3.414823
C	-2.092777	0.647028 1.239935
C	-0.865243	1.314939 1.505284
H	-2.576377	0.090225 2.057965
H	-2.795026	1.057282 0.498225
H	-0.395160	1.172579 2.492143
C	-0.494471	2.612483 0.854632
H	-0.700050	0.485007 -0.875073
O	0.615931	3.128033 1.034599
C	-1.496162	3.379891 0.015589
C	-2.838307	3.574459 0.416551
C	-1.024413	4.053761 -1.134409
C	-3.693834	4.401526 -0.332344
H	-3.209004	3.106125 1.340961
C	-1.886783	4.855072 -1.896715
H	0.032526	3.933973 -1.415995
C	-3.225672	5.030512 -1.498641
H	-4.732141	4.558084 0.001611
H	-1.510958	5.357388 -2.802665
H	-3.900548	5.668907 -2.091312

$E_g(\text{BP86/SVP}) = -2131.8561943$
 $G_g(\text{BP86/SVP}) = -2131.304529$
 $E_s(\text{M06//TZVP//BP86/SVP}) = -2132.2092659$

G (R = Ph)				E _g (BP86/SVP) = -2131.8880428 G _g (BP86/SVP) = -2131.341265 E _s (M06//TZVP//BP86/SVP) = -2131.341265
Ru	-0.222716	-0.116388	0.247984	
P	1.994513	0.370605	-0.149383	
C	-1.967909	-1.521187	0.639300	
C	-0.568210	-0.794069	2.404577	
C	-3.197892	-1.811322	-0.138889	
C	2.384153	-1.950997	-1.746013	
C	3.308787	1.001934	3.737447	
C	1.266694	-2.656285	2.084875	
C	2.581658	1.024765	2.535619	
C	2.230669	3.515392	-2.832915	
C	1.987906	2.274946	-2.220935	
C	-5.551283	-2.516882	-1.553871	
C	-0.785954	-2.381247	0.686463	
C	3.046310	0.325470	1.395643	
C	0.068946	-1.930306	1.779575	
C	2.888992	4.537123	-2.124365	
C	3.084927	-2.777885	-2.643087	
C	-1.826029	-0.581869	1.732995	
C	2.931811	-0.720076	-1.334231	
C	1.548528	-3.814516	1.375536	
C	-4.422614	-2.009709	0.543986	
C	4.337610	-2.381226	-3.140228	
C	4.241245	-0.419213	1.499553	
C	-5.588420	-2.359257	-0.156874	
C	0.686448	-4.279563	0.329346	
C	4.192968	-0.325023	-1.840791	
C	2.402910	2.035148	-0.888834	
C	3.067877	3.063865	-0.187913	
C	3.307906	4.306911	-0.803674	
C	4.499452	0.257545	3.829866	
C	4.890460	-1.151781	-2.736873	
C	-0.452932	-3.573822	-0.030869	
C	-4.341849	-2.316655	-2.243490	
C	-3.175882	-1.964063	-1.544977	
C	4.958359	-0.455651	2.710254	
H	-0.203659	-0.262313	3.291534	
H	1.396427	-2.254750	-1.367377	
H	2.936915	1.561094	4.611137	
H	1.923392	-2.314103	2.899203	
H	1.631522	1.579288	2.481371	
H	1.901897	3.683716	-3.870772	
H	1.483019	1.477190	-2.790081	
H	-6.465235	-2.789588	-2.105506	
H	3.077988	5.510582	-2.604137	
H	2.641504	-3.735545	-2.959168	
H	-2.587122	0.160107	2.010396	
H	2.450877	-4.396392	1.621990	
H	-4.450899	-1.903567	1.640235	
H	4.882164	-3.025811	-3.848771	
H	4.614819	-0.986701	0.634376	
H	-6.530643	-2.514064	0.393128	
H	0.938408	-5.214711	-0.195495	
H	4.628645	0.641956	-1.543118	
H	3.413491	2.895215	0.843513	
H	3.831999	5.097935	-0.243529	
H	5.064015	0.229825	4.775478	
H	5.868322	-0.829177	-3.129084	
H	-1.123526	-3.936747	-0.825179	
H	-4.308558	-2.416155	-3.340010	
H	-2.242269	-1.758351	-2.089847	
H	5.883981	-1.050040	2.774834	
C	-0.498967	1.970599	0.629383	
C	-1.044140	1.665903	-0.672950	
H	0.393872	2.619449	0.676952	
H	-1.171909	2.100308	1.492481	
H	-0.439880	1.946162	-1.551645	
C	-2.482408	1.542211	-1.070971	
H	-0.125669	-0.415287	-1.325718	
O	-2.782009	1.081297	-2.178302	
C	-3.598773	2.035180	-0.170165	
C	-4.864793	1.414614	-0.286570	
C	-3.469684	3.162946	0.673814	
C	-5.958631	1.876241	0.459483	
H	-4.967811	0.566677	-0.980162	
C	-4.573204	3.640198	1.403191	
H	-2.509210	3.696325	0.730926	
C	-5.815829	2.989742	1.309403	
H	-6.933872	1.371018	0.371337	
H	-4.462621	4.530615	2.043009	
H	-6.677743	3.358691	1.888624	

GH (R = Ph)				E _g (BP86/SVP) = -2131.8550402 G _g (BP86/SVP) = -2131.8550402 E _s (M06//TZVP//BP86/SVP) = -2132.2092931
Ru	0.481551	-0.580410	-0.452391	
P	-1.781430	0.018778	-0.144255	
C	2.230265	-2.051880	-0.421366	
C	0.072697	-2.815564	-1.004066	
C	3.680244	-1.802582	-0.565667	
C	-1.383406	0.045726	2.673292	
C	-3.659736	-2.615378	-2.751326	
C	-0.754104	-3.194775	1.467204	
C	-2.826968	-1.638340	-2.181631	
C	-2.937460	3.984090	-0.557544	
C	-2.388969	2.779255	-0.091879	
C	6.485196	-1.393308	-0.869991	
C	1.492798	-2.301334	0.813258	
C	-2.944769	-1.287665	-0.814235	
C	0.153441	-2.756973	0.452237	
C	-3.625186	4.022770	-1.781350	
C	-1.764647	0.234627	4.015125	
C	1.328951	-2.435992	-1.519102	
C	-2.319987	0.214792	1.634308	
C	-0.335445	-3.200544	2.789864	
C	4.386865	-2.339555	-1.672380	
C	-3.085634	0.590306	4.331457	
C	-3.894140	-1.974233	-0.026652	
C	5.767501	-2.135621	-1.823740	
C	0.978326	-2.763590	3.148311	
C	-3.647261	0.586268	1.960484	
C	-2.530829	1.585972	-0.836126	
C	-3.221122	1.634873	-2.066696	
C	-3.760387	2.845772	-2.535427	
C	-4.608106	-3.286720	-1.957374	
C	-4.027690	0.765758	3.299972	
C	1.879753	-2.313671	2.192828	
C	5.801578	-0.851106	0.233015	
C	4.419865	-1.046954	0.380175	
C	-4.713716	-2.969438	-0.593879	
H	-0.789610	-3.167019	-1.581287	
H	-0.345274	-0.219059	2.417169	
H	-3.558226	-2.862372	-3.820388	
H	-1.753225	-3.560342	1.185180	
H	-2.051918	-1.158133	-2.800993	
H	-2.811806	4.901902	0.037890	
H	-1.845296	2.770836	0.865420	
H	7.568790	-1.234593	-0.986806	
H	-4.052002	4.969446	-2.148909	
H	-1.018558	0.106039	4.815324	
H	1.598120	-2.430278	-2.582625	
H	-1.017070	-3.557525	3.577735	
H	3.847755	-2.946682	-2.415933	
H	-3.382930	0.741068	5.381740	
H	-3.995862	-1.740764	1.043451	
H	6.288694	-2.569158	-2.692417	
H	1.286360	-2.803525	4.205342	
H	-4.384194	0.755825	1.159444	
H	-3.367478	0.722823	-2.663253	
H	-4.300300	2.861602	-3.495815	
H	-5.254477	-4.060932	-2.400278	
H	-5.062878	1.057688	3.539433	
H	2.900151	-2.026863	2.484217	
H	6.348936	-0.257818	0.982932	
H	3.897325	-0.586273	1.231305	
H	-5.442031	-3.498154	0.041927	
C	1.754173	0.448430	-1.878102	
C	0.659811	1.325690	-1.643750	
H	1.777298	-0.112801	-2.826541	
H	2.752917	0.687105	-1.476818	
H	-0.153507	1.337594	-2.388088	
C	0.807798	2.724873	-1.100777	
H	0.794775	0.499062	0.670630	
O	0.046246	3.578863	-1.567799	
C	1.891134	3.185983	-0.141053	
C	2.033516	4.588304	0.000539	
C	2.756415	2.347307	0.598618	
C	3.008578	5.136319	0.844382	
H	1.350400	5.227693	-0.578887	
C	3.734493	2.896489	1.445355	
H	2.641203	1.256776	0.535849	
C	3.866382	4.289829	1.571414	
H	3.103363	6.230370	0.936658	
H	4.397657	2.226563	2.015919	
H	4.634819	4.716118	2.236528	

H (R = Ph)			E _g (BP86/SVP) = -2131.8839856 G _g (BP86/SVP) = -2131.337281 E _s (M06//TZVP//BP86/SVP) = -2132.2350278
Ru	-0.986668	-0.164421	0.095515
P	1.138282	-1.007608	-0.081307
C	-3.226725	-0.001565	0.656372
C	-1.676988	-1.140332	2.035272
C	-4.170259	1.038437	0.194677
C	0.317354	-2.859114	-2.109509
C	2.144327	-1.682475	3.882008
C	-1.786625	-3.429652	0.737505
C	1.765321	-1.084173	2.668172
C	3.606586	1.476214	-2.290179
C	2.559322	0.650510	-1.851442
C	-6.005024	3.041907	-0.657135
C	-3.037677	-1.344243	0.117176
C	1.717831	-1.851890	1.478559
C	-2.078672	-2.047813	0.970474
C	4.685725	1.761002	-1.434523
C	0.525827	-3.842726	-3.094835
C	-2.418663	0.064978	1.860897
C	1.404115	-2.329068	-1.385094
C	-2.447493	-4.093882	-0.285098
C	-4.824130	1.879329	1.130920
C	1.822540	-4.308172	-3.367071
C	2.023493	-3.229246	1.540201
C	-5.726343	2.869351	0.710110
C	-3.393265	-3.412115	-1.116889
C	2.708109	-2.800811	-1.669816
C	2.570751	0.098035	-0.548708
C	3.657113	0.389254	0.303022
C	4.707082	1.214305	-0.140684
C	2.452858	-3.054862	3.935539
C	2.914868	-3.784226	-2.650601
C	-3.682945	-2.065867	-0.941273
C	-5.363588	2.218182	-1.599804
C	-4.453357	1.234831	-1.181865
C	2.383494	-3.826029	2.763771
H	-1.014000	-1.382680	2.873504
H	-0.699292	-2.488857	-1.905800
H	2.189784	-1.069397	4.796708
H	-1.070098	-3.952624	1.389468
H	1.492230	-0.014760	2.635492
H	3.581679	1.894924	-3.308876
H	1.733706	0.406390	-2.539550
H	-6.715865	3.816014	-0.986822
H	5.509043	2.407239	-1.777710
H	-0.335083	-4.242087	-3.654421
H	-2.363498	0.932059	2.531844
H	-2.248180	-5.162300	-0.462677
H	-4.638652	1.736690	2.207170
H	1.985831	-5.074964	-4.141428
H	1.976896	-3.847429	0.631343
H	-6.223883	3.505634	1.459626
H	-3.912054	-3.976372	-1.908531
H	3.572175	-2.387015	-1.125830
H	3.694440	-0.033499	1.317984
H	5.551661	1.426044	0.534650
H	2.740612	-3.522474	4.890852
H	3.936796	-4.137786	-2.862640
H	-4.438261	-1.569473	-1.568276
H	-5.564598	2.350468	-2.675178
H	-3.928648	0.623119	-1.931575
H	2.613327	-4.903402	2.795474
C	-0.793471	1.681286	-0.998909
C	-0.495102	1.917831	0.388136
H	-1.770983	2.000605	-1.404745
H	0.025087	1.725936	-1.734665
H	-1.331076	2.314922	0.999963
C	0.784091	2.448446	0.986816
H	-0.944656	-0.406060	-1.477592
O	1.217390	2.017385	2.061511
C	1.464868	3.638900	0.348363
C	2.698739	4.063951	0.896282
C	0.894086	4.388153	-0.706882
C	3.354338	5.194497	0.391865
H	3.114501	3.482842	1.732960
C	1.547374	5.527186	-1.206266
H	-0.076716	4.088986	-1.127671
C	2.780160	5.929684	-0.663172
H	4.316985	5.511565	0.824366
H	1.088365	6.107093	-2.022948
H	3.292216	6.822161	-1.057898

HI (R = Ph)				E _g (BP86/SVP) = -2131.8768895 G _g (BP86/SVP) = -2131.331276 E _s (M06//TZVP//BP86/SVP) = -2132.2290307
Ru	-0.941881	-0.334474	0.138664	
P	1.293322	-0.859711	-0.037515	
C	-3.147000	-0.482404	0.667539	
C	-1.463439	-1.525228	1.954891	
C	-4.185915	0.488292	0.259716	
C	0.710342	-2.711576	-2.121373	
C	2.332627	-1.390142	3.936198	
C	-1.370314	-3.745048	0.544167	
C	1.889856	-0.850418	2.716702	
C	3.470996	1.903737	-2.237284	
C	2.547342	0.932415	-1.818378	
C	-6.183835	2.377311	-0.489615	
C	-2.840205	-1.781352	0.055524	
C	1.976590	-1.613223	1.524930	
C	-1.812856	-2.429190	0.864036	
C	4.438482	2.389666	-1.339959	
C	1.023271	-3.632403	-3.139386	
C	-2.332382	-0.391507	1.865625	
C	1.733457	-2.115470	-1.356271	
C	-1.953335	-4.413501	-0.528293	
C	-4.880705	1.248902	1.235023	
C	2.361779	-3.967613	-3.401410	
C	2.483634	-2.929182	1.590922	
C	-5.862271	2.182080	0.865147	
C	-2.967810	-3.790177	-1.314861	
C	3.080190	-2.452142	-1.633176	
C	2.569884	0.432128	-0.494161	
C	3.545973	0.925196	0.397402	
C	4.473251	1.895104	-0.025535	
C	2.842100	-2.701088	3.993499	
C	3.390836	-3.375126	-2.644863	
C	-3.405541	-2.494688	-1.045944	
C	-5.06335	1.631550	-1.470931	
C	-4.518251	0.704445	-1.103473	
C	2.908957	-3.469351	2.819854	
H	-0.763201	-1.742129	2.769898	
H	-0.337836	-2.439998	-1.915777	
H	2.268462	-0.781414	4.852649	
H	-0.597288	-4.226827	1.162503	
H	1.458325	0.165391	2.684504	
H	3.439228	2.276784	-3.273479	
H	1.819935	0.530441	-2.542862	
H	-6.957269	3.106092	-0.779195	
H	5.166189	3.149117	-1.666950	
H	0.212046	-4.086301	-3.730644	
H	-2.352807	0.438223	2.583997	
H	-1.637279	-5.439305	-0.772245	
H	-4.660573	1.087942	2.301958	
H	2.607380	-4.686302	-4.199840	
H	2.543573	-3.545045	0.680977	
H	-6.388375	2.755427	1.645361	
H	-3.422346	-4.350869	-2.147464	
H	3.894255	-1.979083	-1.060635	
H	3.594089	0.545234	1.428385	
H	5.233934	2.261469	0.682621	
H	3.178791	-3.124611	4.953349	
H	4.443747	-3.627104	-2.850632	
H	-4.214170	-2.046494	-1.641928	
H	-5.743154	1.779093	-2.537080	
H	-3.975751	0.152155	-1.885939	
H	3.295169	-4.500944	2.854647	
C	-0.932550	1.453331	-1.148640	
C	-0.794023	1.768617	0.276809	
H	-1.901054	1.695670	-1.628388	
H	-0.073417	1.693604	-1.801004	
H	-1.732047	2.104563	0.770929	
C	0.345905	2.528715	0.915035	
H	-0.922000	0.012485	-1.482111	
O	0.815813	2.183908	2.003731	
C	0.832598	3.813429	0.282308	
C	0.147187	4.468151	-0.767000	
C	1.990528	4.420231	0.823682	
C	0.614348	5.695075	-1.267486	
H	-0.773087	4.029027	-1.179839	
C	2.462541	5.638362	0.317665	
H	2.498264	3.906844	1.654110	
C	1.775580	6.279098	-0.731411	
H	0.065641	6.200797	-2.078059	
H	3.369138	6.097542	0.743676	
H	2.142971	7.239745	-1.127189	

I (R = Ph)			E _g (BP86/SVP) = -2131.8789452 G _g (BP86/SVP) = -2131.330587 E _s (M06//TZVP//BP86/SVP) = -2132.234431
Ru	-0.783015	-0.627383	
P	1.521263	-0.466064	
C	-2.843728	-1.365624	
C	-0.900294	-1.973907	1.839502
C	-4.112769	-0.688611	0.306943
C	1.548252	-2.390569	-2.098861
C	2.562779	-0.623956	3.996599
C	-0.312367	-4.073784	0.370502
C	2.009809	-0.256856	2.758175
C	2.861924	2.800088	-2.191083
C	2.252846	1.602717	-1.781903
C	-6.562627	0.628469	-0.317819
C	-2.237742	-2.531023	-0.016438
C	2.356332	-0.969605	1.583059
C	-1.063600	-2.928989	0.746467
C	3.614328	3.557199	-1.275550
C	2.134385	-3.172903	-3.112158
C	-2.040714	-1.097890	1.830945
C	2.341622	-1.540365	-1.301120
C	-0.731216	-4.830126	-0.725558
C	-4.949142	-0.168202	1.327945
C	3.519841	-3.115475	-3.335414
C	3.232138	-2.071886	1.683417
C	-6.153962	0.483335	1.019676
C	-1.880394	-4.450766	-1.472670
C	3.735741	-1.482185	-1.539347
C	2.378362	1.141414	-0.449210
C	3.135993	1.908645	0.460871
C	3.750484	3.105109	0.047627
C	3.443186	-1.718612	4.088225
C	4.320313	-2.268332	-2.545316
C	-2.626535	-3.317377	-1.141260
C	-5.746214	0.120191	-1.344154
C	-4.537338	-0.524649	-1.037892
C	3.767866	-2.445260	2.931073
H	-0.145692	-2.036299	2.633061
H	0.460609	-2.429319	-1.920924
H	2.293512	-0.054087	4.900567
H	0.570414	-4.367428	0.959697
H	1.289492	0.577520	2.694301
H	2.754973	3.138516	-3.234171
H	1.700155	0.999141	-2.520633
H	-7.510677	1.134597	-0.559085
H	4.096219	4.494677	-1.595191
H	1.499833	-3.828867	-3.729213
H	-2.254290	-0.336205	2.591802
H	-0.170681	-5.733065	-1.014306
H	-4.657186	-0.297693	2.381767
H	3.979138	-3.726212	-4.129370
H	3.494789	-2.652747	0.786405
H	-6.784731	0.872927	1.834927
H	-2.196816	-5.072269	-2.325896
H	4.367945	-0.806771	-0.940617
H	3.261050	1.569015	1.499605
H	4.346877	3.684702	0.770685
H	3.867527	-2.009443	5.062589
H	5.406904	-2.213043	-2.720595
H	-3.532549	-3.065146	-1.711698
H	-6.050366	0.232585	-2.397465
H	-3.897417	-0.890577	-1.855321
H	4.444861	-3.312595	2.993713
C	-1.239558	1.125522	-1.291334
C	-1.250303	1.404460	0.178448
H	-2.225771	1.174144	-1.796795
H	-0.470340	1.674302	-1.868544
H	-2.276900	1.479745	0.604619
C	-0.440568	2.498439	0.838997
H	-0.914268	-0.040445	-1.558559
O	0.094596	2.325639	1.937958
C	-0.390630	3.875466	0.212344
C	0.541878	4.806333	0.727302
C	-1.278783	4.293164	-0.805617
C	0.601845	6.112140	0.222677
H	1.209755	4.470732	1.534851
C	-1.228536	5.606550	-1.301917
H	-2.035694	3.597024	-1.196318
C	-0.283838	6.516086	-0.794860
H	1.338858	6.825091	0.626103
H	-1.934812	5.923394	-2.085930
H	-0.241978	7.544563	-1.188350

IJ (R = Ph)				E _g (BP86/SVP) = -2131.8536803 G _g (BP86/SVP) = -2131.308544 E _s (M06//TZVP//BP86/SVP) = -2132.209951
Ru	0.056169	0.770701	-0.667294	
P	0.692636	-1.343757	0.373225	
C	0.726907	2.819966	-0.877033	
C	0.408566	1.342241	-2.676717	
C	0.508843	3.920553	0.087264	
C	2.669416	-0.120422	1.981056	
C	1.004163	-3.244125	-3.295043	
C	2.861823	0.381709	-2.709510	
C	0.541998	-2.517613	-2.185181	
C	-1.688782	-3.134079	3.279613	
C	-0.758489	-2.323743	2.607635	
C	0.064834	6.053989	1.919444	
C	1.990650	2.085181	-1.113041	
C	1.351272	-2.382650	-1.029865	
C	1.799832	1.202299	-2.250886	
C	-2.371468	-4.150116	2.587702	
C	3.697167	-0.078135	2.940944	
C	-0.179697	2.454485	-1.953685	
C	2.071389	-1.344084	1.622152	
C	4.112361	0.485905	-2.097026	
C	-0.252930	5.057303	-0.283017	
C	4.138385	-1.263816	3.551362	
C	2.637915	-2.962364	-1.025459	
C	-0.473369	6.108726	0.622187	
C	4.319885	1.395526	-1.022383	
C	2.516528	-2.533783	2.247281	
C	-0.490710	-2.515298	1.230945	
C	-1.178873	-3.540481	0.547108	
C	-2.110450	-4.349740	1.221647	
C	2.286693	-3.824487	-3.281377	
C	3.545693	-2.491989	3.202035	
C	3.282926	2.184345	-0.522134	
C	0.823407	4.932272	2.303642	
C	1.039104	3.879661	1.402236	
C	3.101576	-3.675179	-2.147112	
H	-0.042105	0.829340	-3.538607	
H	2.312496	0.796770	1.486639	
H	0.358963	-3.348457	-4.182438	
H	2.702550	-0.305292	-3.554978	
H	-0.446210	-2.032370	-2.209893	
H	-1.877383	-2.970574	4.352875	
H	-0.221229	-1.542836	3.169339	
H	-0.107199	6.878685	2.629135	
H	-3.100928	-4.786727	3.113209	
H	4.153605	0.887249	3.212298	
H	-1.161694	2.902486	-2.155621	
H	4.952063	-0.126886	-2.459547	
H	-0.659925	5.123658	-1.304153	
H	4.942325	-1.233738	4.304286	
H	3.294779	-2.846849	-0.150598	
H	-1.066826	6.982236	0.307237	
H	5.325511	1.484468	-0.580719	
H	2.045874	-3.497725	1.996415	
H	-0.986898	-3.716986	-0.521281	
H	-2.633444	-5.147523	0.669932	
H	2.651246	-4.385998	-4.156506	
H	3.883919	-3.424788	3.681293	
H	3.471426	2.904317	0.288471	
H	1.242337	4.872372	3.321125	
H	1.597297	2.989371	1.727565	
H	4.111777	-4.115263	-2.129868	
C	-1.954728	1.029885	1.653964	
C	-1.891405	1.018669	0.112426	
H	-2.972248	1.274307	2.039781	
H	-1.673841	0.049047	2.083761	
H	-2.278570	2.001443	-0.248090	
C	-2.735019	-0.052993	-0.534134	
H	-1.260248	1.794982	2.057567	
O	-2.178639	-0.966440	-1.172521	
C	-4.240883	-0.046123	-0.457911	
C	-4.973506	1.077605	-0.008591	
C	-4.946334	-1.203643	-0.865158	
C	-6.376901	1.042219	0.033942	
H	-4.441609	1.991347	0.296178	
C	-6.345859	-1.243077	-0.810585	
H	-4.360391	-2.065941	-1.218240	
C	-7.065178	-0.118496	-0.361718	
H	-6.937587	1.925718	0.378548	
H	-6.884135	-2.152927	-1.121473	
H	-8.166089	-0.146480	-0.323047	

J (R = Ph)			E _g (BP86/SVP) = -2131.8795348 G _g (BP86/SVP) = -2131.329122 E _s (M06//TZVP//BP86/SVP) = -2132.235098
Ru	0.904153	-0.267459	
P	-1.389890	-0.461138	
C	3.130997	-0.778102	
C	1.294199	-2.129138	-1.144544
C	4.249339	0.173888	-0.677374
C	-1.896979	-0.979554	2.369076
C	-2.387938	-2.951201	-3.598039
C	1.130166	-3.431789	1.136822
C	-2.069751	-1.818394	-2.826661
C	-3.948620	2.618535	-1.651175
C	-3.401538	1.580027	-0.877406
C	6.407173	2.014704	-1.023524
C	2.793704	-1.635431	0.601529
C	-1.917194	-1.918539	-1.426338
C	1.656642	-2.469380	0.227997
C	-3.298608	3.054635	-2.818196
C	-2.667705	-1.311855	3.498685
C	2.215466	-1.134661	-1.611309
C	-2.498885	-0.814307	1.105947
C	1.736877	-3.596452	2.379615
C	4.725273	0.524974	-1.969221
C	-4.055332	-1.490200	3.373202
C	-2.101656	-3.183709	-0.819788
C	5.783555	1.427677	-2.139712
C	2.866591	-2.806498	2.739576
C	-3.891541	-1.035802	0.982142
C	-2.194597	0.957772	-1.264030
C	-1.522207	1.436812	-2.414106
C	-2.078187	2.466264	-3.192205
C	-2.559230	-4.204517	-2.985952
C	-4.663597	-1.359385	2.110444
C	3.390681	-1.838122	1.885195
C	5.952934	1.683605	0.263618
C	4.892356	0.779092	0.435176
C	-2.416666	-4.315327	-1.591600
H	0.539696	-2.644852	-1.749405
H	-0.802925	-0.873671	2.442154
H	-2.508481	-2.847147	-4.688414
H	0.279698	-4.060112	0.831671
H	-1.952291	-0.845174	-3.325914
H	-4.889821	3.093701	-1.331581
H	-3.915433	1.272274	0.044329
H	7.239732	2.723258	-1.157259
H	-3.733193	3.865159	-3.425026
H	-2.178275	-1.439641	4.477611
H	2.242721	-0.731832	-2.631064
H	1.353282	-4.349911	3.085074
H	4.267039	0.066909	-2.858512
H	-4.663503	-1.748635	4.254892
H	-2.009379	-3.283950	0.272870
H	6.128926	1.672247	-3.157133
H	3.348081	-2.975279	3.716531
H	-4.375839	-0.977925	-0.005252
H	-0.541380	1.014640	-2.681702
H	-1.543276	2.820406	-4.088088
H	-2.809661	-5.089967	-3.591525
H	-5.747906	-1.522614	2.000898
H	4.287403	-1.277295	2.182333
H	6.425286	2.137135	1.149857
H	4.552149	0.555626	1.455702
H	-2.558569	-5.289501	-1.096370
C	1.219524	0.988986	3.047445
C	1.429120	1.149904	1.561586
H	1.379412	1.955401	3.579976
H	0.212101	0.626729	3.324243
H	2.493634	1.229107	1.277450
C	0.590172	1.851733	0.624026
H	1.949544	0.259506	3.453606
O	1.007997	1.781708	-0.631938
C	-0.552399	2.768086	0.938014
C	-0.754681	3.844091	0.038696
C	-1.357297	2.704633	2.100102
C	-1.716906	4.829759	0.299380
H	-0.133188	3.888156	-0.867600
C	-2.333956	3.683195	2.348895
H	-1.246478	1.873600	2.807673
C	-2.513624	4.754037	1.455955
H	-1.848823	5.663289	-0.408918
H	-2.959578	3.605971	3.252706
H	-3.273113	5.525714	1.660517

JK (R = Ph)				E _g (BP86/SVP) = -2555.7209778 G _g (BP86/SVP) = -2555.022777 E _s (M06//TZVP//BP86/SVP) = -2556.2315258
Ru	0.642953	-0.721028	-0.908755	
P	1.996445	0.011785	0.814180	
C	-0.518276	-2.629000	-1.340185	
C	1.801131	-2.510187	-1.102000	
C	-1.943306	-2.914049	-1.064352	
C	4.368335	0.162813	-0.732833	
C	1.798190	-3.161213	3.485639	
C	2.298846	-1.738768	-3.589488	
C	1.486439	-2.079804	2.645626	
C	0.333308	3.412871	2.509365	
C	0.746667	2.413147	1.613773	
C	-4.666580	-3.542602	-0.583004	
C	0.028768	-2.168504	-2.615891	
C	2.504922	-1.402524	1.933659	
C	1.482556	-2.083430	-2.461558	
C	0.575536	3.271357	3.887278	
C	5.650443	0.619660	-1.081283	
C	0.581730	-2.938046	-0.460091	
C	3.674908	0.715466	0.367574	
C	1.680589	-1.459232	-4.797473	
C	-2.300755	-0.049995	-0.296007	
C	6.253102	1.655901	-0.345843	
C	3.839103	-1.837677	2.081919	
C	-3.649534	-4.361469	-0.060369	
C	0.251777	-1.520048	-4.943614	
C	4.289918	1.754198	1.100299	
C	1.420169	1.262483	2.075458	
C	1.665402	1.130424	3.461361	
C	1.241725	2.126927	4.359346	
C	3.130414	-3.597828	3.616390	
C	5.566602	2.223677	0.741099	
C	-0.568199	-1.874933	-3.881469	
C	-4.323988	-2.407081	-1.339442	
C	-2.977195	-2.092950	-1.580213	
C	4.147019	-2.934029	2.911457	
H	2.809574	-2.658753	-0.693414	
H	3.883471	-0.625095	-1.328795	
H	0.992881	-3.667854	4.041875	
H	3.395875	-1.718016	-3.496982	
H	0.440008	-1.746433	2.548947	
H	-0.189493	4.301535	2.121926	
H	0.537965	2.528337	0.540919	
H	-5.724668	-3.785000	-0.396080	
H	0.245355	4.051143	4.592231	
H	6.176175	0.172828	-1.940499	
H	0.501952	-3.391379	0.534098	
H	2.293976	-1.198911	-5.675058	
H	-1.510485	-4.708654	0.096981	
H	7.253800	2.023791	-0.623386	
H	4.651414	-1.317320	1.552265	
H	-3.908077	-5.254431	0.531145	
H	-0.193891	-1.301598	-5.926680	
H	3.769794	2.202452	1.960245	
H	2.195185	0.247171	3.848039	
H	1.439764	2.006664	5.436816	
H	3.373370	-4.451606	4.269001	
H	6.027672	3.039768	1.320511	
H	-1.657299	-1.948755	-4.013191	
H	-5.113609	-1.748041	-1.732715	
H	-2.708962	-1.176715	-2.128734	
H	5.194067	-3.263392	3.009188	
C	1.896683	1.974925	-2.351129	
C	0.657065	1.096465	-2.246043	
H	1.921030	2.582630	-3.283807	
H	2.000092	2.676145	-1.497151	
H	0.546479	0.440180	-3.132709	
C	-0.654314	1.686758	-1.946215	
H	2.808599	1.348932	-2.364016	
O	-1.697424	0.969667	-1.894914	
C	-2.073505	-1.458672	3.678471	
C	-2.135059	-0.374754	2.883591	
H	-1.707009	-1.392182	4.715609	
H	-2.392733	-2.452595	3.319015	
H	-1.806917	0.613769	3.252936	
C	-2.659458	-0.381870	1.465885	
H	-2.771905	-1.444572	1.136348	
O	-1.683954	0.278352	0.657146	
H	-1.988773	0.375154	-0.283561	
C	-0.857411	3.167150	-1.677814	
C	-1.683600	3.574169	-0.603001	
C	-0.358310	4.154227	-2.558223	
C	-1.978509	4.930972	-0.399732	
H	-2.077147	2.810149	0.083891	
C	-0.677025	5.510279	-2.369981	
H	0.259765	3.859533	-3.418542	
C	-1.478920	5.904243	-1.285424	
H	-2.614036	5.229721	0.449558	
H	-0.295392	6.263807	-3.077539	
H	-1.720093	6.968554	-1.132971	
C	-4.058664	0.263070	1.372116	
C	-5.029046	0.002137	2.365140	
C	-4.427995	1.064251	0.270024	
C	-6.326444	0.531379	2.266051	
H	-4.759945	-0.621658	3.231930	
C	-5.727470	1.595514	0.171467	
H	-3.705043	1.283469	-0.531947	
C	-6.682171	1.334160	1.167860	
H	-7.064040	0.316830	3.056423	
H	-5.989959	2.221341	-0.696820	
H	-7.698075	1.753617	1.090348	

K (R = Ph)				E _g (BP86/SVP) = -2555.7425925 G _g (BP86/SVP) = -2555.044856 E _s (M06//TZVP//BP86/SVP) = -2556.2437245
Ru	-0.157001	-1.033683	-0.247878	
P	1.751662	-0.280671	0.801897	
C	-1.978075	-2.465973	-0.580268	
C	0.028600	-3.055115	0.514052	
C	-3.402989	-2.140706	-0.792047	
C	3.644045	-0.981287	-1.183426	
C	1.859112	-2.691227	4.191146	
C	1.291738	-3.851641	-1.654118	
C	1.467423	-1.809217	3.171344	
C	1.195336	3.723630	1.824021	
C	1.217981	2.494256	1.143232	
C	-6.171806	-1.581786	-1.176176	
C	-1.034313	-2.929624	-1.582040	
C	2.366262	-1.449968	2.137064	
C	0.214925	-3.277408	-0.915257	
C	1.637938	3.806996	3.156169	
C	4.836388	-0.880185	-1.921152	
C	-1.322494	-2.608984	0.717186	
C	3.335343	-0.039707	-0.175110	
C	1.121683	-4.104430	-3.011836	
C	-4.377473	-2.565056	0.150210	
C	5.732373	0.175590	-1.673760	
C	3.663036	-2.005154	2.151026	
C	-5.741024	-2.289125	-0.038990	
C	-0.110145	-3.783126	-3.662292	
C	4.244483	1.013794	0.069723	
C	1.697246	1.324050	1.774635	
C	2.148467	1.421989	3.111523	
C	2.113198	2.650550	3.796662	
C	3.152739	-3.247204	4.189612	
C	5.431167	1.121787	-0.678447	
C	-1.170371	-3.193213	-2.980344	
C	-5.220422	-1.150677	-2.118699	
C	-3.857101	-1.423927	-1.929994	
C	4.049513	-2.902904	3.165929	
H	0.732680	-3.357484	1.297951	
H	2.937181	-1.800360	-1.390369	
H	1.145561	-2.952058	4.989381	
H	2.220022	-4.138325	-1.134628	
H	0.444951	-1.396109	3.172298	
H	0.825640	4.620854	1.302717	
H	0.857380	2.457537	0.108113	
H	-7.241538	-1.366904	-1.326770	
H	1.614825	4.769704	3.691511	
H	5.061131	-1.626292	-2.700233	
H	-1.798708	-2.465522	1.695427	
H	1.932971	-4.570609	-3.592381	
H	-4.057528	-3.144756	1.030449	
H	6.663382	0.260788	-2.256798	
H	4.385536	-1.738026	1.365642	
H	-6.475408	-2.639709	0.704138	
H	-0.223812	-4.017950	-4.733010	
H	4.028339	1.756128	0.852654	
H	2.539624	0.534234	3.629303	
H	2.469275	2.700358	4.838401	
H	3.457497	-3.947066	4.983977	
H	6.126869	1.952201	-0.476517	
H	-2.117336	-2.980769	-3.498028	
H	-5.541733	-0.583920	-3.007190	
H	-3.126120	-1.046418	-2.661263	
H	5.065170	-3.330361	3.153668	
C	0.857757	-0.289205	-3.237082	
C	-0.133694	0.220592	-2.197516	
H	0.819363	0.306879	-4.177829	
H	1.907869	-0.279626	-2.889920	
H	-1.158704	-0.157398	-2.390071	
C	-0.289766	1.649316	-1.967373	
H	0.624394	-1.336286	-3.502886	
O	-1.325222	2.089264	-1.354803	
C	-2.419570	-0.601290	3.753370	
C	-1.895015	0.275283	2.876154	
H	-2.049528	-0.672133	4.788808	
H	-3.258278	-1.263979	3.476574	
H	-1.067950	0.942618	3.179635	
C	-2.407021	0.493885	1.468581	
H	-3.056488	-0.358939	1.172916	
O	-1.289696	0.600943	0.561692	
H	-1.499305	1.250533	-0.272366	
C	-3.257132	1.763366	1.407605	
C	-4.638654	1.669677	1.140935	
C	-2.689760	3.034067	1.647871	
C	-5.442883	2.822291	1.123992	
H	-5.085051	0.682569	0.936921	
C	-3.492954	4.185206	1.625479	
H	-1.609628	3.121677	1.842842	
C	-4.872221	4.083316	1.367417	
H	-6.520437	2.734125	0.911547	
H	-3.038517	5.171650	1.811532	
H	-5.500787	4.988193	1.351739	
C	0.658702	2.714499	-2.460133	
C	2.044671	2.531675	-2.679766	
C	0.105346	4.000231	-2.691653	
C	2.845475	3.598026	-3.122891	
H	2.517207	1.563751	-2.471606	
C	0.901127	5.055306	-3.158058	
H	-0.967259	4.143584	-2.493642	
C	2.277774	4.858276	-3.375810	
H	3.925361	3.437759	-3.269529	
H	0.447122	6.041264	-3.348470	
H	2.907415	5.687952	-3.735783	

KL (R = Ph)				$E_g(\text{BP86/SVP}) = -2555.7359027$ $G_g(\text{BP86/SVP}) = -2555.040612$ $E_s(\text{M06//TZVP//BP86/SVP}) = -2556.2368135$
Ru	0.201286	-1.200341	-0.173195	
P	1.980777	0.149058	0.640625	
C	-0.926697	-2.914937	-1.078022	
C	1.131474	-3.104696	0.073428	
C	-2.366034	-3.059000	-1.388169	
C	2.638269	1.044549	-1.960788	
C	4.336344	-2.622287	2.646510	
C	2.681329	-2.664341	-2.012381	
C	3.274720	-1.801177	2.232149	
C	0.550654	3.091339	3.189719	
C	0.720451	2.196306	2.119647	
C	-5.134321	-3.412960	-1.952165	
C	0.175660	-2.601479	-2.009353	
C	3.438499	-0.894993	1.156360	
C	1.443423	-2.785580	-1.310274	
C	1.425195	3.061572	4.290320	
C	3.236807	1.888689	-2.913088	
C	-0.304494	-3.257534	0.180118	
C	2.751516	1.327148	-0.582234	
C	2.660698	-2.390104	-3.374432	
C	-3.115076	-4.093725	-0.769934	
C	3.942780	3.032333	-2.499441	
C	4.687476	-0.838225	0.503096	
C	-4.480898	-4.265924	-1.045159	
C	1.421510	-2.216519	-4.066002	
C	3.462776	2.478196	-0.173847	
C	1.778966	1.259280	2.129945	
C	2.659143	1.241094	3.236150	
C	2.479526	2.133202	4.309373	
C	5.576835	-2.562809	1.983574	
C	4.051904	3.325334	-1.128377	
C	0.198497	-2.312488	-3.410389	
C	-4.406331	-2.383484	-2.575626	
C	-3.042559	-2.205842	-2.296500	
C	5.746988	-1.671255	0.911731	
H	1.863571	-3.362195	0.847815	
H	2.074090	0.155603	-2.284295	
H	4.193027	-3.314721	3.491576	
H	3.629409	-2.825329	-1.477017	
H	2.304440	-1.858234	2.752621	
H	-0.278598	3.815789	3.156619	
H	0.012276	2.239163	1.279380	
H	-6.205124	-3.548675	-2.171641	
H	1.287146	3.761631	5.129906	
H	3.143908	1.652783	-3.985308	
H	-0.826469	-3.574241	1.091714	
H	3.606221	-2.316432	-3.934012	
H	-2.607949	-4.787067	-0.080733	
H	4.404797	3.698155	-3.245935	
H	4.839106	-0.135971	-0.330561	
H	-5.036639	-5.080771	-0.553889	
H	1.436751	-2.021049	-5.150290	
H	3.552323	2.719798	0.896605	
H	3.501627	0.534588	3.263502	
H	3.177310	2.103439	5.161799	
H	6.408264	-3.210051	2.304899	
H	4.597585	4.223088	-0.796312	
H	-0.743002	-2.225066	-3.971550	
H	-4.908503	-1.700113	-3.278870	
H	-2.504600	-1.367097	-2.761115	
H	6.715169	-1.614266	0.388682	
C	-0.805594	1.068588	-3.439288	
C	-1.108323	1.055634	-1.965956	
H	-1.310381	0.221074	-3.951956	
H	-1.156607	2.001233	-3.924697	
H	-1.207385	0.051863	-1.490295	
C	-1.459193	2.126387	-1.181220	
H	0.277912	0.962435	-3.671722	
O	-1.838010	1.999456	0.113675	
C	-1.767648	-2.907205	3.519183	
C	-1.463397	-1.679420	3.057514	
H	-1.308451	-3.312163	4.435632	
H	-2.511660	-3.545912	3.010711	
H	-0.728389	-1.048088	3.590429	
C	-2.082827	-1.015949	1.836327	
H	-2.545330	-1.802652	1.191662	
O	-1.090362	-0.287085	1.121923	
H	-1.544004	1.100312	0.510138	
C	-1.544619	3.541870	-1.645763	
C	-2.594504	4.360740	-1.161368	
C	-0.587500	4.117291	-2.514623	
C	-2.705862	5.698769	-1.567427	
H	-3.321624	3.926592	-0.458977	
C	-0.697234	5.460330	-2.913417	
H	0.273249	3.519576	-2.849333	
C	-1.760628	6.254072	-2.449826	
H	-3.536387	6.316615	-1.189052	
H	0.064228	5.893406	-3.582079	
H	-1.846131	7.306447	-2.765044	
C	-3.214452	-0.080569	2.276036	
C	-4.546682	-0.358180	1.906842	
C	-2.952164	1.052668	3.077082	
C	-5.598132	0.472559	2.331842	
H	-4.759593	-1.235399	1.273687	
C	-4.001042	1.884775	3.499521	
H	-1.914973	1.289114	3.361551	
C	-5.327975	1.596722	3.130882	
H	-6.633368	0.242678	2.031987	
H	-3.781990	2.767258	4.122252	
H	-6.150044	2.250440	3.464251	

L (R = Ph)			$E_g(\text{BP86/SVP}) = -2555.7402885$ $G_g(\text{BP86/SVP}) = -2555.047049$ $E_s(\text{M06//TZVP//BP86/SVP}) = -2556.2413122$
Ru	-0.931207	1.135825	
P	-2.070518	-0.903150	
C	-0.408096	3.165262	
C	-2.564186	2.526710	
C	0.899796	3.853150	
C	-1.504632	-1.796078	
C	-5.755547	0.490379	
C	-3.372400	1.497974	
C	-4.381017	0.236660	
C	-0.033448	-3.300908	
C	-0.390367	-2.516065	
C	3.379006	5.240094	
C	-1.089973	2.428064	
C	-3.907083	-0.629970	
C	-2.448167	2.110822	
C	-0.941800	-3.503502	
C	-1.417711	-2.739512	
C	-1.341561	3.227355	
C	-1.948440	-2.185723	
C	-2.968994	1.237972	
C	1.046010	5.143706	
C	-1.765875	-4.080553	
C	-4.842792	-1.222026	
C	2.271460	5.826749	
C	-1.640319	1.556196	
C	-2.296210	-3.537381	
C	-1.675512	-1.927407	
C	-2.585619	-2.142087	
C	-2.218335	-2.921653	
C	-6.679705	-0.103202	
C	-2.204601	-4.477721	
C	-0.709562	2.131479	
C	3.249875	3.959800	
C	2.028079	3.271692	
C	-6.218363	-0.955447	
H	-3.472448	2.460481	
H	-1.218477	-0.746538	
H	-6.106317	1.159747	
H	-4.397701	1.277514	
H	-3.663691	0.718827	
H	0.967996	-3.759016	
H	0.340275	-2.375230	
H	4.339425	5.776993	
H	-0.657036	-4.118523	
H	-1.065158	-2.422853	
H	-1.155747	3.714984	
H	-3.675622	0.788193	
H	0.176221	5.623028	
H	-1.688818	-4.821458	
H	-4.497161	-1.895672	
H	2.358288	6.830259	
H	-1.356936	1.350137	
H	-2.632945	-3.857642	
H	-3.597934	-1.714112	
H	-2.944113	-3.081156	
H	-7.756906	0.100346	
H	-2.472233	-5.529453	
H	0.291544	2.404686	
H	4.114016	3.483286	
H	1.959811	2.250801	
H	-6.933466	-1.424472	
C	2.528432	-0.310408	
C	1.993605	-0.550391	
H	2.584246	0.779382	
H	3.545815	-0.726285	
H	1.128170	0.070590	
C	2.463606	-1.416124	
H	1.877418	-0.746363	
O	1.969214	-1.459927	
C	0.542056	3.295408	
C	0.611658	2.007953	
H	0.026349	3.591263	
H	1.018003	4.099491	
H	0.141891	1.213213	
C	1.342739	1.509064	
H	1.571898	2.381900	
O	0.517565	0.560663	
H	1.446607	-0.645310	
C	3.561741	-2.405105	
C	4.465831	-2.650552	
C	3.713792	-3.144829	
C	5.508897	-3.577221	
H	4.336229	-2.097542	
C	4.757052	-4.074741	
H	2.984968	-3.015544	
C	5.663491	-4.290089	
H	6.209009	-3.746379	
H	4.853853	-4.646225	
H	6.481430	-5.019881	
C	2.671106	0.868481	
C	3.889231	1.504720	
C	2.702192	-0.341645	
C	5.115304	0.951441	
H	3.873962	2.443313	
C	3.926477	-0.896359	
H	1.758191	-0.857156	
C	5.137380	-0.250859	
H	6.058663	1.459866	
H	3.936899	-1.841459	
H	6.097156	-0.686424	

LF (R = Ph)			E _g (BP86/SVP) = -2131.8266585 G _g (BP86/SVP) = -2131.279751 E _s (M06//TZVP//BP86/SVP) = -2132.1862094
Ru	0.106336	-0.592648	
P	-2.102842	0.145461	
C	1.925888	-2.015404	
C	-0.349689	-2.729394	-0.151612
C	3.324668	-1.947094	-0.627396
C	-1.832431	1.177051	2.403909
C	-4.266652	-3.077489	-1.671491
C	-0.726708	-2.375629	2.432616
C	-3.342844	-2.030942	-1.516915
C	-2.113344	3.528147	-2.586703
C	-1.852554	2.571790	-1.593181
C	6.032959	-1.957027	-1.512942
C	1.414216	-1.887763	1.182288
C	-3.387221	-1.187875	-0.379559
C	0.007338	-2.328077	1.193708
C	-3.060287	3.265411	-3.594340
C	-2.232764	1.912224	3.534322
C	0.790905	-2.473994	-0.980685
C	-2.656692	1.128919	1.260819
C	-0.086016	-2.029027	3.604718
C	3.753724	-2.802861	-1.675732
C	-3.455716	2.603867	3.531887
C	-4.363064	-1.436352	0.609170
C	5.087126	-2.806199	-2.113682
C	1.295301	-1.614645	3.601641
C	-3.879598	1.839252	1.257545
C	-2.541929	1.334899	-1.590294
C	-3.498613	1.081446	-2.597087
C	-3.750833	2.042317	-3.594581
C	-5.238130	-3.314196	-0.680737
C	-4.278415	2.567798	2.390339
C	2.033079	-1.533542	2.436205
C	5.624137	-1.099092	-0.475333
C	4.289983	-1.088380	-0.042349
C	-5.278156	-2.495899	0.459919
H	-1.307119	-3.161515	-0.464999
H	-0.865715	0.651517	2.389263
H	-4.222522	-3.717402	-2.567395
H	-1.775377	-2.711424	2.429260
H	-2.565026	-1.868449	-2.281369
H	-1.571745	4.487604	-2.573351
H	-1.110152	2.764796	-0.801705
H	7.080502	-1.960256	-1.853792
H	-3.262152	4.015735	-4.375409
H	-1.576895	1.950730	4.418621
H	0.840121	-2.680828	-2.058605
H	-0.629213	-2.070637	4.561824
H	3.033699	-3.495864	-2.138432
H	-3.766499	3.181820	4.417124
H	-4.411360	-0.797856	1.504158
H	5.390915	-3.485693	-2.926375
H	1.775024	-1.365578	4.561834
H	-4.520893	1.830429	0.361249
H	-4.064510	0.137805	-2.604544
H	-4.501424	1.830747	-4.373218
H	-5.958060	-4.139730	-0.797451
H	-5.233242	3.117714	2.378635
H	3.093883	-1.248155	2.465322
H	6.347763	-0.413732	-0.006164
H	3.983944	-0.363257	0.724972
H	-6.030135	-2.678014	1.244421
C	2.730227	0.653105	-2.524535
C	1.623369	1.069469	-1.875128
H	2.653603	0.001039	-3.409284
H	3.743540	0.921956	-2.187730
H	0.625896	0.804506	-2.297582
C	1.489435	1.952617	-0.631554
O	0.517549	1.406584	0.219464
H	1.078789	2.931058	-1.016704
C	2.794580	2.337497	0.071872
C	3.786529	3.095795	-0.590249
C	2.991559	2.006729	1.427491
C	4.960957	3.482224	0.077419
H	3.632416	3.399121	-1.639086
C	4.164728	2.397126	2.099278
H	2.193624	1.451069	1.943313
C	5.157770	3.129610	1.425669
H	5.725206	4.070922	-0.455890
H	4.300138	2.134600	3.161586
H	6.075503	3.438658	1.951566

With [RuCl(η⁵-indenyl)(PPh₃)₂] (4):

Ru	0.108637	-1.224786	-0.055440
Cl	0.087545	-1.479273	-2.500341
P	-1.911637	-0.154830	0.084621
P	1.510069	0.675478	-0.143498
C	-0.343106	-3.379320	0.340716
C	0.624284	-1.980195	1.965775
C	-2.206808	0.278706	2.903406
C	-1.903526	2.286763	1.572499
C	-3.805574	1.769746	-0.873582
C	-2.717580	0.932817	-1.220785
C	3.304012	-0.701679	-1.877155
C	2.184091	1.474515	3.877153
C	-5.482446	-3.210252	0.057895
C	3.122900	-2.532471	1.324367
C	1.583693	1.240671	2.628747
C	-0.134961	3.749920	-2.350544
C	0.318374	2.501670	-1.895656
C	-4.417096	-1.266043	1.076128
C	1.104473	-3.447785	0.187652
C	-3.347437	-2.398059	-0.796752
C	-4.156002	2.338846	-3.217524
C	-4.510133	2.474310	-1.863339
C	2.373973	1.001614	1.480015
C	1.705992	-2.600344	1.205115
C	-2.379702	0.788070	-2.583120
C	-0.013294	4.888230	-1.532552
C	4.402978	-0.810009	-2.748534
C	-5.480239	-2.187046	1.020318
C	-2.066470	0.881819	1.629215
C	-1.902821	3.060994	2.746166
C	-0.610400	-2.567095	1.499034
C	-4.417204	-3.306433	-0.856358
C	2.947589	0.548465	-1.332579
C	3.908265	-3.295237	0.460780
C	-2.209771	1.054321	4.075200
C	5.153744	0.327054	-3.089303
C	3.779091	0.984488	1.616846
C	3.318355	-4.102126	-0.554430
C	3.703683	1.691504	-1.685146
C	-2.060778	2.451186	4.002138
C	-3.096385	1.488107	-3.571255
C	0.901102	2.373229	-0.614359
C	-3.332876	-1.373629	0.178899
C	1.030227	3.520408	0.198324
C	0.572394	4.770146	-0.260443
C	3.585361	1.453777	4.004154
C	4.800660	1.580015	-2.555441
C	1.934344	-4.172572	-0.711040
C	4.378276	1.203821	2.871913
H	0.752297	-1.375188	2.871469
H	-2.322503	-0.811437	2.991661
H	-1.771202	2.787815	0.602698
H	-4.120299	1.870808	0.176155
H	2.701363	-1.590327	-1.641712
H	1.549443	1.668939	4.756455
H	-6.317057	-3.928115	0.014629
H	3.581776	-1.911626	2.108346
H	0.486510	1.240726	2.542668
H	-0.591691	3.830737	-3.349421
H	0.232391	1.612206	-2.539240
H	-4.444775	-0.457131	1.821971
H	-2.514346	-2.469125	-1.516958
H	-4.714367	2.886790	-3.993625
H	-5.349578	3.125951	-1.571705
H	-1.560167	0.106884	-2.867809
H	-0.370476	5.867461	-1.889581
H	4.661991	-1.793136	-3.172515
H	-6.315449	-2.096206	1.733476
H	-1.775618	4.152657	2.671496
H	-1.595783	-2.461961	1.969320
H	-4.417850	-4.095545	-1.625418
H	5.005120	-3.270634	0.558063
H	-2.332300	0.560199	5.052373
H	6.009549	0.241026	-3.778236
H	4.413876	0.794570	0.738726
H	3.971124	-4.683758	-1.224746
H	3.432301	2.679663	-1.281525
H	-2.066796	3.059817	4.920291
H	-2.819670	1.358194	-4.630074
H	1.495205	3.445110	1.192814
H	0.682227	5.658481	0.382612
H	4.056684	1.629943	4.984308
H	5.378204	2.479562	-2.823096
H	1.482806	-4.798973	-1.494847
H	5.476549	1.181549	2.959844
H	-1.073793	-3.976896	-0.215893

E_g(BP86/SVP) = -2973.6068512
G_g(BP86/SVP) = -2973.021086
E_s(M06//TZVP//BP86/SVP) = -2974.0962819

B				E_g(BP86/SVP) = -1937.85509 G_g(BP86/SVP) = -1937.520943 E_s(M06//TZVP//BP86/SVP) = -1938.1057466
Ru	1.329549	-0.016775	0.031257	
Cl	1.466473	-2.352530	0.058832	
P	-0.950431	-0.020774	0.012445	
C	2.152555	1.649528	1.103477	
C	2.191804	1.486003	-1.225705	
C	-0.965712	-1.293329	-2.502149	
C	-2.265385	3.880437	0.573121	
C	4.417752	0.068287	-1.357384	
C	-1.728819	2.598422	0.775568	
C	-1.765411	-2.108370	3.509809	
C	-1.152912	-1.617103	2.344260	
C	3.366860	0.911316	0.731713	
C	-1.758809	1.632838	-0.259457	
C	3.393731	0.811915	-0.715609	
C	-3.015151	-1.611931	3.920170	
C	-1.504389	-2.055914	-3.552582	
C	1.534108	2.128857	-0.110299	
C	-1.710569	-1.073992	-1.322903	
C	5.396884	-0.543551	-0.571276	
C	-2.787247	-2.617847	-3.429579	
C	-2.329987	1.984459	-1.501160	
C	5.369675	-0.447501	0.846866	
C	-2.995749	-1.645969	-1.203128	
C	-1.790427	-0.623217	1.567589	
C	-3.051355	-0.132848	1.982246	
C	-3.656774	-0.624570	3.152520	
C	-2.831661	4.222404	-0.669326	
C	-3.529208	-2.414084	-2.252521	
C	4.363080	0.262219	1.506249	
C	-2.860226	3.272371	-1.703726	
H	1.952320	1.644148	-2.286114	
H	0.051627	-0.874604	-2.576575	
H	-2.240592	4.617972	1.391333	
H	4.438347	-0.017283	-2.454929	
H	-1.286748	2.341173	1.752041	
H	-1.256003	-2.884459	4.103171	
H	-0.175244	-2.011061	2.022549	
H	-3.489414	-1.993058	4.838787	
H	-0.911286	-2.223917	-4.465674	
H	0.685095	2.819755	-0.174863	
H	6.203398	-1.116283	-1.055532	
H	-3.206031	-3.224757	-4.248260	
H	-2.365167	1.245865	-2.316947	
H	6.155757	-0.947737	1.434173	
H	-3.581571	-1.504573	-0.281637	
H	-3.566107	0.642288	1.393611	
H	-4.637483	-0.230473	3.464431	
H	-3.250346	5.228786	-0.828611	
H	-4.530088	-2.862273	-2.145333	
H	4.342347	0.326420	2.605261	
H	-3.303568	3.529972	-2.678942	
H	1.877087	1.943812	2.125218	

Ru	-1.305648	-0.216766	0.275539
Cl	-1.569562	0.054590	-2.156292
P	0.944001	0.427341	0.018642
C	-3.034634	-1.644672	0.453960
C	-1.317012	-1.520188	2.050795
C	1.409107	-1.458861	-2.050765
C	2.396583	-0.027629	3.890344
C	0.208824	-3.365703	0.953996
C	1.640782	0.358766	2.771214
C	0.863341	4.242852	-1.542002
C	0.660905	2.873447	-1.306240
C	-1.981064	-2.576574	0.061662
C	2.006357	-0.063199	1.470087
C	-0.929248	-2.517582	1.062661
C	1.681889	4.998422	-0.682028
C	2.130004	-2.024843	-3.116776
C	-2.666672	-1.097038	1.725873
C	1.872940	-0.283974	-1.424830
C	0.272366	-4.266503	-0.107804
C	3.313361	-1.419933	-3.573001
C	3.137922	-0.895862	1.323281
C	-0.750682	-4.311067	-1.099752
C	3.060966	0.325012	-1.891434
C	1.285013	2.242169	-0.202864
C	2.109657	3.002773	0.653523
C	2.303595	4.376293	0.413485
C	3.520358	-0.859689	3.733026
C	3.776947	-0.242389	-2.959011
C	-1.858440	-3.466089	-1.041036
C	3.884603	-1.293897	2.448085
H	-0.783505	-1.318269	2.987856
H	0.468754	-1.919925	-1.717516
H	2.101218	0.319553	4.893493
H	1.002984	-3.326859	1.715220
H	0.752711	0.993093	2.911082
H	0.374745	4.723380	-2.404619
H	0.019082	2.279047	-1.979358
H	1.835883	6.073388	-0.867704
H	1.751880	-2.938194	-3.602544
H	-3.304926	-0.466676	2.357745
H	1.131395	-4.950671	-0.191501
H	3.871535	-1.860069	-4.414914
H	3.439782	-1.241193	0.322316
H	-0.660204	-5.029181	-1.930298
H	3.427624	1.251674	-1.422646
H	2.610837	2.524255	1.508972
H	2.949757	4.960243	1.088459
H	4.108361	-1.169342	4.611606
H	4.698583	0.243896	-3.316855
H	-2.641187	-3.499420	-1.813378
H	4.761095	-1.947793	2.313043
C	-1.488603	1.585323	1.463133
C	-2.286530	1.697501	0.278937
H	-0.583704	2.212130	1.541061
H	-1.975850	1.403730	2.438909
H	-1.862329	2.305802	-0.541760
C	-3.808009	1.693052	0.261444
H	-4.178280	1.139833	1.161684
C	-4.350217	3.130572	0.355984
H	-3.969983	3.745590	-0.486227
H	-5.458037	3.116365	0.296476
H	-4.053681	3.612155	1.311548
O	-4.336201	1.075340	-0.909594
H	-3.572979	0.705367	-1.418121
H	-3.987365	-1.487999	-0.066346

E_g(BP86/SVP) = -2016.9442678
G_g(BP86/SVP) = -2016.9442678
E_s(M06//TZVP//BP86/SVP) = -2170.5067898

D				E _g (BP86/SVP) = -2403.0816726 G _g (BP86/SVP) = -2402.532824 E _s (M06//TZVP//BP86/SVP) = -2403.5641756
Ru	-0.311487	-1.227141	-0.318326	
Cl	0.553973	-1.059665	1.964903	
P	-1.008070	0.979820	-0.081130	
C	-0.512170	-3.478754	-0.287360	
C	-1.782286	-2.115843	-1.707852	
C	-2.407254	0.469302	2.328185	
C	-3.147919	1.550673	-3.603961	
C	-3.880406	-1.958258	-0.124064	
C	-2.146170	1.251964	-2.666169	
C	2.520153	3.106266	0.133799	
C	1.472930	2.196714	0.355803	
C	-1.777544	-3.186307	0.382594	
C	-2.366641	1.448666	-1.281361	
C	-2.576180	-2.361621	-0.507810	
C	2.329752	4.195572	-0.734920	
C	-3.039544	0.811777	3.535433	
C	-0.590153	-2.935751	-1.613887	
C	-1.773332	1.460361	1.549695	
C	-4.382889	-2.378050	1.115012	
C	-3.031537	2.143300	3.987768	
C	-3.624503	1.935539	-0.863978	
C	-3.592175	-3.161872	1.995607	
C	-1.763584	2.794867	2.010500	
C	0.242220	2.337146	-0.327239	
C	0.058745	3.434373	-1.198654	
C	1.095703	4.366632	-1.387604	
C	-4.399402	2.033162	-3.176212	
C	-2.389275	3.133821	3.224049	
C	-2.292491	-3.555525	1.649372	
C	-4.633930	2.219363	-1.804121	
H	-2.159349	-1.632941	-2.618749	
H	-2.389840	-0.577277	1.991808	
H	-2.950901	1.398242	-4.677797	
H	-4.487876	-1.336050	-0.800023	
H	-1.179100	0.852459	-3.007933	
H	3.498134	2.902360	0.596061	
H	1.620044	1.350926	1.047413	
H	3.153499	4.904883	-0.918488	
H	-3.526350	0.024318	4.132949	
H	0.126217	-3.119938	-2.422491	
H	-5.401336	-2.085026	1.417905	
H	-3.517384	2.408124	4.941503	
H	-3.821329	2.091308	0.207409	
H	-4.009501	-3.465145	2.969882	
H	-1.255541	3.574050	1.420615	
H	-0.892345	3.559405	-1.739461	
H	0.941820	5.220569	-2.068359	
H	-5.188841	2.259117	-3.911568	
H	-2.367574	4.178358	3.576064	
H	-1.679167	-4.152271	2.341732	
H	-5.611332	2.591621	-1.455256	
C	0.951799	-0.483092	-1.910077	
C	1.818774	-0.931971	-0.860030	
H	0.879625	0.604201	-2.098029	
H	0.883681	-1.071619	-2.844974	
H	2.150704	-0.161471	-0.148592	
C	2.958976	-1.962698	-0.969479	
H	3.118178	-2.391457	0.065947	
O	3.980323	-1.149587	-1.403746	
H	4.416217	-0.030312	-0.467692	
C	5.981344	0.212362	0.745042	
C	6.563414	1.331874	1.630141	
H	7.519829	1.027940	2.109021	
H	6.748154	2.240942	1.018881	
H	5.839861	1.599573	2.429344	
C	6.975338	-0.148913	-0.388186	
H	6.494496	-0.897403	-1.052374	
H	7.197369	0.754051	-0.996400	
H	7.934497	-0.561276	-0.001699	
C	5.695938	-1.045254	1.603548	
H	4.958827	-0.801243	2.396862	
H	5.252125	-1.832256	0.960295	
H	6.614734	-1.452653	2.082565	
O	4.780964	0.707267	0.186388	
C	2.760778	-3.161328	-1.918976	
H	2.040316	-3.917770	-1.537540	
H	2.444925	-2.827422	-2.932374	
H	3.746346	-3.658490	-2.038559	
H	0.277910	-4.131621	0.103274	

DE				E _g (BP86/SVP) = -2403.0591369 G _g (BP86/SVP) = -2402.509757 E _s (M06//TZVP//BP86/SVP) = -2403.5436666
Ru	0.438504	0.172756	-0.861152	
Cl	1.511198	0.691464	1.278100	
P	-1.583183	0.295525	0.174784	
C	2.184474	-1.349893	-1.542624	
C	0.073811	-1.316050	-2.507822	
C	-0.861016	-1.472141	2.269809	
C	-4.258447	-1.050457	-2.737478	
C	-0.887675	-3.345867	-1.120323	
C	-3.226427	-0.380445	-2.058564	
C	-2.012976	4.181680	1.525240	
C	-1.560421	2.874683	1.280386	
C	1.371510	-2.358320	-0.867439	
C	-3.006698	-0.590686	-0.676057	
C	0.072349	-2.387760	-1.508994	
C	-3.212427	4.638928	0.946859	
C	-0.961346	-2.054471	3.545033	
C	1.439602	-0.835659	-2.629866	
C	-1.710023	-0.407535	1.902845	
C	-0.554637	-4.275063	-0.116392	
C	-1.899918	-1.573832	4.474828	
C	-3.841412	-1.509890	-0.001238	
C	0.707994	-4.231405	0.524669	
C	-2.653433	0.069610	2.840517	
C	-2.316911	1.992766	0.468123	
C	-3.518063	2.459606	-0.107508	
C	-3.960103	3.776675	0.127814	
C	-5.082457	-1.962921	-2.053372	
C	-2.746229	-0.508704	4.119394	
C	1.671025	-3.270359	0.174299	
C	-4.865544	-2.191592	-0.684067	
H	-0.717725	-1.178584	-3.256117	
H	-0.109433	-1.842983	1.557745	
H	-4.412267	-0.864137	-3.813146	
H	-1.874184	-3.378151	-1.609377	
H	-2.571499	0.309447	-2.611394	
H	-1.416043	4.851558	2.165337	
H	-0.611958	2.521871	1.721338	
H	-3.560772	5.668222	1.132881	
H	-0.286117	-2.882838	3.812762	
H	1.827645	-0.103413	-3.347502	
H	-1.286879	-5.045056	0.176935	
H	-1.968177	-2.024491	5.478894	
H	-3.686392	-1.703212	1.070509	
H	0.938603	-4.968037	1.312592	
H	-3.320751	0.903678	2.572834	
H	-4.124456	1.789593	-0.736757	
H	-4.900530	4.125215	-0.330541	
H	-5.884770	-2.497588	-2.587730	
H	-3.483026	-0.119963	4.841854	
H	2.652435	-3.223435	0.671463	
H	-5.497559	-2.909975	-0.136206	
C	-0.279619	1.665648	-2.219116	
C	0.609299	2.292779	-1.288885	
H	-1.356977	1.923085	-2.183929	
H	0.091503	1.481681	-3.244979	
H	0.161901	2.849823	-0.445414	
C	2.043503	2.682229	-1.700941	
H	1.904192	3.362838	-2.614398	
O	2.738986	1.542373	-1.967949	
H	3.530781	-0.317312	0.936770	
C	5.499609	-0.073530	0.795141	
C	6.687545	-0.985946	1.148953	
H	7.654689	-0.453899	1.027281	
H	6.605439	-1.341609	2.197915	
H	6.691291	-1.876318	0.485696	
C	5.434179	1.122209	1.768906	
H	4.561976	1.763518	1.526206	
H	5.319158	0.762252	2.813217	
H	6.350260	1.749085	1.709555	
C	5.606820	0.423091	-0.662384	
H	5.752259	-0.441284	-1.345925	
H	4.677784	0.953476	-0.981708	
H	6.474502	1.107115	-0.794152	
O	4.334597	-0.897410	0.961280	
C	2.709817	3.583396	-0.630061	
H	3.739249	3.843168	-0.957218	
H	2.145728	4.532968	-0.469740	
H	2.773961	3.034665	0.332845	
H	3.216180	-1.094330	-1.281938	

E				E _g (BP86/SVP) = -2403.0962973 G _g (BP86/SVP) = -2402.545931 E _s (M06//TZVP//BP86/SVP) = -2403.572583
Ru	0.521192	0.488241	-1.281844	
Cl	2.144225	1.339148	0.466643	
P	-1.114548	0.322195	0.393474	
C	1.205893	-1.932935	-0.893742	
C	0.004370	-1.188793	-2.724199	
C	0.483977	-1.013198	2.351453	
C	-4.737030	-0.851252	-1.295337	
C	-2.008776	-2.867134	-2.395053	
C	-3.448597	-0.331666	-1.086078	
C	-1.207691	4.263263	1.721137	
C	-0.813548	2.960992	1.372007	
C	-0.075340	-2.665209	-0.895185	
C	-2.764027	-0.549569	0.132903	
C	-0.805489	-2.238793	-2.059709	
C	-2.540604	4.678418	1.543669	
C	0.854158	-1.405648	3.650264	
C	1.340698	-1.291071	-2.151634	
C	-0.669018	-0.233728	2.133893	
C	-2.504622	-3.906730	-1.567117	
C	0.073402	-1.025123	4.754268	
C	-3.380971	-1.366965	1.104538	
C	-1.804332	-4.300196	-0.416288	
C	-1.441025	0.156966	3.253914	
C	-1.752280	2.040840	0.843518	
C	-3.087843	2.465348	0.672551	
C	-3.477280	3.774874	1.016535	
C	-5.353372	-1.636757	-0.305463	
C	-1.077119	-0.240658	4.552062	
C	-0.579779	-3.676921	-0.069123	
C	-4.661884	-1.906373	0.886888	
H	-0.179609	-0.861947	-3.758864	
H	1.116205	-1.290540	1.499202	
H	-5.254872	-0.654176	-2.248518	
H	-2.566640	-2.565796	-3.297461	
H	-2.959191	0.252154	-1.880144	
H	-0.459689	4.961848	2.131111	
H	0.237551	2.646974	1.495995	
H	-2.846252	5.702672	1.814437	
H	1.776598	-1.992032	3.785973	
H	2.271000	-0.935352	-2.612517	
H	-3.452786	-4.404824	-1.828678	
H	0.366899	-1.325837	5.773870	
H	-2.858382	-1.586014	2.046849	
H	-2.204717	-5.107123	0.219885	
H	-2.332394	0.788644	3.112415	
H	-3.840820	1.769080	0.273866	
H	-4.526062	4.084064	0.872661	
H	-6.361723	-2.050854	-0.470826	
H	-1.691559	0.075369	5.411638	
H	-0.020577	-4.004681	0.822700	
H	-5.120385	-2.543519	1.661220	
C	-0.814211	1.786346	-2.383799	
C	0.286039	2.547967	-1.892329	
H	-1.813422	1.966415	-1.949601	
H	-0.827573	1.484261	-3.447023	
H	0.155715	3.274054	-1.071322	
C	1.548039	2.545994	-2.757402	
H	1.282451	2.871734	-3.807701	
O	1.915842	1.184694	-2.737113	
H	3.261318	-0.425973	0.993791	
C	5.132054	-1.072923	0.900741	
C	5.848556	-2.349340	1.372229	
H	6.935231	-2.309220	1.147739	
H	5.717316	-2.481825	2.466606	
H	5.416694	-3.237989	0.866607	
C	5.688785	0.165902	1.636521	
H	5.135978	1.073771	1.316652	
H	5.556545	0.051093	2.732807	
H	6.769013	0.321674	1.424412	
C	5.282460	-0.897735	-0.626042	
H	4.892965	-1.792101	-1.155411	
H	4.701230	-0.018179	-0.972383	
H	6.345265	-0.754194	-0.919486	
O	3.753705	-1.256854	1.246643	
C	2.666085	3.477931	-2.265961	
H	3.563542	3.356141	-2.909283	
H	2.348351	4.544964	-2.315694	
H	2.943373	3.221421	-1.223588	
H	2.042910	-2.104650	-0.199877	

EF			E _g (BP86/SVP) = -2403.0633595 G _g (BP86/SVP) = -2402.51169 E _s (M06//TZVP//BP86/SVP) = -2403.5418069
Ru	1.135940	-0.991499	-1.563165
Cl	-3.485533	-0.304267	-0.421766
P	1.103493	-0.245076	0.654910
C	1.808833	0.751311	-3.062183
C	3.356419	-0.241919	-1.676544
C	-0.532967	1.871034	-0.233340
C	4.879430	-0.674696	2.339397
C	4.179306	2.002357	-0.557272
C	3.692761	-0.863363	1.610760
C	-1.870965	-2.457337	2.501280
C	-1.166201	-1.538713	1.705596
C	2.391491	1.823709	-2.235179
C	2.665483	0.109649	1.625838
C	3.384344	1.215672	-1.393278
C	-1.191810	-3.290182	3.408667
C	-1.438153	2.935847	-0.082116
C	2.640476	-0.411768	-2.927484
C	0.022371	1.242571	0.897117
C	3.977829	3.407400	-0.536977
C	-1.785401	3.388144	1.198832
C	2.876368	1.293592	2.363536
C	2.987584	3.997613	-1.336313
C	-0.360808	1.678766	2.188260
C	0.242431	-1.444115	1.810703
C	0.921822	-2.279712	2.724602
C	0.206655	-3.196909	3.518223
C	5.069346	0.501920	3.087074
C	-1.247242	2.755964	2.335949
C	2.182813	3.207711	-2.195143
C	4.066486	1.485391	3.089259
H	4.137204	-0.930870	-1.323682
H	-0.275943	1.499469	-1.237424
H	5.662872	-1.449885	2.316616
H	4.952798	1.543460	0.079290
H	3.568879	-1.776018	1.006338
H	-2.965539	-2.506638	2.382451
H	-1.757867	-0.917008	0.995747
H	-1.748858	-4.010480	4.030802
H	-1.893304	3.392625	-0.973992
H	2.759756	-1.229283	-3.654682
H	4.602825	4.036379	0.117874
H	-2.504647	4.214575	1.316136
H	2.112763	2.084978	2.359186
H	2.835749	5.089167	-1.303437
H	0.011945	1.154040	3.082321
H	2.013938	-2.210927	2.840552
H	0.752198	-3.837629	4.230981
H	6.000793	0.654485	3.656238
H	-1.542445	3.086431	3.345237
H	1.418038	3.680794	-2.832514
H	4.211293	2.421472	3.652981
C	1.779519	-3.013085	-1.171783
C	0.353644	-2.943988	-1.118873
H	2.342033	-3.214162	-0.242312
H	2.284706	-3.377593	-2.088133
H	-0.187327	-3.093557	-0.170819
C	-0.430742	-2.943049	-2.439148
H	-0.043583	-3.730059	-3.142403
C	-1.942119	-3.090759	-2.290059
H	-2.364316	-2.266502	-1.669454
H	-2.428409	-3.052943	-3.286796
H	-2.184994	-4.069669	-1.822336
O	-0.085450	-1.653224	-2.962543
H	-5.114646	0.998158	-0.860648
C	-6.844290	1.016075	0.052901
C	-6.221414	1.230529	1.452462
H	-6.865697	0.833458	2.268673
H	-5.235203	0.720023	1.479781
H	-6.054649	2.314703	1.629273
C	-7.097357	-0.492161	-0.184750
H	-7.542140	-0.646296	-1.191146
H	-6.121376	-1.022555	-0.153743
H	-7.781074	-0.930868	0.576247
C	-8.151898	1.815315	-0.089169
H	-7.952868	2.899427	0.049316
H	-8.575873	1.677021	-1.106517
H	-8.909549	1.495247	0.658020
O	-5.966885	1.521754	-0.947790
H	1.097229	0.910531	-3.885416

F				E_g(BP86/SVP) = -1709.3742274 G_g(BP86/SVP) = -1708.941871 E_s(M06//TZVP//BP86/SVP) = -1709.6252261
Ru	-1.185083	-0.847937	-0.768765	
P	0.823506	0.212584	-0.020223	
C	-3.279825	-0.915324	-1.478176	
C	-1.900790	0.924890	-1.954608	
C	-0.236827	0.216946	2.594944	
C	1.426004	3.107077	-2.949817	
C	-2.407925	2.203263	0.305558	
C	1.214696	1.898563	-2.266268	
C	4.279281	-2.017256	0.735798	
C	3.057057	-1.336349	0.873599	
C	-3.361272	-0.006973	-0.353331	
C	1.109085	1.865678	-0.854100	
C	-2.501178	1.134451	-0.635347	
C	4.982740	-1.977963	-0.479797	
C	-0.244399	0.501634	3.974223	
C	-2.428909	-0.291368	-2.487176	
C	0.853897	0.623857	1.796565	
C	-3.145169	2.129618	1.483717	
C	0.826914	1.191171	4.564611	
C	1.168825	3.089952	-0.153334	
C	-3.966310	0.997144	1.770997	
C	1.943392	1.297931	2.402078	
C	2.511565	-0.597037	-0.203099	
C	3.228017	-0.569750	-1.421499	
C	4.450988	-1.249989	-1.557477	
C	1.502171	4.317817	-2.237433	
C	1.925396	1.585332	3.776318	
C	-4.073105	-0.067167	0.881691	
C	1.359514	4.304164	-0.840864	
H	-1.281120	1.652896	-2.489406	
H	-1.047173	-0.374656	2.135378	
H	1.515513	3.103767	-0.048078	
H	-1.780721	3.079620	0.081288	
H	1.089449	0.966973	-2.840975	
H	4.683036	-2.581222	1.591936	
H	2.529321	-1.374563	1.838212	
H	5.940957	-2.510775	-0.586272	
H	-1.096216	0.171167	4.589753	
H	-2.262709	-0.664435	-3.505890	
H	-3.093737	2.954552	2.211506	
H	0.815923	1.413665	5.643938	
H	1.057731	3.105505	0.940509	
H	-4.529745	0.971678	2.717495	
H	2.818147	1.589193	1.798487	
H	2.842775	-0.003566	-2.280795	
H	4.991552	-1.204892	-2.516552	
H	1.658043	5.268238	-2.772002	
H	2.776537	2.112978	4.236301	
H	-4.711174	-0.934954	1.107011	
H	1.397054	5.247230	-0.272120	
C	-0.938278	-2.743846	-1.846470	
C	0.120971	-2.630971	-0.921593	
H	-0.729046	-2.636262	-2.923678	
H	-1.829845	-3.340710	-1.591773	
H	1.150943	-2.469281	-1.279086	
C	-0.149013	-2.995884	0.538384	
O	-1.253537	-2.173767	0.848859	
H	0.753433	-2.693081	1.137859	
C	-0.413868	-4.479108	0.823762	
H	0.486226	-5.097892	0.616484	
H	-0.684857	-4.609681	1.892531	
H	-1.257163	-4.858741	0.210165	
H	-3.865650	-1.835151	-1.595261	

FG				E_g(BP86/SVP) = -1709.3735467 G_g(BP86/SVP) = -1708.943943 E_s(M06//TZVP//BP86/SVP) = -1709.6271871
Ru	-1.155553	-0.957693	-0.697842	
P	0.752290	0.328427	-0.090967	
C	-3.223954	-1.370727	-1.507561	
C	-2.208248	0.672530	-1.954637	
C	0.608381	-0.430181	2.645897	
C	-0.192281	4.261935	-1.188739	
C	-2.929083	1.811871	0.332815	
C	0.104440	2.888830	-1.226355	
C	4.303795	-1.067027	-1.762224	
C	3.137951	-0.923336	-0.989889	
C	-3.456532	-0.525949	-0.359930	
C	0.399014	2.169802	-0.042384	
C	-2.804069	0.751039	-0.616984	
C	4.692542	-0.066246	-2.668740	
C	1.077550	-0.545597	3.966431	
C	-2.537221	-0.585857	-2.522441	
C	1.440363	0.084428	1.630570	
C	-3.688542	1.602197	1.477877	
C	2.387951	-0.152977	4.286737	
C	0.368335	2.872323	1.183578	
C	-4.321994	0.345248	1.732271	
C	2.754423	0.485857	1.962543	
C	2.327707	0.234041	-1.114907	
C	2.742649	1.245116	-2.011744	
C	3.909486	1.093913	-2.782557	
C	-0.218843	4.946607	0.039285	
C	3.224409	0.363355	3.280772	
C	-4.205602	-0.715516	0.844661	
C	0.058816	4.243973	1.223186	
H	-1.717578	1.499550	-2.475929	
H	-0.414621	-0.747511	2.385128	
H	-0.407861	4.798053	-2.126965	
H	-2.459969	2.787868	0.139822	
H	0.102505	2.372127	-2.197052	
H	4.915891	-1.975614	-1.642275	
H	2.870359	-1.719141	-0.272508	
H	5.606547	-0.183183	-3.272798	
H	0.414612	-0.952454	4.746851	
H	-2.312762	-0.911227	-3.546135	
H	-3.811305	2.420979	2.204324	
H	2.759937	-0.251845	5.319160	
H	0.584724	2.344343	2.123225	
H	-4.920956	0.223933	2.649094	
H	3.418399	0.897783	1.186956	
H	2.175767	2.180840	-2.103392	
H	4.210038	1.901235	-3.469883	
H	-0.455769	6.021908	0.071114	
H	4.254022	0.672698	3.522300	
H	-4.707740	-1.676871	1.035714	
H	0.038273	4.765141	2.193702	
C	-0.940143	-2.980622	-1.426329	
C	0.303455	-2.646597	-0.821785	
H	-1.005464	-3.000403	-2.527301	
H	-1.614147	-3.694150	-0.923078	
H	1.146327	-2.366055	-1.473959	
C	0.745839	-3.265337	0.472331	
H	-1.177982	-1.529946	0.778132	
O	1.912898	-3.155856	0.857462	
C	-0.228931	-4.125019	1.272890	
H	-0.290063	-5.131407	0.804187	
H	0.165969	-4.247227	2.298790	
H	-1.251353	-3.701432	1.305872	
H	-3.648980	-2.371547	-1.651064	

G				E_g(BP86/SVP) = -1709.4023541 G_g(BP86/SVP) = -1708.975465 E_s(M06//TZVP//BP86/SVP) = -1709.6566427
Ru	-1.363829	0.237348	0.228351	
P	0.920497	0.164380	0.007663	
C	-3.504463	-0.505062	0.393636	
C	-1.877270	-1.119168	1.980292	
C	0.774452	-1.545398	-2.261176	
C	2.028329	-0.725103	3.904839	
C	-0.950188	-3.176691	0.610125	
C	1.458433	-0.144021	2.760254	
C	2.246371	3.735851	-1.610457	
C	1.622901	2.495642	-1.398657	
C	-2.782734	-1.643809	-0.131497	
C	1.769223	-0.633320	1.468286	
C	-1.766615	-2.023933	0.847640	
C	3.088277	4.282393	-0.624493	
C	1.293261	-2.237413	-3.371058	
C	-2.978762	-0.236328	1.709528	
C	1.619217	-0.758436	-1.453198	
C	-1.167194	-3.928047	-0.536072	
C	2.659748	-2.149563	-3.684229	
C	2.640096	-1.738810	1.355578	
C	-2.156483	-3.548836	-1.500782	
C	2.993995	-0.669531	-1.777874	
C	1.833301	1.780442	-0.195268	
C	2.683163	2.333840	0.786096	
C	3.305838	3.577959	0.570963	
C	2.896841	-1.825743	3.781183	
C	3.510050	-1.363244	-2.884703	
C	-2.942006	-2.418160	-1.325437	
C	3.193652	-2.333053	2.505806	
H	-1.312582	-1.193159	2.917338	
H	-0.299178	-1.603536	-2.024373	
H	1.783687	-0.322646	4.901066	
H	-0.192153	-3.475389	1.350404	
H	0.747606	0.691054	2.866555	
H	2.073312	4.277927	-2.553752	
H	0.976795	2.069702	-2.183608	
H	3.576854	5.255546	-0.791303	
H	0.619207	-2.843397	-3.997051	
H	-3.373305	0.510892	2.410548	
H	-0.564326	-4.831935	-0.716874	
H	3.063959	-2.687536	-4.556756	
H	2.886015	-2.148654	0.364585	
H	-2.292808	-4.171796	-2.399143	
H	3.664968	-0.042711	-1.168883	
H	2.873317	1.788603	1.723229	
H	3.970154	3.993816	1.345490	
H	3.334707	-2.290047	4.679136	
H	4.581238	-1.281679	-3.129632	
H	-3.705156	-2.132994	-2.066161	
H	3.863749	-3.201239	2.398670	
C	-1.186932	2.197542	1.091071	
C	-1.671088	2.326925	-0.262191	
H	-0.171331	2.567735	1.315829	
H	-1.885688	2.332362	1.935366	
H	-0.960948	2.665039	-1.034483	
C	-3.072554	2.646456	-0.681950	
H	-1.236731	0.371422	-1.357852	
O	-3.361530	2.754344	-1.873993	
C	-4.125743	2.948765	0.386868	
H	-4.069319	2.288067	1.273019	
H	-3.964398	3.987104	0.751400	
H	-5.133907	2.894823	-0.066520	
H	-4.371138	-0.023991	-0.075421	

GH				E_g(BP86/SVP) = -1709.370516 G_g(BP86/SVP) = -1708.943129 E_s(M06//TZVP//BP86/SVP) = -1709.625953
Ru	-1.091070	-1.115821	-0.600435	
P	0.678626	0.357977	-0.046189	
C	-3.171001	-1.633059	-1.231300	
C	-2.247975	0.382604	-1.959855	
C	-0.321544	0.569890	2.605914	
C	0.549667	3.080322	-3.202119	
C	-2.846412	1.737890	0.234769	
C	0.608333	1.910245	-2.427318	
C	4.560787	-0.996108	0.659891	
C	3.214636	-0.625493	0.814236	
C	-3.352421	-0.675159	-0.165165	
C	0.593430	1.968131	-1.012264	
C	-2.752628	0.580669	-0.599706	
C	5.191304	-0.876106	-0.587541	
C	-0.324302	1.012962	3.941941	
C	-2.566631	-0.936216	-2.363629	
C	0.705614	0.961370	1.723283	
C	-3.522436	1.640984	1.444304	
C	0.698339	1.853398	4.410377	
C	0.469321	3.234681	-0.400477	
C	-4.099903	0.404487	1.876972	
C	1.735049	1.807220	2.205263	
C	2.477269	-0.109362	-0.274477	
C	3.117797	-0.007892	-1.530369	
C	4.461429	-0.387218	-1.684740	
C	0.440376	4.336707	-2.578728	
C	1.729440	2.250111	3.537866	
C	-4.012284	-0.745034	1.103616	
C	0.388721	4.406348	-1.177650	
H	-1.797801	1.162661	-2.583323	
H	-1.115868	-0.097995	2.235315	
H	0.575554	3.007825	-4.301368	
H	-2.412635	2.692699	-0.099404	
H	0.632209	0.930787	-2.931574	
H	5.111317	-1.399303	1.524193	
H	2.738862	-0.744922	1.797909	
H	6.246045	-1.170051	-0.708715	
H	-1.132525	0.693408	4.618895	
H	-2.388742	-1.364376	-3.358691	
H	-3.620628	2.530571	2.086178	
H	0.698240	2.197096	5.457327	
H	0.426897	3.315531	0.695350	
H	-4.632219	0.371786	2.841100	
H	2.556515	2.111566	1.537509	
H	2.579095	0.387354	-2.402503	
H	4.941277	-0.290864	-2.671953	
H	0.383945	5.254878	-3.184683	
H	2.539951	2.903254	3.899364	
H	-4.473403	-1.689454	1.432640	
H	0.285723	5.381995	-0.675843	
C	-0.788325	-3.140315	-1.298860	
C	0.484128	-2.704819	-0.830504	
H	-0.965553	-3.190775	-2.386121	
H	-1.348407	-3.893083	-0.718277	
H	1.248649	-2.374398	-1.553241	
C	1.106423	-3.343668	0.379786	
H	-0.960807	-1.685774	0.874963	
O	2.328184	-3.339513	0.521873	
C	0.233981	-4.115537	1.370913	
H	-0.778686	-3.687057	1.497177	
H	0.129525	-5.161928	1.009667	
H	0.757015	-4.151511	2.345595	
H	-3.582427	-2.649556	-1.247087	

H				E_g(BP86/SVP) = -1709.3946296 G_g(BP86/SVP) = -1708.966373 E_s(M06//TZVP//BP86/SVP) = -1709.6485357
Ru	0.799265	-1.359322	-0.555766	
P	-0.483441	0.459893	0.026459	
C	2.675489	-2.628847	-0.795794	
C	1.984870	-1.871883	1.323112	
C	1.251376	2.206678	-1.432573	
C	-0.935960	-0.103086	4.109116	
C	3.188079	0.471577	1.158938	
C	-0.951951	-0.268067	2.713350	
C	-3.866637	0.853196	-2.324873	
C	-2.546730	0.725567	-1.862913	
C	3.186110	-1.286585	-0.620729	
C	-0.508681	0.777579	1.866235	
C	2.751465	-0.809877	0.691449	
C	-4.938990	0.829534	-1.413125	
C	1.650080	3.441441	-1.978446	
C	2.007610	-2.993317	0.426077	
C	0.068229	2.107113	-0.674880	
C	4.043394	1.221428	0.364322	
C	0.870760	4.591082	-1.771948	
C	-0.020733	1.968414	2.448651	
C	4.464614	0.756196	-0.923591	
C	-0.716057	3.269536	-0.478414	
C	-2.277356	0.578632	-0.480777	
C	-3.357233	0.552288	0.425751	
C	-4.679746	0.675661	-0.041252	
C	-0.453663	1.088175	4.682253	
C	-0.315659	4.501802	-1.019622	
C	4.034874	-0.463468	-1.428294	
C	0.009921	2.118721	3.848074	
H	1.586613	-1.859827	2.344454	
H	1.857110	1.304274	-1.606742	
H	-1.297405	-0.920886	4.753274	
H	2.873290	0.830153	2.150861	
H	-1.307292	-1.220299	2.280667	
H	-4.058765	0.976315	-3.402860	
H	-1.711200	0.759438	-2.581416	
H	-5.974936	0.931822	-1.773702	
H	2.575957	3.498838	-2.572793	
H	1.583812	-3.982517	0.643497	
H	4.405708	2.197373	0.723887	
H	1.180962	5.556814	-2.202470	
H	0.347909	2.785090	1.810615	
H	5.145101	1.383177	-1.521729	
H	-1.655256	3.209176	0.094297	
H	-3.170993	0.442235	1.504444	
H	-5.512568	0.656655	0.679886	
H	-0.433536	1.209671	5.777231	
H	-0.938800	5.396537	-0.860322	
H	4.369491	-0.820669	-2.414943	
H	0.400004	3.052227	4.285156	
C	-0.422513	-2.416822	-1.977147	
C	-0.804485	-2.813246	-0.646208	
H	0.190884	-3.095019	-2.596705	
H	-1.123083	-1.807540	-2.571750	
H	-0.346082	-3.736332	-0.244474	
C	-2.173742	-2.698667	-0.031993	
H	0.793459	-0.573398	-1.946474	
O	-2.334045	-2.732570	1.190280	
C	-3.369155	-2.707640	-0.972852	
H	-3.345917	-1.837263	-1.659773	
H	-3.330928	-3.616605	-1.611653	
H	-4.307215	-2.697300	-0.387440	
H	2.874498	-3.288509	-1.649837	

H1				E _g (BP86/SVP) = -1709.3873546 G _g (BP86/SVP) = -1708.960919 E _s (M06//TZVP//BP86/SVP) = -1709.6422531
Ru	0.900552	-1.260672	-0.428211	
P	-0.543991	0.466496	0.074469	
C	2.720802	-2.577014	-0.360365	
C	1.986512	-1.398043	1.527588	
C	1.157922	2.320737	-1.257430	
C	-1.418985	-0.415071	4.020459	
C	3.312882	0.818732	0.980752	
C	-1.272735	-0.467197	2.624066	
C	-3.725687	0.855161	-2.557459	
C	-2.448566	0.795440	-1.976121	
C	3.284090	-1.239195	-0.433194	
C	-0.778702	0.655802	1.913611	
C	2.843755	-0.507056	0.749381	
C	-4.872414	0.660002	-1.764949	
C	1.536725	3.585467	-1.746767	
C	1.997893	-2.679418	0.882991	
C	-0.021738	2.171189	-0.500915	
C	4.205423	1.385698	0.074435	
C	0.742328	4.712604	-1.481092	
C	-0.399625	1.807694	2.636739	
C	4.620979	0.679296	-1.094249	
C	-0.825517	3.309741	-0.251930	
C	-2.293241	0.538535	-0.591917	
C	-3.449180	0.347143	0.194039	
C	-4.728434	0.407768	-0.390675	
C	-1.047947	0.740753	4.733139	
C	-0.441778	4.572054	-0.732198	
C	4.162780	-0.607624	-1.365465	
C	-0.529950	1.845777	4.038435	
H	1.540207	-1.171033	2.503304	
H	1.773600	1.431442	-1.468038	
H	-1.814605	-1.293272	4.555544	
H	2.990362	1.366930	1.879490	
H	-1.523647	-1.397215	2.085795	
H	-3.826090	1.062976	-3.634961	
H	-1.558841	0.976087	-2.601883	
H	-5.874961	0.709312	-2.218793	
H	2.459322	3.685340	-2.340442	
H	1.509033	-3.583391	1.269643	
H	4.594399	2.400046	0.255568	
H	1.038683	5.702414	-1.864165	
H	0.010339	2.682572	2.110057	
H	5.324557	1.162722	-1.790941	
H	-1.767825	3.205523	0.309684	
H	-3.358136	0.157511	1.274064	
H	-5.619566	0.260590	0.240436	
H	-1.153327	0.774516	5.829352	
H	-1.076316	5.450236	-0.530907	
H	4.502534	-1.152537	-2.260475	
H	-0.221880	2.750165	4.587706	
C	-0.111811	-2.092541	-2.205931	
C	-0.460323	-2.802252	-0.974998	
H	0.543452	-2.609866	-2.931280	
H	-0.920685	-1.534364	-2.712244	
H	0.099397	-3.737894	-0.775662	
C	-1.842362	-2.945776	-0.403896	
H	0.745526	-0.869523	-2.027441	
O	-2.006084	-3.277911	0.772556	
C	-3.031861	-2.808872	-1.345361	
H	-3.052156	-1.821826	-1.849317	
H	-2.952599	-3.576241	-2.146596	
H	-3.971755	-2.957607	-0.782061	
H	2.917831	-3.395417	-1.065984	

I				E_g(BP86/SVP) = -1709.3898108 G_g(BP86/SVP) = -1708.961232 E_s(M06//TZVP//BP86/SVP) = -1709.648867
Ru	0.955172	-1.228284	-0.349737	
P	-0.566851	0.464250	0.076276	
C	2.750129	-2.531849	-0.165252	
C	1.980497	-1.172505	1.576835	
C	1.112474	2.358020	-1.224848	
C	-1.504001	-0.411408	4.008154	
C	3.402324	0.948214	0.906783	
C	-1.307297	-0.475830	2.618445	
C	-3.707505	0.714934	-2.628985	
C	-2.441164	0.710525	-2.021126	
C	3.351451	-1.213377	-0.332543	
C	-0.866773	0.667310	1.904691	
C	2.913484	-0.378687	0.776273	
C	-4.861305	0.474174	-1.859597	
C	1.464869	3.626061	-1.725396	
C	1.986231	-2.519238	1.057246	
C	-0.091208	2.179015	-0.512555	
C	4.314946	1.428886	-0.034954	
C	0.619462	4.727703	-1.516137	
C	-0.593526	1.854071	2.618119	
C	4.724004	0.624669	-1.136086	
C	-0.945613	3.291734	-0.321679	
C	-2.303259	0.464722	-0.633126	
C	-3.466630	0.226799	0.129114	
C	-4.734966	0.231780	-0.481753	
C	-1.237521	0.778586	4.711338	
C	-0.588619	4.557799	-0.812992	
C	4.245250	-0.676139	-1.304244	
C	-0.773666	1.905734	4.013880	
H	1.518029	-0.853434	2.519318	
H	1.772254	1.490672	-1.390948	
H	-1.856433	-1.306092	4.546136	
H	3.078127	1.573997	1.752864	
H	-1.476922	-1.428452	2.087441	
H	-3.794276	0.916026	-3.708971	
H	-1.547761	0.927750	-2.629943	
H	-5.855534	0.480645	-2.333878	
H	2.406866	3.748276	-2.283317	
H	1.481075	-3.379344	1.516155	
H	4.720244	2.447657	0.069167	
H	0.895083	5.720176	-1.907696	
H	-0.228058	2.746535	2.088356	
H	5.439464	1.036747	-1.865919	
H	-1.906247	3.162964	0.202531	
H	-3.390217	0.044870	1.211574	
H	-5.631843	0.049085	0.131707	
H	-1.381508	0.822267	5.802810	
H	-1.262219	5.415692	-0.655946	
H	4.582681	-1.296749	-2.149571	
H	-0.547120	2.837921	4.556285	
C	-0.038947	-2.080861	-2.264407	
C	-0.333985	-2.764798	-0.967321	
H	0.553602	-2.666829	-2.995188	
H	-0.914313	-1.615890	-2.758343	
H	0.239531	-3.700006	-0.795148	
C	-1.721967	-2.991043	-0.436594	
H	0.678513	-1.091813	-2.132052	
O	-1.897223	-3.318032	0.739672	
C	-2.898027	-2.933866	-1.405662	
H	-3.829689	-3.192748	-0.869043	
H	-3.006222	-1.929772	-1.863437	
H	-2.734103	-3.652158	-2.238680	
H	2.955136	-3.409813	-0.793063	

IJ				$E_g(\text{BP86/SVP}) = -1709.3652523$ $G_g(\text{BP86/SVP}) = -1708.938579$ $E_s(\text{M06//TZVP//BP86/SVP}) = -1709.6276259$
Ru	0.721624	-1.490236	-0.430212	
P	-0.506229	0.541148	0.011680	
C	2.450466	-2.185275	-1.519301	
C	2.203374	-2.369304	0.794857	
C	0.734280	1.832149	-2.179207	
C	0.258807	0.507121	4.069343	
C	3.317675	-0.043406	1.371652	
C	-0.123807	0.159652	2.762979	
C	-4.474867	0.726397	-1.211820	
C	-3.071022	0.699505	-1.177504	
C	3.018947	-0.976832	-0.913222	
C	-0.021666	1.108243	1.715260	
C	2.872208	-1.093279	0.525677	
C	-5.212323	0.690946	-0.013716	
C	0.975758	2.893303	-3.070978	
C	2.119343	-3.105608	-0.456337	
C	-0.171626	1.987117	-1.111242	
C	3.940473	1.067989	0.799909	
C	0.314608	4.120919	-2.900657	
C	0.501242	2.388669	1.993754	
C	4.115352	1.167511	-0.609274	
C	-0.845541	3.222000	-0.954216	
C	-2.377273	0.641468	0.055252	
C	-3.126063	0.609315	1.251011	
C	-4.532664	0.633368	1.214352	
C	0.771447	1.789306	4.343556	
C	-0.597349	4.282979	-1.840526	
C	3.653581	0.168026	-1.467630	
C	0.897323	2.723699	3.302208	
H	1.989685	-2.773870	1.794241	
H	1.240576	0.860731	-2.299015	
H	0.164151	-0.235876	4.877648	
H	3.193617	-0.120248	2.462876	
H	-0.492943	-0.856844	2.542763	
H	-4.995545	0.779989	-2.181528	
H	-2.507032	0.744686	-2.123665	
H	-6.313446	0.712049	-0.039181	
H	1.682166	2.756480	-3.905427	
H	1.811177	-4.153564	-0.570821	
H	4.312381	1.876594	1.448341	
H	0.501869	4.952436	-3.598966	
H	0.616472	3.127696	1.187009	
H	4.628294	2.048471	-1.026987	
H	-1.579833	3.350465	-0.143113	
H	-2.611810	0.570639	2.222751	
H	-5.099121	0.610594	2.159188	
H	1.079000	2.056254	5.367398	
H	-1.125868	5.240656	-1.707575	
H	3.807391	0.245049	-2.555905	
H	1.309179	3.725616	3.504675	
C	-1.481662	-2.599941	-2.290089	
C	-0.904645	-2.784063	-0.880297	
H	-2.249534	-3.367931	-2.546241	
H	-1.960507	-1.606976	-2.419982	
H	-0.433250	-3.793463	-0.809770	
C	-1.867180	-2.749209	0.275213	
H	-0.680540	-2.680607	-3.053532	
O	-1.450561	-2.595696	1.434111	
C	-3.357453	-2.932467	0.026322	
H	-3.549897	-3.827780	-0.602537	
H	-3.892425	-3.021573	0.990394	
H	-3.757034	-2.058986	-0.531769	
H	2.480836	-2.423755	-2.591972	

J				E _g (BP86/SVP) = -1709.3962054 G _g (BP86/SVP) = -1708.9664 E _s (M06//TZVP//BP86/SVP) = -1709.6525226
Ru	-1.117638	-0.842342	-0.611350	
P	0.886923	0.140770	0.050217	
C	-2.927888	-1.165117	-1.893027	
C	-1.538740	0.702746	-2.115968	
C	-0.032700	0.803189	2.631756	
C	2.400483	2.629565	-2.973060	
C	-2.717867	2.129045	-0.219432	
C	2.125865	1.506386	-2.172049	
C	4.548581	-1.876013	0.586650	
C	3.455518	-1.019629	0.809586	
C	-3.364105	-0.179088	-0.924796	
C	1.367743	1.632840	-0.986964	
C	-2.500068	0.990628	-1.051059	
C	4.617106	-2.651609	-0.583829	
C	0.010316	1.401502	3.905025	
C	-1.847200	-0.590255	-2.663128	
C	1.055152	0.917688	1.743449	
C	-3.770122	2.110736	0.693011	
C	1.142803	2.132927	4.299356	
C	0.898448	2.916455	-0.623108	
C	-4.612492	0.964561	0.819093	
C	2.179250	1.683001	2.138064	
C	2.410491	-0.926874	-0.136458	
C	2.472866	-1.737088	-1.296109	
C	3.573390	-2.581119	-1.522870	
C	1.922712	3.899547	-2.605748	
C	2.224362	2.278370	3.409816	
C	-4.420704	-0.171670	0.038568	
C	1.171663	4.038254	-1.425549	
H	-0.791640	1.405399	-2.503558	
H	-0.925610	0.255130	2.292714	
H	3.000213	2.508124	-3.889486	
H	-2.080705	3.019388	-0.331210	
H	2.519079	0.523522	-2.472880	
H	5.352346	-1.936712	1.338205	
H	3.415847	-0.436632	1.741248	
H	5.475378	-3.320647	-0.756116	
H	-0.850273	1.302129	4.585891	
H	-1.353809	-1.057070	-3.525338	
H	-3.959990	2.991177	1.326686	
H	1.179661	2.604034	5.294753	
H	0.321704	3.043434	0.306069	
H	-5.439920	0.987645	1.546816	
H	3.017710	1.835065	1.440023	
H	1.627596	-1.732894	-2.001410	
H	3.602934	-3.203214	-2.431728	
H	2.139888	4.778665	-3.233038	
H	3.106611	2.868736	3.705767	
H	-5.088464	-1.042228	0.133195	
H	0.798512	5.029364	-1.120550	
C	-2.235005	-2.070708	2.386356	
C	-1.861881	-2.309240	0.943336	
H	-2.643712	-3.001973	2.843433	
H	-1.377678	-1.750413	3.009673	
H	-2.691863	-2.677321	0.316262	
C	-0.557706	-2.715734	0.514334	
H	-3.028477	-1.298614	2.472729	
O	-0.368781	-2.842385	-0.784291	
C	0.546860	-3.104362	1.476792	
H	0.642778	-2.405997	2.331266	
H	0.297667	-4.103087	1.899279	
H	1.516332	-3.178781	0.954513	
H	-3.382396	-2.149288	-2.064948	

JK				E _g (BP86/SVP) = -1941.650167 G _g (BP86/SVP) = -1941.119447 E _s (M06//TZVP//BP86/SVP) = -1942.0050926
Ru	0.841908	-0.671617	-0.042361	
P	-1.321116	-0.046754	-0.132984	
C	1.851175	-0.174524	-2.002991	
C	1.119350	-2.319076	-1.401738	
C	-2.362279	-2.646154	-0.641186	
C	-0.925097	2.945049	-2.987139	
C	3.448066	-3.153132	-0.501701	
C	-0.751678	2.096687	-1.881842	
C	-3.174566	1.185919	3.406514	
C	-2.701528	0.408867	2.335693	
C	2.984801	-0.890459	-1.409836	
C	-1.656234	1.038935	-1.630295	
C	2.547635	-2.229480	-1.079147	
C	-2.936697	2.570869	3.434642	
C	-3.369220	-3.610115	-0.831310	
C	0.760322	-1.100948	-2.125651	
C	-2.687375	-1.317489	-0.302893	
C	4.767006	-2.751389	-0.253497	
C	-4.720085	-3.256964	-0.679536	
C	-2.718694	0.831173	-2.537971	
C	5.194386	-1.436811	-0.566291	
C	-4.052844	-0.970727	-0.156439	
C	-1.989908	1.002249	1.266755	
C	-1.753004	2.394382	1.308988	
C	-2.222639	3.169902	2.382926	
C	-1.990488	2.735257	-3.880822	
C	-5.058833	-1.933978	-0.340574	
C	4.319631	-0.503970	-1.136709	
C	-2.879914	1.671798	-3.655675	
H	0.561383	-3.265343	-1.424001	
H	-1.302914	-2.919782	-0.739839	
H	-0.212590	3.769679	-3.150206	
H	3.119273	-4.178097	-0.266717	
H	0.109169	2.245333	-1.212030	
H	-3.732930	0.702436	4.224153	
H	-2.901862	-0.673635	2.330964	
H	-3.308002	3.181279	4.273194	
H	-3.093655	-4.644240	-1.093141	
H	-0.148105	-0.948423	-2.724036	
H	5.481980	-3.463103	0.188204	
H	-5.510387	-4.011175	-0.822378	
H	-3.425961	0.002906	-2.386127	
H	6.237521	-1.147007	-0.362248	
H	-4.334778	0.060975	0.105363	
H	-1.205493	2.886403	0.493770	
H	-2.031354	4.254901	2.391984	
H	-2.121671	3.393133	-4.754802	
H	-6.115973	-1.647681	-0.219175	
H	4.672273	0.507252	-1.393649	
H	-3.710678	1.487506	-4.355876	
C	-0.341337	-2.898484	2.176295	
C	0.842136	-2.054766	1.744829	
H	-0.134026	-3.431451	3.133908	
H	-1.269862	-2.309982	2.320393	
H	1.715160	-2.655033	1.429306	
C	1.244212	-0.859979	2.434485	
H	-0.573932	-3.676666	1.421463	
O	2.403827	-0.335172	2.204496	
C	2.192472	4.438328	-1.231582	
C	1.934845	3.850571	-0.048154	
H	1.731838	5.399096	-1.513565	
H	2.888150	3.985626	-1.960147	
H	1.237733	4.326983	0.667326	
C	2.582886	2.582234	0.454921	
H	3.109584	2.088855	-0.397569	
O	1.571074	1.709319	0.977248	
H	2.032311	1.040390	1.602992	
C	3.622688	2.903638	1.544935	
H	3.146276	3.433134	2.396681	
H	4.078490	1.968023	1.929051	
H	4.427964	3.548880	1.137790	
C	0.389552	-0.190868	3.497329	
H	-0.601465	-0.656531	3.637152	
H	0.950253	-0.261375	4.454419	
H	0.255235	0.887187	3.274814	
H	1.902128	0.819551	-2.464714	

K				E _g (BP86/SVP) = -1941.6617573 G _g (BP86/SVP) = -1941.6617573 E _s (M06//TZVP//BP86/SVP) = -1942.0172142
Ru	1.040851	-0.764159	0.106489	
P	-0.785362	0.664825	0.096308	
C	2.669370	-2.074825	0.997641	
C	1.599062	-0.354738	2.173936	
C	0.517776	3.060662	-0.636461	
C	-1.945528	0.605213	4.079810	
C	3.272462	1.544357	1.422280	
C	-1.592234	0.254000	2.767604	
C	-3.856765	-1.211415	-2.037467	
C	-2.592254	-0.806818	-1.571481	
C	3.400639	-0.860512	0.747309	
C	-1.249900	1.247688	1.819200	
C	2.726566	0.226931	1.450827	
C	-5.027847	-0.741457	-1.419367	
C	0.676973	4.301710	-1.274948	
C	1.609867	-1.775140	1.946658	
C	-0.664638	2.303410	-0.807386	
C	4.459914	1.768343	0.730288	
C	-0.332931	4.795334	-2.121252	
C	-1.264438	2.599045	2.221369	
C	5.117491	0.702140	0.038951	
C	-1.673966	2.809238	-1.656812	
C	-2.476940	0.080336	-0.477786	
C	-3.663730	0.549418	0.135564	
C	-4.925897	0.141764	-0.330368	
C	-1.948503	1.957186	4.474933	
C	-1.503572	4.042605	-2.313990	
C	4.604248	-0.590580	0.025852	
C	-1.604214	2.949624	3.543518	
H	0.967156	0.176532	2.895528	
H	1.326166	2.659884	-0.003702	
H	-2.214951	-0.182217	4.802127	
H	2.780955	2.355027	1.983692	
H	-1.569380	-0.807340	2.468595	
H	-3.920299	-1.904727	-2.891609	
H	-1.693968	-1.205747	-2.057664	
H	-6.017007	-1.062038	-1.784022	
H	1.602871	4.879273	-1.122146	
H	0.953115	-2.499714	2.444112	
H	4.907859	2.774239	0.717347	
H	-0.204236	5.762188	-2.633598	
H	-1.013894	3.391402	1.499986	
H	6.059864	0.914564	-0.491478	
H	-2.603290	2.239050	-1.807187	
H	-3.606682	1.246022	0.985607	
H	-5.835535	0.521422	0.162558	
H	-2.218699	2.233099	5.506737	
H	-2.298260	4.417842	-2.978970	
H	5.130647	-1.402583	-0.499560	
H	-1.605000	4.010943	3.840395	
C	2.421559	0.754527	-2.374903	
C	1.747279	-0.576405	-2.073848	
H	2.968938	0.726513	-3.347546	
H	1.695594	1.588840	-2.431907	
H	2.463469	-1.413476	-1.942838	
C	0.683829	-0.987642	-2.967373	
H	3.164894	1.021537	-1.600715	
O	0.225891	-2.182781	-2.980678	
C	-1.427892	-4.011992	2.359301	
C	-1.449550	-3.463128	1.130536	
H	-2.262520	-3.879473	3.066422	
H	-0.578302	-4.629009	2.702567	
H	-2.312812	-2.855203	0.801973	
C	-0.391793	-3.670636	0.069229	
H	0.542731	-4.052008	0.546722	
O	-0.129491	-2.426004	-0.595645	
H	0.093002	-2.526966	-1.641187	
C	-0.861740	-4.701937	-0.972272	
H	-0.099285	-4.838277	-1.766428	
H	-1.037335	-5.679871	-0.481062	
H	-1.807956	-4.375360	-1.450011	
C	0.069106	0.001553	-3.942223	
H	0.834697	0.347311	-4.669906	
H	-0.762709	-0.477834	-4.491318	
H	-0.299882	0.910985	-3.423595	
H	2.950999	-3.071053	0.631344	

KL				E _g (BP86/SVP) = -1941.660034 G _g (BP86/SVP) = -1941.126979 E _s (M06//TZVP//BP86/SVP) = -1942.0142854
Ru	1.044657	-0.753307	0.078103	
P	-0.801013	0.655024	0.103909	
C	2.714140	-2.039198	0.936109	
C	1.620255	-0.352539	2.139144	
C	0.467613	3.056918	-0.664413	
C	-1.887550	0.598943	4.108232	
C	3.254291	1.584644	1.400687	
C	-1.567298	0.247833	2.787595	
C	-3.934076	-1.291405	-1.883604	
C	-2.655031	-0.878883	-1.465044	
C	3.425260	-0.809805	0.700075	
C	-1.226503	1.239662	1.836557	
C	2.733410	0.257228	1.416820	
C	-5.086448	-0.782070	-1.262500	
C	0.606446	4.293911	-1.315706	
C	1.656016	-1.770192	1.895293	
C	-0.711121	2.288199	-0.810561	
C	4.438909	1.836632	0.712923	
C	-0.420577	4.772047	-2.150072	
C	-1.209769	2.589128	2.244462	
C	5.117255	0.789027	0.014252	
C	-1.737670	2.779435	-1.647184	
C	-2.506728	0.056811	-0.416386	
C	-3.675847	0.565336	0.200178	
C	-4.951746	0.149759	-0.218263	
C	-1.859327	1.949040	4.508859	
C	-1.587998	4.008323	-2.317020	
C	4.625536	-0.512354	-0.014480	
C	-1.517112	2.939513	3.574691	
H	0.986525	0.157979	2.873871	
H	1.289575	2.670774	-0.039619	
H	-2.156188	-0.186990	4.832444	
H	2.747260	2.380922	1.968818	
H	-1.570244	-0.812420	2.484081	
H	-4.022895	-2.022030	-2.703753	
H	-1.772715	-1.307670	-1.955629	
H	-6.086432	-1.109358	-1.589723	
H	1.529611	4.880424	-1.181565	
H	1.016536	-2.512410	2.388892	
H	4.868601	2.850537	0.710277	
H	-0.308109	5.735518	-2.672518	
H	-0.961053	3.380557	1.521404	
H	6.057632	1.022865	-0.510680	
H	-2.664909	2.201570	-1.778874	
H	-3.593459	1.299215	1.016190	
H	-5.846438	0.561016	0.276636	
H	-2.104267	2.224992	5.546921	
H	-2.396237	4.371161	-2.972492	
H	5.166182	-1.309406	-0.548177	
H	-1.494527	3.999435	3.875675	
C	2.429150	0.769783	-2.405482	
C	1.719778	-0.546351	-2.122657	
H	3.202314	0.985195	-1.645616	
H	2.947054	0.752883	-3.393660	
H	2.411397	-1.406434	-2.012807	
C	0.613352	-0.921631	-2.972370	
H	1.731968	1.629760	-2.410570	
O	0.144653	-2.117843	-2.988037	
C	-1.248069	-4.148406	2.335667	
C	-1.330067	-3.571116	1.122598	
H	-2.065979	-4.070491	3.069958	
H	-0.362467	-4.735355	2.638353	
H	-2.228262	-2.993924	0.835103	
C	-0.295959	-3.701052	0.026340	
H	0.666985	-4.055700	0.466341	
O	-0.108304	-2.429095	-0.609868	
H	0.069759	-2.487559	-1.679700	
C	-0.750802	-4.724074	-1.030368	
H	-0.006545	-4.805395	-1.848837	
H	-0.870296	-5.721488	-0.561919	
H	-1.723574	-4.426773	-1.472755	
C	-0.074971	0.062491	-3.903622	
H	-1.113843	0.247502	-3.558049	
H	0.440250	1.034139	-4.000608	
H	-0.156692	-0.414986	-4.901883	
H	3.012531	-3.025963	0.558025	

L				E _g (BP86/SVP) = -1941.6554213 G _g (BP86/SVP) = -1941.6554213 E _s (M06//TZVP//BP86/SVP) = -1942.0080863
Ru	0.496636	-0.529162	-1.080661	
P	-1.150840	0.431430	0.327192	
C	1.649824	-1.959781	-2.290318	
C	-0.630001	-1.498975	-2.618109	
C	-0.400973	-1.326672	2.405465	
C	-4.864494	0.207989	-2.124048	
C	-1.528862	-3.232183	-0.833765	
C	-3.212153	0.477734	-1.597860	
C	0.004426	4.239185	1.461280	
C	-0.056289	2.851324	1.254525	
C	0.877167	-2.751307	-1.332212	
C	-2.872843	0.077427	-0.282789	
C	-0.542274	-2.514162	-1.584262	
C	-1.033258	5.075028	1.010029	
C	-0.387880	-1.817863	3.723138	
C	0.721050	-1.231735	-3.102267	
C	-1.162846	-0.185679	2.079335	
C	-1.113580	-4.159406	0.111082	
C	-1.129985	-1.169808	4.725401	
C	-3.835064	-0.612073	0.485573	
C	0.279463	-4.384806	0.365297	
C	-1.903170	0.465951	3.092584	
C	-1.169197	2.277036	0.594217	
C	-2.210665	3.120645	0.150097	
C	-2.141012	4.511080	0.356193	
C	-5.437944	-0.482974	-1.350781	
C	-1.886934	-0.026509	4.408141	
C	1.266026	-3.693507	-0.325653	
C	-5.106720	-0.893238	-0.048599	
H	-1.558798	-1.118999	-3.062774	
H	0.191572	-1.819236	1.616559	
H	-4.736118	0.534994	-3.146286	
H	-2.598228	-3.067909	-1.036062	
H	-2.464071	1.003840	-2.213333	
H	0.875808	4.669844	1.980284	
H	0.765020	2.215499	1.619216	
H	-0.979814	6.163630	1.171961	
H	0.215152	-2.706889	3.967220	
H	0.971525	-0.558346	-3.932640	
H	-1.861750	-4.733795	0.679333	
H	-1.113581	-1.550440	5.759377	
H	-3.591170	-0.937689	1.508132	
H	0.569539	-5.128014	1.125252	
H	-2.487198	1.368899	2.852904	
H	-3.093432	2.696604	-0.351332	
H	-2.965599	5.153565	0.007253	
H	-6.434928	-0.702222	-1.764936	
H	-2.463660	0.490037	5.192237	
H	2.333164	-3.884608	-0.133976	
H	-5.844389	-1.436604	0.563651	
C	5.730706	-1.234905	1.002140	
C	4.425937	-0.498152	0.862122	
H	5.630489	-2.312666	0.737371	
H	6.512758	-0.823597	0.323567	
H	3.971021	-0.503115	-0.145868	
C	3.740114	0.161121	1.835862	
H	6.140414	-1.191188	2.031368	
O	2.563224	0.822357	1.609986	
C	1.900880	2.139428	-4.356656	
C	1.672446	2.308584	-3.040900	
H	1.328320	2.690652	-5.120514	
H	2.683743	1.450956	-4.722232	
H	0.888725	3.008348	-2.694246	
C	2.443431	1.634910	-1.923015	
H	3.040096	0.792052	-2.356863	
O	1.527510	1.158828	-0.935148	
H	2.309893	0.838783	0.641275	
C	3.412219	2.631176	-1.258501	
H	3.989496	2.137462	-0.450013	
H	4.128294	3.030387	-2.005888	
H	2.848196	3.480007	-0.820476	
C	4.137207	0.280205	3.283077	
H	4.262871	1.349563	3.558425	
H	3.327712	-0.121208	3.929731	
H	5.074718	-0.257457	3.514625	
H	2.742462	-1.969480	-2.394727	

LF	
IND8-6Me SCF Done: -1709.34411775 A.U.	
Ru	1.286030 0.182034 -0.548777
P	-0.981503 0.093882 -0.021725
C	3.323840 -0.284928 -1.302346
C	1.379038 -1.338802 -2.148066
C	-0.336933 -0.807607 2.580661
C	-2.730133 -1.880304 -3.221073
C	1.155751 -3.080528 -0.169801
C	-2.046412 -0.952471 -2.418356
C	-2.091520 4.042492 0.417484
C	-1.432540 2.805121 0.489342
C	2.942478 -1.316838 -0.371582
C	-1.965773 -1.130141 -1.015575
C	1.728255 -1.972740 -0.890798
C	-3.264760 4.178744 -0.348191
C	-0.611373 -1.153628 3.916306
C	2.341977 -0.296059 -2.377379
C	-1.373773 -0.347365 1.742665
C	1.760939 -3.506732 0.996945
C	-1.916914 -1.042275 4.423891
C	-2.569353 -2.269851 -0.441675
C	2.936003 -2.853013 1.515099
C	-2.683012 -0.222175 2.262027
C	-1.945442 1.680948 -0.201741
C	-3.129038 1.819992 -0.958280
C	-3.780815 3.065690 -1.032284
C	-3.327234 -3.014240 -2.638835
C	-2.953343 -0.573635 3.594750
C	3.516571 -1.779797 0.865691
C	-3.239868 -3.207343 -1.250387
H	0.556793 -1.629334 -2.812636
H	0.688470 -0.866565 2.183265
H	-2.791525 -1.720326 -4.309596
H	0.265130 -3.589243 -0.569427
H	-1.561740 -0.079455 -2.885660
H	-1.683839 4.909011 0.962546
H	-0.511177 2.682359 1.083925
H	-3.777466 5.152100 -0.408539
H	0.206524 -1.503826 4.566115
H	2.362507 0.361093 -3.258103
H	1.339663 -4.360202 1.551117
H	-2.128203 -1.311675 5.471377
H	-2.514932 -2.428944 0.646007
H	3.379614 -3.224837 2.452589
H	-3.495940 0.160206 1.623469
H	-3.554318 0.955515 -1.490475
H	-4.703200 3.161152 -1.627794
H	-3.856854 -3.746417 -3.268903
H	-3.976893 -0.473430 3.990522
H	4.423793 -1.298240 1.261252
H	-3.700839 -4.093818 -0.785730
C	3.105581 3.208393 -1.551465
C	2.171540 2.699536 -0.715499
H	2.914972 3.308542 -2.632216
H	4.089264 3.547149 -1.185400
H	1.158023 2.465701 -1.140757
C	2.247361 2.494090 0.795839
O	1.448473 1.388116 1.139270
H	1.778140 3.403922 1.268634
C	3.677787 2.403257 1.352152
H	4.213883 1.540098 0.906316
H	4.263233 3.326381 1.153703
H	3.632941 2.253901 2.449394
H	4.200116 0.369778 -1.234230

E_g(BP86/SVP) = -1709.3441177
G_g(BP86/SVP) = -1708.91616
E_s(M06//TZVP//BP86/SVP) = -1709.6006092

With [RuCl(Cp)(PPh₃)₂] (5):

A	
Ru	0.036068 -0.902649 -1.191465
Cl	-0.051403 1.035595 -2.717406
P	-1.782230 -0.055597 0.035803
P	1.819414 0.091611 -0.048387
C	-0.654902 -2.347608 -2.762948
C	0.046980 -3.061151 -0.645267
C	-2.901683 -2.173993 1.633214
C	-1.249781 -0.772626 2.731455
C	-2.493055 2.080692 1.882485
C	-2.068160 1.713580 0.587638
C	3.274294 0.448530 -2.472948
C	2.693993 -2.915803 2.689397
C	-5.855868 -0.282655 -2.302584
C	2.040568 -1.953824 1.901159
C	0.969917 3.843927 1.458347
C	1.123490 2.726527 0.622624
C	-4.650930 -0.182128 -0.186143
C	0.793967 -2.328842 -2.741838
C	-3.416918 -0.250010 -2.283231
C	-2.746279 4.400815 1.171347
C	-2.822566 3.417940 2.171478
C	2.763715 -1.155058 0.984532
C	1.216692 -2.769506 -1.442960
C	-1.989407 2.709427 -0.415602
C	1.269916 3.752255 2.829667
C	4.325303 0.936290 -3.269893
C	-5.861770 -0.227613 -0.896612
C	-2.038188 -1.054876 1.588829
C	-1.344912 -1.566647 3.887130
C	-1.104127 -2.802616 -1.482431
C	-4.632140 -0.281077 -2.992235
C	3.180798 0.807582 -1.112730
C	-2.983556 -2.976923 2.785525
C	5.290313 1.796515 -2.719766
C	4.155695 -1.360896 0.863234

E_g(BP86/SVP) = -2820.0811259
G_g(BP86/SVP) = -2819.538126
E_s(M06//TZVP//BP86/SVP) = -2820.5350636

C	4.149119	1.683760	-0.569100
C	-2.212284	-2.673481	3.919791
C	-2.329374	4.039756	-0.122665
C	1.595373	1.501722	1.148848
C	-3.414530	-0.216849	-0.872622
C	1.901142	1.416426	2.524908
C	1.731894	2.536523	3.360854
C	4.080858	-3.113816	2.559746
C	5.197820	2.171739	-1.367316
C	4.806214	-2.337264	1.641348
H	0.032469	-3.479628	0.367648
H	-3.529429	-2.422676	0.763944
H	-0.545702	0.074969	2.719089
H	-2.586549	1.326038	2.677050
H	2.493411	-0.188153	-2.911716
H	2.111748	-3.520449	3.403338
H	-6.806623	-0.312246	-2.858724
H	0.951122	-1.823052	1.990329
H	0.604052	4.791939	1.034465
H	0.885081	2.797985	-0.450928
H	-4.673032	-0.108558	0.912641
H	-2.456077	-0.205621	-2.820299
H	-3.016003	5.444893	1.398294
H	-3.151562	3.686297	3.188446
H	-1.644274	2.433101	-1.426548
H	1.145228	4.630251	3.483376
H	4.378326	0.653291	-4.333359
H	-6.816981	-0.209083	-0.347443
H	-0.730625	-1.318082	4.767455
H	-2.152960	-2.943993	-1.192048
H	-4.617799	-0.296492	-4.003959
H	-3.664032	-3.843589	2.794764
H	6.109418	2.184353	-3.346543
H	4.741408	-0.759123	0.152723
H	4.084331	1.990723	0.486572
H	-2.285223	-3.296892	4.825040
H	-2.267601	4.800861	-0.917309
H	2.291805	0.478180	2.947400
H	1.978005	2.457734	4.432246
H	4.592394	-3.875517	3.169618
H	5.944781	2.853224	-0.929179
H	5.891615	-2.487840	1.525227
H	-1.288147	-2.073176	-3.615018
H	2.257434	-2.884838	-1.112911
H	1.443283	-2.056058	-3.582555

Ru	-1.894872	-0.263942	-0.165919
Cl	-1.777361	-2.605295	-0.270796
P	0.427493	0.014452	-0.010512
C	-2.928579	1.323170	-1.181684
C	-3.052117	0.991197	1.120422
C	0.423047	-1.315240	2.475344
C	1.100336	4.068992	-0.555777
C	0.757503	2.721101	-0.748390
C	1.826062	-2.086018	-3.301215
C	1.065075	-1.650139	-2.203266
C	-3.889818	0.251292	-0.928190
C	0.978554	1.767278	0.274148
C	-3.970309	0.051936	0.479361
C	2.970598	-1.373770	-3.701882
C	0.988591	-1.997340	3.566515
C	-2.470586	1.822658	0.091340
C	1.229398	-0.912365	1.389111
C	2.363093	-2.291257	3.577602
C	1.538855	2.196839	1.495705
C	2.608713	-1.215663	1.403520
C	1.449506	-0.494223	-1.485546
C	2.603361	0.215737	-1.890113
C	3.356809	-0.222777	-2.993876
C	1.656655	4.489152	0.667417
C	3.170848	-1.901341	2.493747
C	1.871365	3.551127	1.690437
H	-2.900260	1.105027	2.202127
H	-0.658561	-1.103857	2.445386
H	0.930691	4.796989	-1.365322
H	0.317697	2.401008	-1.707382
H	1.515776	-2.989519	-3.850145
H	0.167993	-2.209553	-1.889339
H	3.560884	-1.714794	-4.567505
H	0.347846	-2.311786	4.405697
H	-1.770757	2.652683	0.249525
H	2.805511	-2.834013	4.428287
H	1.720144	1.469945	2.302479
H	3.246994	-0.923844	0.554720
H	2.918113	1.119355	-1.345795
H	4.252701	0.341198	-3.299918
H	1.922438	5.547225	0.820110
H	4.246794	-2.138829	2.492816
H	2.306696	3.870590	2.650874
H	-2.665315	1.726045	-2.168693
H	-4.409722	-0.338819	-1.694522
H	-4.560292	-0.720455	0.989887

E_g(BP86/SVP) = -1784.3234915
G_g(BP86/SVP) = -1784.030613
E_s(M06//TZVP//BP86/SVP) = -1784.030613

C				$E_g(\text{BP86/SVP}) = -2016.6251266$ $G_g(\text{BP86/SVP}) = -2016.225951$ $E_s(\text{M06//TZVP//BP86/SVP}) = -2016.9442678$
Ru	1.308021	-0.710939	0.070683	
Cl	1.498704	0.448401	2.233972	
P	-0.870037	0.110561	-0.046114	
C	2.947826	-2.261277	0.377018	
C	1.057957	-2.642938	-0.961277	
C	-1.589484	-0.917476	2.512449	
C	-2.157359	-1.547357	-3.638182	
C	-1.430141	-0.852708	-2.657916	
C	-0.596535	4.227819	0.104980	
C	-0.468166	2.854221	0.366949	
C	1.840443	-2.622867	1.224934	
C	-1.894245	-0.789317	-1.321349	
C	0.691422	-2.885758	0.417672	
C	-1.345391	4.674496	-0.999334	
C	-2.417663	-1.051279	3.640579	
C	2.458477	-2.273751	-0.974067	
C	-1.927961	-0.017885	1.480734	
C	-3.587789	-0.281531	3.754427	
C	-3.093782	-1.457666	-0.991704	
C	-3.100786	0.761695	1.606755	
C	-1.096183	1.907270	-0.478311	
C	-1.849268	2.360553	-1.583093	
C	-1.970472	3.739193	-1.840767	
C	-3.351206	-2.210466	-3.298377	
C	-3.926242	0.627445	2.735979	
C	-3.812187	-2.166947	-1.972937	
H	0.417291	-2.804472	-1.836603	
H	-0.655046	-1.490893	2.439528	
H	-1.784147	-1.575786	-4.674530	
H	-0.485967	-0.359388	-2.933467	
H	-0.104965	4.955044	0.770767	
H	0.119176	2.504917	1.233313	
H	-1.442129	5.752893	-1.202919	
H	-2.136222	-1.752047	4.442622	
H	3.055729	-2.071462	-1.872676	
H	-4.232242	-0.382361	4.642320	
H	-3.474125	-1.428556	0.040209	
H	-3.372135	1.481271	0.818444	
H	-2.351504	1.638851	-2.245282	
H	-2.561978	4.080507	-2.705475	
H	-3.917018	-2.762091	-4.065852	
H	-4.836762	1.241814	2.821771	
H	-4.742286	-2.687067	-1.693109	
C	1.703902	0.554660	-1.677463	
C	2.487753	1.009647	-0.579383	
H	0.856955	1.177101	-2.011864	
H	2.179102	-0.020307	-2.493146	
H	2.120246	1.905724	-0.045747	
C	3.996083	0.838678	-0.472231	
H	4.299101	-0.035689	-1.103716	
C	4.726139	2.077457	-1.019366	
H	4.416687	2.987261	-0.463572	
H	5.821525	1.955181	-0.891427	
H	4.510741	2.229063	-2.098116	
O	4.424359	0.607027	0.869795	
H	3.612972	0.550973	1.430659	
H	3.959966	-1.997842	0.707504	
H	1.870973	-2.648310	2.322315	
H	-0.289999	-3.223936	0.773477	

D				E _g (BP86/SVP) = -2249.5470861 G _g (BP86/SVP) = -2249.041358 E _s (M06//TZVP//BP86/SVP) = -2249.9995086
Ru	0.294253	-1.351667	-0.378387	
Cl	-0.290199	-0.165412	-2.483020	
P	1.709988	0.407337	0.066669	
C	-0.348012	-3.484310	-0.793088	
C	1.493613	-2.931931	0.548912	
C	3.059073	0.144559	-2.430502	
C	3.012858	-0.473366	3.915992	
C	2.238775	-0.085597	2.810867	
C	-0.583462	3.848689	-0.068937	
C	-0.030361	2.581804	-0.318437	
C	0.769517	-3.184777	-1.650426	
C	2.818606	0.028434	1.523099	
C	1.907428	-2.863625	-0.844534	
C	-0.097377	4.644645	0.983848	
C	4.009979	0.484498	-3.410510	
C	0.104997	-3.320350	0.568671	
C	2.962329	0.893708	-1.240259	
C	4.870539	1.577900	-3.214759	
C	4.189381	-0.278543	1.375098	
C	3.818479	2.003839	-1.058440	
C	1.023510	2.094378	0.490529	
C	1.508730	2.898421	1.546323	
C	0.949845	4.166816	1.789952	
C	4.378850	-0.775981	3.756768	
C	4.770554	2.340014	-2.036023	
C	4.960523	-0.683066	2.481911	
H	2.138941	-2.793417	1.426089	
H	2.347905	-0.679369	-2.590717	
H	2.541713	-0.547033	4.909734	
H	1.166137	0.122114	2.945333	
H	-1.412896	4.207841	-0.698798	
H	-0.412910	1.953828	-1.142855	
H	-0.540977	5.634191	1.181480	
H	4.065842	-0.103842	-4.340927	
H	-0.500743	-3.484361	1.468484	
H	5.612159	1.845630	-3.985394	
H	4.662425	-0.202603	0.383973	
H	3.738217	2.616892	-0.146525	
H	2.323616	2.533915	2.191290	
H	1.335240	4.781163	2.620522	
H	4.983978	-1.087611	4.623611	
H	5.432515	3.207496	-1.878858	
H	6.027173	-0.923902	2.341361	
C	-0.953740	-0.515896	1.252236	
C	-1.870979	-0.659750	0.179945	
H	-0.650113	0.501700	1.555220	
H	-1.012577	-1.218687	2.105362	
H	-2.001996	0.201731	-0.492518	
C	-3.172049	-1.494022	0.185650	
H	-3.341041	-1.882515	-0.865944	
O	-4.073938	-0.543486	0.579455	
H	-5.083371	-0.003311	-0.449666	
C	-6.784099	0.920758	-0.090511	
C	-7.956383	1.498563	-0.907730	
H	-8.741811	1.942821	-0.257403	
H	-7.583844	2.282371	-1.601443	
H	-8.416565	0.697028	-1.524233	
C	-6.106443	2.040408	0.742349	
H	-5.228922	1.610932	1.268409	
H	-5.738493	2.839425	0.063428	
H	-6.793383	2.499312	1.489689	
C	-7.288283	-0.194812	0.862075	
H	-7.789107	-0.991798	0.271114	
H	-6.404717	-0.643763	1.362249	
H	-8.003053	0.179516	1.630054	
O	-5.866256	0.384113	-1.016723	
C	-3.216215	-2.722404	1.125173	
H	-2.593051	-3.582978	0.796420	
H	-2.931896	-2.438540	2.162312	
H	-4.270784	-3.065735	1.163767	
H	-1.356820	-3.762392	-1.119832	
H	2.917242	-2.637652	-1.210311	
H	0.732848	-3.152108	-2.747466	

DE				E _g (BP86/SVP) = -2249.5398527 G _g (BP86/SVP) = -2249.032508 E _s (M06//TZVP//BP86/SVP) = -2249.9860611
Ru	0.503028	-0.228932	0.014217	
Cl	0.513489	1.349325	1.901214	
P	-1.721585	-0.008476	-0.037362	
C	2.417110	-1.931893	0.813967	
C	0.698288	-2.412545	-0.668897	
C	-2.089066	-0.490997	2.752259	
C	-2.895401	-2.657755	-3.040870	
C	-2.273518	-1.629011	-2.313774	
C	-2.464557	3.995519	-0.744815	
C	-1.991692	2.775268	-0.233995	
C	1.159983	-1.972136	1.536630	
C	-2.640912	-1.358305	-0.972864	
C	0.127182	-2.405956	0.654669	
C	-3.352198	4.015381	-1.836661	
C	-2.815708	-0.532848	3.955872	
C	2.130764	-2.199761	-0.527222	
C	-2.684949	0.004612	1.574256	
C	-4.142157	-0.069848	4.001032	
C	-3.628435	-2.174870	-0.376733	
C	-4.014319	0.480958	1.630823	
C	-2.414266	1.550684	-0.806873	
C	-3.304459	1.577352	-1.901839	
C	-3.768419	2.804211	-2.414782	
C	-3.881139	-3.459423	-2.436221	
C	-4.739706	0.441236	2.834801	
C	-4.237945	-3.217894	-1.099598	
H	0.190141	-2.759334	-1.577777	
H	-1.037548	-0.807549	2.722235	
H	-2.597393	-2.840759	-4.086332	
H	-1.480786	-1.030338	-2.787307	
H	-2.127982	4.940443	-0.287888	
H	-1.285025	2.753016	0.615456	
H	-3.716594	4.975221	-2.238531	
H	-2.331646	-0.915143	4.869257	
H	2.844653	-2.110481	-1.354443	
H	-4.707351	-0.096350	4.947365	
H	-3.928294	-1.997629	0.667042	
H	-4.488826	0.889883	0.724349	
H	-3.648378	0.635388	-2.356280	
H	-4.462906	2.808734	-3.271300	
H	-4.361358	-4.273587	-3.003210	
H	-5.775788	0.817518	2.861415	
H	-5.000681	-3.844456	-0.608338	
C	0.606618	0.507561	-2.009446	
C	1.077325	1.544715	-1.152595	
H	-0.349291	0.649305	-2.549128	
H	1.353775	-0.102646	-2.548785	
H	0.420938	2.414089	-0.962431	
C	2.593791	1.718978	-0.979822	
H	2.979904	2.033695	-2.005014	
O	3.090282	0.484937	-0.602430	
H	4.273736	0.291701	0.294595	
C	6.221733	-0.211897	0.081572	
C	7.308337	-0.837596	0.979844	
H	8.251173	-1.030135	0.422241	
H	7.531253	-0.159358	1.830703	
H	6.943537	-1.797840	1.401594	
C	6.733203	1.137090	-0.489454	
H	5.949866	1.593185	-1.129513	
H	6.945677	1.840477	0.343216	
H	7.658067	1.018685	-1.098352	
C	5.878402	-1.164031	-1.091637	
H	5.584215	-2.161424	-0.700377	
H	5.010080	-0.741340	-1.639693	
H	6.732488	-1.301709	-1.792010	
O	5.090060	0.002357	0.898351	
C	2.959369	2.876810	-0.024121	
H	4.063591	2.967782	0.046921	
H	2.555454	3.850511	-0.387904	
H	2.556041	2.678373	0.988732	
H	3.379353	-1.558295	1.194471	
H	-0.895749	-2.697311	0.926070	
H	1.050626	-1.790698	2.614761	

E				E _g (BP86/SVP) = -2249.5444764 G _g (BP86/SVP) = -2249.038648 E _s (M06//TZVP//BP86/SVP) = -2249.9850598
44	0.650183	0.416184	-0.869881	
17	1.628877	1.135671	1.282949	
15	-1.347662	0.012802	0.206720	
6	0.412723	-3.040312	-1.293505	
6	0.784160	-1.082083	-2.469355	
6	-0.212685	-1.674828	2.191890	
6	-4.242789	-1.326726	-2.481967	
6	-3.229659	-0.596553	-1.840913	
6	-2.188788	3.819002	1.651704	
6	-1.561229	2.614084	1.292845	
6	-0.629800	-2.921882	-2.289985	
6	-2.733916	-0.990579	-0.574917	
6	-0.414174	-1.747668	-2.994761	
6	-3.550570	4.028352	1.365860	
6	-0.131977	-2.312727	3.442397	
6	1.297521	-1.960837	-1.420824	
6	-1.277797	-0.795511	1.901415	
6	-1.108499	-2.073162	4.425078	
6	-3.261871	-2.161487	0.009553	
6	-2.252447	-0.557905	2.896045	
6	-2.290881	1.584570	0.648986	
6	-3.660280	1.800940	0.375783	
6	-4.282945	3.014736	0.726015	
6	-4.763660	-2.490777	-1.885769	
6	-2.169271	-1.191982	4.148670	
6	-4.262164	-2.908252	-0.642091	
1	1.473234	-0.521933	-3.125426	
1	0.563662	-1.852001	1.432335	
1	-4.618160	-0.992591	-3.463454	
1	-2.808684	0.293038	-2.334509	
1	-1.602337	4.604336	2.156686	
1	-0.491815	2.455213	1.516541	
1	-4.038407	4.978142	1.641245	
1	0.713067	-2.988602	3.651241	
1	2.253503	-1.845188	-0.883729	
1	-1.038654	-2.565296	5.409442	
1	-2.885264	-2.499554	0.986509	
1	-3.085154	0.134103	2.692108	
1	-4.254562	1.012898	-0.111084	
1	-5.351991	3.162495	0.498269	
1	-5.551179	-3.071947	-2.392280	
1	-2.936633	-0.990666	4.914859	
1	-4.652862	-3.823539	-0.166859	
6	-0.305005	1.680831	-2.285247	
6	0.615529	2.433377	-1.475693	
1	-1.387984	1.865771	-2.158513	
1	-0.019537	1.420967	-3.322541	
1	0.252659	3.169952	-0.735680	
6	2.085506	2.430817	-1.912871	
1	2.151433	2.736877	-3.000323	
8	2.449368	1.072409	-1.756617	
1	3.198203	-0.488197	1.042630	
6	5.127244	-0.845476	0.746343	
6	6.045195	-2.016010	1.139951	
1	7.106280	-1.794224	0.898537	
1	5.963484	-2.223952	2.227728	
1	5.745484	-2.934087	0.592694	
6	5.487049	0.415773	1.560949	
1	4.792185	1.243319	1.308187	
1	5.394592	0.210874	2.648525	
1	6.524827	0.755164	1.352436	
6	5.227746	-0.557297	-0.766410	
1	5.044534	-1.488534	-1.343453	
1	4.456625	0.183132	-1.075631	
1	6.234898	-0.173488	-1.042679	
8	3.799367	-1.275739	1.082010	
6	2.979723	3.390401	-1.114247	
1	4.038643	3.268680	-1.426251	
1	2.687468	4.451349	-1.289722	
1	2.904038	3.163329	-0.030994	
1	0.496103	-3.854536	-0.556073	
1	-1.048691	-1.349627	-3.800296	
1	-1.488867	-3.600506	-2.398365	

EF				E _g (BP86/SVP) = -2249.5586489 G _g (BP86/SVP) = -2249.049806 E _s (M06//TZVP//BP86/SVP) = -2250.0107191
Ru	1.555122	-1.638544	-0.444567	
Cl	-3.096730	-1.518468	0.791925	
P	1.045978	0.667378	-0.058375	
C	0.853674	-3.670271	-0.971984	
C	0.892956	-1.959012	-2.585883	
C	-1.603664	1.110948	-0.918911	
C	4.076118	3.553583	0.387908	
C	2.943636	2.754561	0.638293	
C	-0.304922	0.619982	3.864261	
C	0.253850	0.245524	2.627220	
C	-0.298747	-2.827107	-0.738262	
C	2.492648	1.824640	-0.322392	
C	-0.257245	-1.784207	-1.722289	
C	-0.765634	1.929164	4.074550	
C	-2.627076	1.637294	-1.728436	
C	1.572140	-3.131536	-2.103038	
C	-0.249621	1.442902	-1.168997	
C	-2.313470	2.515031	-2.782555	
C	3.217805	1.703440	-1.533784	
C	0.055687	2.325852	-2.228094	
C	0.356834	1.197845	1.591231	
C	-0.129253	2.511513	1.797413	
C	-0.678817	2.876577	3.036528	
C	4.770056	3.445283	-0.828319	
C	-0.973170	2.860432	-3.027232	
C	4.335125	2.514099	-1.790631	
H	1.142338	-1.370070	-3.476545	
H	-1.896947	0.401009	-0.114741	
H	4.416410	4.266804	1.156735	
H	2.411343	2.851210	1.596832	
H	-0.394628	-0.132597	4.664304	
H	0.613563	-0.788143	2.443022	
H	-1.211786	2.211935	5.042496	
H	-3.666714	1.318756	-1.529398	
H	2.488948	-3.558146	-2.532098	
H	-3.116128	2.927595	-3.416451	
H	2.909607	0.936845	-2.265418	
H	1.096790	2.617776	-2.431110	
H	-0.095852	3.248132	0.978344	
H	-1.058784	3.900659	3.186554	
H	5.654411	4.073836	-1.022647	
H	-0.716648	3.553002	-3.846623	
H	4.879481	2.407640	-2.743442	
C	3.700922	-2.180626	-0.480493	
C	3.569122	-1.102386	0.412506	
H	4.196743	-2.019765	-1.453525	
H	3.717478	-3.217289	-0.101825	
H	3.994691	-0.121129	0.154174	
C	3.075036	-1.385274	1.828702	
O	1.871662	-2.077286	1.621646	
H	-4.524521	-0.683508	-0.455474	
H	2.894322	-0.386913	2.329177	
C	-6.337940	-0.093138	0.029799	
C	-5.867621	0.755381	1.233708	
H	-6.653989	0.841721	2.016479	
H	-4.962692	0.281795	1.670941	
H	-5.595212	1.778838	0.897778	
C	-6.749160	-1.504611	0.510129	
H	-7.091684	-2.113798	-0.353510	
H	-5.860098	-2.000874	0.954492	
H	-7.565388	-1.469069	1.265399	
C	-7.504309	0.593936	-0.701022	
H	-7.195555	1.598539	-1.060575	
H	-7.807335	-0.005504	-1.585612	
H	-8.385659	0.715011	-0.035234	
O	-5.284985	-0.210963	-0.928249	
H	1.142613	-4.551067	-0.384252	
H	-1.018928	-1.001652	-1.806301	
H	-1.097170	-2.902687	0.019894	
C	4.049084	-2.164262	2.728971	
H	4.975819	-1.580260	2.925633	
H	3.563387	-2.384321	3.703295	
H	4.329460	-3.132447	2.262528	

F				E _g (BP86/SVP) = -1555.8500596 G _g (BP86/SVP) = -1555.459651 E _s (M06//TZVP//BP86/SVP) = -1556.0666373
Ru	-1.763266	0.310719	-0.082646	
P	0.590985	0.041147	-0.010462	
C	-3.608575	1.289465	0.666110	
C	-1.969626	2.552511	-0.447565	
C	0.324681	-0.858981	2.645306	
C	1.803267	3.626506	-1.748923	
C	1.191245	2.388804	-1.489766	
C	2.467625	-3.313993	-1.651003	
C	1.831526	-2.420909	-0.771110	
C	-2.523119	1.518137	1.595350	
C	1.458982	1.679818	-0.293758	
C	-1.514449	2.273964	0.902972	
C	2.818715	-2.904952	-2.948782	
C	0.777907	-1.301598	3.903153	
C	-3.248069	1.922743	-0.581290	
C	1.253630	-0.537646	1.631789	
C	2.153084	-1.428298	4.157968	
C	2.322707	2.271834	0.653893	
C	2.638459	-0.698132	1.884210	
C	1.536154	-1.095559	-1.170196	
C	1.893660	-0.697713	-2.478507	
C	2.529534	-1.592128	-3.357463	
C	2.673730	4.197739	-0.803294	
C	3.083782	-1.132791	3.143107	
C	2.920745	3.521061	0.401757	
H	-1.461685	3.175176	-1.191804	
H	-0.751234	-0.825105	2.402141	
H	1.587694	4.154067	-2.692076	
H	0.467249	1.979111	-2.211171	
H	2.690811	-4.338774	-1.313285	
H	1.574109	-2.761265	0.243215	
H	3.317910	-3.605092	-3.637276	
H	0.044972	-1.561066	4.683917	
H	-3.868478	1.933964	-1.487171	
H	2.504718	-1.772790	5.143952	
H	2.527583	1.762826	1.606815	
H	3.373733	-0.490737	1.090195	
H	1.690538	0.326231	-2.822808	
H	2.804162	-1.253411	-4.369384	
H	3.146767	5.172644	-1.001392	
H	4.163433	-1.246780	3.332152	
H	3.585077	3.965560	1.160183	
C	-2.808221	-0.712912	-1.761456	
C	-1.689439	-1.492205	-1.427942	
H	-2.813558	-0.147649	-2.708560	
H	-3.798879	-0.949283	-1.337960	
H	-0.839931	-1.557311	-2.127527	
C	-1.762757	-2.419795	-0.211276	
O	-2.116589	-1.549730	0.839226	
H	-0.733041	-2.847097	-0.053099	
C	-2.730017	-3.604434	-0.341135	
H	-2.406918	-4.303763	-1.142846	
H	-2.763880	-4.165943	0.616004	
H	-3.758927	-3.254709	-0.567219	
H	-4.529184	0.730179	0.872722	
H	-0.571101	2.625275	1.340386	
H	-2.481272	1.181497	2.638563	

FG				E _g (BP86/SVP) = -1555.8533918 G _g (BP86/SVP) = -1555.466518 E _s (M06//TZVP//BP86/SVP) = -1556.0717804
Ru	1.854561	0.286410	-0.040306	
P	-0.512844	0.124865	0.024464	
C	3.842170	1.276454	-0.376438	
C	2.209409	2.522188	0.732279	
C	-0.679646	-1.426365	-2.350179	
C	-1.782955	4.110843	-0.079149	
C	-1.158767	2.904280	0.278267	
C	-1.967645	-1.984173	3.317941	
C	-1.380005	-1.640659	2.087702	
C	2.906881	1.727736	-1.367273	
C	-1.372267	1.719658	-0.467980	
C	1.866623	2.438939	-0.682204	
C	-2.562970	-1.002583	4.128500	
C	-1.310670	-2.253799	-3.295323	
C	3.400072	1.790433	0.917888	
C	-1.334971	-1.071216	-1.153139	
C	-2.605697	-2.741981	-3.052914	
C	-2.216241	1.790737	-1.598667	
C	-2.641590	-1.558153	-0.921396	
C	-1.377429	-0.294003	1.642941	
C	-1.995762	0.681866	2.457787	
C	-2.578497	0.331265	3.688883	
C	-2.622818	4.165459	-1.205771	
C	-3.268740	-2.391000	-1.863441	
C	-2.830235	3.002899	-1.965112	
H	1.658190	3.062686	1.510827	
H	0.341373	-1.051344	-2.527610	
H	-1.604605	5.015733	0.523770	
H	-0.482147	2.885838	1.145104	
H	-1.960106	-3.038475	3.638944	
H	-0.926437	-2.434261	1.467719	
H	-3.021440	-1.276758	5.092166	
H	-0.781783	-2.523384	-4.223622	
H	3.921729	1.644355	1.872757	
H	-3.098296	-3.397960	-3.788465	
H	-2.398607	0.892246	-2.205508	
H	-3.176045	-1.286053	0.001474	
H	-2.052101	1.729180	2.131007	
H	-3.057624	1.112140	4.301400	
H	-3.108160	5.112099	-1.491667	
H	-4.284200	-2.769321	-1.663959	
H	-3.480403	3.031592	-2.854222	
C	3.054032	-1.169760	1.046639	
C	1.752524	-1.731912	0.985889	
H	3.393763	-0.743474	2.004793	
H	3.862135	-1.586732	0.423177	
H	1.112739	-1.660778	1.879990	
C	1.432834	-2.912257	0.121402	
H	1.798390	-0.676814	-1.299854	
O	0.370174	-3.526005	0.254730	
C	2.474178	-3.420730	-0.871585	
H	3.233185	-4.020602	-0.323614	
H	1.974669	-4.082798	-1.603376	
H	3.001691	-2.600286	-1.395911	
H	4.772572	0.727615	-0.566303	
H	1.008236	2.920493	-1.163970	
H	2.972976	1.563090	-2.449670	

Ru	1.458818	-0.467204	0.240017	$E_g(\text{BP86/SVP}) = -1555.8807532$ $G_g(\text{BP86/SVP}) = -1555.497415$ $E_s(\text{M06//TZVP//BP86/SVP}) = -1556.1001174$
P	-0.742743	0.046648	0.001128	
C	3.336009	-1.690688	0.795717	
C	1.503682	-2.674702	-0.270718	
C	-1.295317	-0.380061	2.772323	
C	-1.739577	-2.304593	-3.268158	
C	-1.126245	-1.388779	-2.398022	
C	-1.107287	4.146957	-0.403092	
C	-0.824505	2.853255	0.063250	
C	2.315924	-1.905116	1.778934	
C	-1.655783	-1.151235	-1.105843	
C	1.178344	-2.505472	1.131672	
C	-1.751465	4.327432	-1.640921	
C	-2.093537	-0.353739	3.930678	
C	2.828029	-2.161911	-0.468882	
C	-1.801304	0.082480	1.540783	
C	-3.406929	0.140905	3.871455	
C	-2.794032	-1.880323	-0.698274	
C	-3.120945	0.591118	1.493339	
C	-1.186575	1.717928	-0.700490	
C	-1.835296	1.907521	-1.939261	
C	-2.114359	3.206418	-2.405336	
C	-2.876273	-3.023359	-2.852860	
C	-3.918025	0.616301	2.649611	
C	-3.394130	-2.814112	-1.564703	
H	0.865952	-3.148277	-1.027256	
H	-0.256003	-0.738411	2.820504	
H	-1.319719	-2.466290	-4.274051	
H	-0.213830	-0.860030	-2.716795	
H	-0.820772	5.019674	0.205049	
H	-0.327021	2.720850	1.037875	
H	-1.971375	5.342747	-2.007448	
H	-1.680194	-0.713267	4.886602	
H	3.373282	-2.152787	-1.421995	
H	-4.030957	0.166278	4.779085	
H	-3.217737	-1.727948	0.305677	
H	-3.526512	0.979880	0.545655	
H	-2.136049	1.038974	-2.544891	
H	-2.624570	3.338323	-3.373039	
H	-3.350981	-3.750347	-3.530897	
H	-4.942996	1.017224	2.597399	
H	-4.276224	-3.380177	-1.224642	
C	1.887173	0.705055	-1.530327	
C	2.342256	1.435352	-0.376488	
H	1.027424	1.113865	-2.089809	
H	2.618444	0.196400	-2.182392	
H	1.737058	2.287293	-0.026024	
C	3.760275	1.580789	0.072558	
H	1.218975	0.499633	1.490241	
O	4.044627	2.257799	1.061737	
C	4.879928	0.965899	-0.773472	
H	4.606197	0.010423	-1.260429	
H	5.129988	1.683846	-1.585247	
H	5.784309	0.834211	-0.148583	
H	4.328328	-1.263446	0.984030	
H	0.261346	-2.854258	1.623526	
H	2.399570	-1.659472	2.845413	

GH				E _g (BP86/SVP) = -1555.8510291 G _g (BP86/SVP) = -1555.466283 E _s (M06//TZVP//BP86/SVP) = -1556.0734132
Ru	1.816945	0.029135	0.268246	
P	-0.496584	-0.181956	-0.006688	
C	3.744093	-0.840382	1.040607	
C	2.554580	-2.096636	-0.546203	
C	-0.791519	-0.912426	2.737870	
C	-0.506585	-2.345828	-3.546462	
C	-0.299127	-1.373272	-2.554910	
C	-2.815431	3.238084	0.127904	
C	-1.954980	2.176817	0.444072	
C	2.624132	-1.435003	1.717786	
C	-0.867018	-1.517878	-1.265418	
C	1.858286	-2.152350	0.727250	
C	-3.353268	3.350355	-1.165490	
C	-1.506760	-1.296980	3.887628	
C	3.678865	-1.259976	-0.351278	
C	-1.451621	-0.735107	1.505958	
C	-2.893721	-1.505271	3.817713	
C	-1.613594	-2.682731	-0.986468	
C	-2.854329	-0.921189	1.451221	
C	-1.624994	1.204925	-0.527594	
C	-2.168239	1.323345	-1.823680	
C	-3.025152	2.393336	-2.138802	
C	-1.257732	-3.500821	-3.258240	
C	-3.566747	-1.311555	2.596540	
C	-1.800111	-3.669031	-1.974476	
H	2.248526	-2.586667	-1.477736	
H	0.289474	-0.713941	2.788009	
H	-0.067650	-2.206232	-4.547486	
H	0.331641	-0.497118	-2.775840	
H	-3.057538	3.989479	0.895903	
H	-1.534819	2.102702	1.459941	
H	-4.025054	4.186897	-1.415300	
H	-0.975285	-1.424723	4.844380	
H	4.408505	-0.983983	-1.124140	
H	-3.455551	-1.805266	4.716768	
H	-2.050260	-2.834171	0.011948	
H	-3.396381	-0.743332	0.508792	
H	-1.940563	0.571829	-2.594141	
H	-3.442931	2.471412	-3.155380	
H	-1.410980	-4.270327	-4.031501	
H	-4.657745	-1.454530	2.538122	
H	-2.377338	-4.575912	-1.732337	
C	2.973037	1.525361	-0.809985	
C	1.628052	1.964866	-0.930500	
H	3.455302	1.069127	-1.690052	
H	3.666124	2.062595	-0.140912	
H	1.086994	1.782275	-1.874118	
C	1.159769	3.229076	-0.274623	
H	1.509322	1.051538	1.452683	
O	0.210221	3.851113	-0.747807	
C	1.942482	3.803371	0.905607	
H	2.366464	3.021138	1.564451	
H	2.778296	4.422809	0.513326	
H	1.274866	4.471404	1.482482	
H	4.545971	-0.251540	1.501692	
H	0.956101	-2.745143	0.929396	
H	2.421704	-1.390400	2.794838	

H				E _g (BP86/SVP) = -1555.8743671 G _g (BP86/SVP) = -1555.48879 E _s (M06//TZVP//BP86/SVP) = -1556.0929596
Ru	-1.634149	-0.497733	-0.723896	
P	0.503406	-0.159495	-0.001849	
C	-3.700756	-1.488515	-0.921906	
C	-2.388940	-1.844833	0.972191	
C	1.484326	-2.379023	-1.542784	
C	-0.044556	0.184014	4.092034	
C	-0.122018	0.356701	2.699488	
C	2.333393	2.964379	-2.009400	
C	1.673654	1.769570	-1.679089	
C	-2.668663	-2.418704	-1.276230	
C	0.703048	-0.409244	1.838628	
C	-1.843906	-2.639609	-0.111040	
C	2.701515	3.870738	-0.997037	
C	2.483021	-3.218743	-2.070892	
C	-3.525122	-1.144995	0.468949	
C	1.821727	-1.291799	-0.712301	
C	3.835257	-2.978872	-1.777081	
C	1.571431	-1.370778	2.401437	
C	3.188665	-1.052000	-0.432208	
C	1.374030	1.460125	-0.330364	
C	1.743997	2.374443	0.677686	
C	2.403128	3.572715	0.342775	
C	0.828778	-0.770369	4.645963	
C	4.185602	-1.890295	-0.956998	
C	1.628342	-1.552087	3.796341	
H	-2.007400	-1.805209	2.000010	
H	0.426756	-2.549010	-1.794335	
H	-0.682880	0.798028	4.747563	
H	-0.838060	1.086818	2.282833	
H	2.564570	3.187392	-3.063435	
H	1.401283	1.058546	-2.476277	
H	3.220065	4.807929	-1.254673	
H	2.199371	-4.060622	-2.722793	
H	-4.153872	-0.453719	1.045245	
H	4.618319	-3.632923	-2.192998	
H	2.207047	-1.991446	1.752578	
H	3.477673	-0.195355	0.197216	
H	1.522837	2.153149	1.732654	
H	2.688091	4.275941	1.141683	
H	0.879612	-0.908958	5.737912	
H	5.244482	-1.687131	-0.729570	
H	2.306515	-2.311783	4.217522	
C	-2.020988	1.203782	-2.006358	
C	-2.370843	1.561626	-0.660023	
H	-2.812259	0.969598	-2.740549	
H	-1.130972	1.666949	-2.462908	
H	-3.424511	1.422531	-0.351901	
C	-1.786248	2.678569	0.153472	
H	-0.814767	-0.701729	-2.074388	
O	-1.912624	2.712041	1.381291	
C	-1.169789	3.853245	-0.592606	
H	-0.344754	3.530836	-1.259014	
H	-1.942561	4.314162	-1.245926	
H	-0.798165	4.602257	0.130987	
H	-4.494217	-1.120961	-1.585682	
H	-1.020271	-3.359260	-0.023510	
H	-2.548006	-2.899945	-2.255301	

H1				E _g (BP86/SVP) = -1555.860287 G _g (BP86/SVP) = -1555.472772 E _s (M06//TZVP//BP86/SVP) = -1555.472772
Ru	-1.666415	-0.449001	-0.706253	
P	0.500669	-0.178033	0.019169	
C	-3.104974	-2.053131	-1.407540	
C	-3.091540	-1.232030	0.780331	
C	1.440518	-2.353039	-1.574744	
C	-0.236778	0.270864	4.069052	
C	-0.223026	0.424467	2.672236	
C	2.586796	2.828751	-1.928991	
C	1.856152	1.670038	-1.618703	
C	-2.031049	-2.705251	-0.716762	
C	0.610835	-0.396370	1.871374	
C	-2.001381	-2.163773	0.626960	
C	2.942523	3.732597	-0.910139	
C	2.408753	-3.225055	-2.107782	
C	-3.774817	-1.164593	-0.492809	
C	1.800202	-1.364322	-0.638522	
C	3.751309	-3.114151	-1.710483	
C	1.393377	-1.390990	2.498489	
C	3.159099	-1.246924	-0.259254	
C	1.467468	1.394748	-0.285277	
C	1.828051	2.306707	0.728710	
C	2.560924	3.467168	0.415450	
C	0.550556	-0.718304	4.686922	
C	4.124735	-2.119867	-0.786285	
C	1.357778	-1.552814	3.896859	
H	-3.362496	-0.698280	1.699346	
H	0.386842	-2.409171	-1.892938	
H	-0.881698	0.926032	4.676539	
H	-0.878191	1.180863	2.206193	
H	2.886958	3.023331	-2.971268	
H	1.602352	0.956333	-2.420298	
H	3.518319	4.640405	-1.150751	
H	2.111235	-3.990537	-2.842682	
H	-4.657523	-0.552522	-0.722061	
H	4.511417	-3.794595	-2.126860	
H	2.029822	-2.057301	1.897123	
H	3.467638	-0.458432	0.445899	
H	1.541771	2.111447	1.773007	
H	2.837753	4.166799	1.220410	
H	0.527189	-0.843535	5.781393	
H	5.178388	-2.017985	-0.479925	
H	1.968240	-2.340383	4.367591	
C	-1.813754	1.280597	-2.178979	
C	-2.262940	1.607756	-0.801655	
H	-2.604271	1.193404	-2.949781	
H	-0.968523	1.889583	-2.556641	
H	-3.354389	1.548934	-0.623360	
C	-1.728488	2.746279	0.009503	
H	-1.233097	0.146613	-2.298961	
O	-1.986862	2.838421	1.214199	
C	-0.977615	3.871135	-0.698441	
H	-0.077716	3.506554	-1.233115	
H	-1.640859	4.335815	-1.460870	
H	-0.679147	4.634756	0.043542	
H	-3.386642	-2.220345	-2.456435	
H	-1.306216	-2.461985	1.422682	
H	-1.386313	-3.499593	-1.110900	

I				E _g (BP86/SVP) = -1555.457179 G _g (BP86/SVP) = -1555.488792 E _s (M06//TZVP//BP86/SVP) = -1556.09296
Ru	-1.634068	-0.497793	-0.724123	
P	0.503399	-0.159475	-0.001797	
C	-3.700757	-1.488426	-0.921488	
C	-2.387841	-1.845818	0.971607	
C	1.484756	-2.378384	-1.543320	
C	-0.044785	0.183338	4.092120	
C	-0.122158	0.356328	2.699608	
C	2.333022	2.964853	-2.008923	
C	1.673415	1.769934	-1.678748	
C	-2.668875	-2.418414	-1.276965	
C	0.702900	-0.409501	1.838642	
C	-1.843435	-2.639978	-0.112388	
C	2.701001	3.871160	-0.996460	
C	2.483615	-3.217819	-2.071581	
C	-3.524324	-1.145701	0.469481	
C	1.821927	-1.291464	-0.712353	
C	3.835772	-2.977953	-1.777429	
C	1.571157	-1.371251	2.401296	
C	3.188799	-1.051645	-0.431928	
C	1.373796	1.460318	-0.330059	
C	1.743629	2.374576	0.678092	
C	2.402613	3.572967	0.343313	
C	0.828438	-0.771230	4.645903	
C	4.185889	-1.889656	-0.956868	
C	1.627975	-1.552853	3.796165	
H	-2.005623	-1.806693	1.999193	
H	0.427237	-2.548329	-1.795116	
H	-0.683099	0.797259	4.747747	
H	-0.838136	1.086570	2.283035	
H	2.564205	3.187996	-3.062930	
H	1.401144	1.058954	-2.476008	
H	3.219446	4.808438	-1.253989	
H	2.200143	-4.059467	-2.723858	
H	-4.152753	-0.454778	1.046550	
H	4.618970	-3.631772	-2.193452	
H	2.206743	-1.991859	1.752350	
H	3.477614	-0.195217	0.197878	
H	1.522479	2.153148	1.733034	
H	2.687460	4.276154	1.142297	
H	0.879200	-0.910034	5.737827	
H	5.244717	-1.686508	-0.729187	
H	2.306054	-2.312699	4.217227	
C	-2.021353	1.203978	-2.006095	
C	-2.370994	1.561477	-0.659620	
H	-2.812700	0.969787	-2.740205	
H	-1.131515	1.667439	-2.462687	
H	-3.424576	1.422192	-0.351277	
C	-1.786354	2.678448	0.153838	
H	-0.814522	-0.701123	-2.074642	
O	-1.912186	2.711716	1.381712	
C	-1.170481	3.853356	-0.592363	
H	-0.799582	4.602796	0.131159	
H	-0.344909	3.531193	-1.258240	
H	-1.943193	4.313556	-1.246243	
H	-4.494620	-1.120487	-1.584580	
H	-1.019887	-3.359838	-0.025713	
H	-2.548865	-2.899221	-2.256334	

IJ				E _g (BP86/SVP) = -1556.0939607 G _g (BP86/SVP) = -1555.457179 E _s (M06//TZVP//BP86/SVP) = -1555.457179
Ru	-1.710910	-0.363461	-0.516273	
P	0.587453	-0.117868	0.002972	
C	-3.498640	-1.405683	-1.197843	
C	-2.494408	-1.795292	0.876185	
C	1.286439	-2.132098	-1.881569	
C	-0.021549	-0.100164	4.096045	
C	-0.046541	0.212502	2.726123	
C	2.628598	3.086308	-1.647988	
C	1.881750	1.914797	-1.449167	
C	-2.316174	-2.244399	-1.386081	
C	0.722509	-0.548093	1.809234	
C	-1.771833	-2.576099	-0.091768	
C	3.113433	3.810449	-0.542052	
C	2.168314	-2.983011	-2.572707	
C	-3.600949	-1.118895	0.197972	
C	1.761612	-1.275969	-0.866926	
C	3.536739	-2.987563	-2.254443	
C	1.480699	-1.638896	2.287645	
C	3.144488	-1.272127	-0.567049	
C	1.614527	1.440587	-0.142739	
C	2.106004	2.170508	0.959478	
C	2.848727	3.349792	0.757890	
C	0.744428	-1.182464	4.567977	
C	4.022655	-2.128997	-1.250654	
C	1.487375	-1.954222	3.659510	
H	-2.294487	-1.760055	1.955368	
H	0.215386	-2.105473	-2.133743	
H	-0.619863	0.503390	4.797226	
H	-0.691081	1.036025	2.370806	
H	2.832262	3.437665	-2.672285	
H	1.506832	1.353854	-2.321807	
H	3.696538	4.732269	-0.696062	
H	1.783026	-3.640228	-3.368712	
H	-4.339716	-0.470154	0.686550	
H	4.228852	-3.652914	-2.794908	
H	2.067544	-2.254589	1.589212	
H	3.539598	-0.585972	0.198918	
H	1.914448	1.819074	1.984829	
H	3.225961	3.908764	1.629373	
H	0.754106	-1.428906	5.641782	
H	5.096537	-2.119265	-1.004250	
H	2.080800	-2.811470	4.016379	
C	-2.026640	2.123245	-2.425467	
C	-2.408374	1.636748	-1.023179	
H	-2.455337	3.127248	-2.659477	
H	-0.928967	2.200903	-2.570512	
H	-3.506298	1.480079	-0.947478	
C	-1.992524	2.446949	0.151745	
H	-2.405588	1.425869	-3.201733	
O	-2.379407	2.170956	1.306035	
C	-1.109629	3.672968	-0.065137	
H	-1.703908	4.451299	-0.593522	
H	-0.776818	4.076372	0.909675	
H	-0.231612	3.459582	-0.705568	
H	-4.159087	-1.040107	-1.995209	
H	-0.909005	-3.223407	0.108751	
H	-1.982825	-2.652471	-2.350657	

J				E _g (BP86/SVP) = -1555.8718277 G _g (BP86/SVP) = -1555.48365 E _s (M06//TZVP//BP86/SVP) = -1556.0939607
Ru	-1.724642	0.392294	-0.236176	
P	0.540590	-0.046442	0.001535	
C	-3.555164	1.640277	-0.483413	
C	-1.427784	2.507267	-0.903680	
C	0.381785	-0.512989	2.784307	
C	2.885357	2.798636	-2.013360	
C	2.145702	1.640196	-1.714055	
C	2.620695	-3.328999	-1.622173	
C	2.164997	-2.360514	-0.709908	
C	-2.920989	1.914190	0.791098	
C	1.612602	1.439243	-0.422077	
C	-1.611386	2.451778	0.540197	
C	2.180720	-3.310063	-2.957129	
C	0.870810	-0.739431	4.084785	
C	-2.611812	1.991580	-1.518591	
C	1.262928	-0.415243	1.689147	
C	2.252927	-0.860740	4.304266	
C	1.847270	2.425773	0.564035	
C	2.656029	-0.504856	1.925464	
C	1.259448	-1.356628	-1.119176	
C	0.796492	-1.366300	-2.457696	
C	1.264739	-2.326834	-3.370464	
C	3.104916	3.776982	-1.028244	
C	3.144872	-0.734890	3.222353	
C	2.583380	3.584885	0.263109	
H	-0.537549	2.881664	-1.423329	
H	-0.695611	-0.381476	2.595382	
H	3.297907	2.931790	-3.026477	
H	1.993200	0.881835	-2.496707	
H	3.324359	-4.106240	-1.282721	
H	2.509514	-2.404330	0.333566	
H	2.539747	-4.069235	-3.670359	
H	0.167346	-0.814027	4.929717	
H	-2.772236	1.869867	-2.597975	
H	2.639654	-1.038132	5.320657	
H	1.462800	2.279913	1.585868	
H	3.367423	-0.372097	1.094897	
H	0.035029	-0.635852	-2.772356	
H	0.893580	-2.316623	-4.407773	
H	3.685781	4.682914	-1.263732	
H	4.231458	-0.805886	3.391895	
H	2.735603	4.339393	1.047649	
C	-2.952875	-1.778570	2.164274	
C	-2.931919	-1.257793	0.744377	
H	-3.681275	-2.617168	2.266941	
H	-1.970180	-2.160716	2.502823	
H	-3.900425	-0.853918	0.402875	
C	-2.138713	-1.851430	-0.292745	
H	-3.273239	-0.992942	2.880362	
O	-2.194531	-1.323977	-1.490447	
C	-1.308390	-3.101036	-0.058728	
H	-0.679838	-3.036245	0.851240	
H	-2.002576	-3.957924	0.088021	
H	-0.665356	-3.311797	-0.931147	
H	-4.566723	1.244867	-0.640673	
H	-0.912676	2.827863	1.296317	
H	-3.373881	1.775042	1.781479	

JK				E _g (BP86/SVP) = -1788.1199111 G _g (BP86/SVP) = -1787.631289 E _s (M06//TZVP//BP86/SVP) = -1788.4454684
Ru	0.611572	-1.216218	-0.795661	
P	-0.933966	0.318949	0.046614	
C	2.160316	-1.405460	-2.405341	
C	-0.035090	-0.790427	-2.800239	
C	-3.131219	-1.137337	-1.008480	
C	0.801405	3.739593	-1.546323	
C	0.569086	2.514226	-0.901037	
C	-1.793832	0.588346	4.134259	
C	-1.833308	0.247576	2.771327	
C	1.384739	-2.604474	-2.365724	
C	-0.732419	1.962921	-0.838292	
C	-0.005748	-2.231572	-2.566787	
C	-0.865295	1.533894	4.601899	
C	-4.487814	-1.407428	-1.265812	
C	1.309990	-0.281685	-2.723057	
C	-2.751240	-0.032825	-0.219628	
C	-5.485035	-0.575519	-0.730752	
C	-1.786189	2.651516	-1.478512	
C	-3.764615	0.798282	0.317471	
C	-0.950345	0.851438	1.845437	
C	-0.019409	1.798124	2.328908	
C	0.021617	2.135510	3.692717	
C	-0.256842	4.423223	-2.171999	
C	-5.119579	0.527045	0.063772	
C	-1.546831	3.869165	-2.143876	
H	-0.925965	-0.200820	-3.057002	
H	-2.341898	-1.794387	-1.402019	
H	1.823829	4.150066	-1.567907	
H	1.414124	1.963591	-0.458693	
H	-2.496867	0.108680	4.834233	
H	-2.571629	-0.493529	2.428131	
H	-0.833858	1.801471	5.670060	
H	-4.765254	-2.277831	-1.881772	
H	1.623474	0.757982	-2.872754	
H	-6.548322	-0.787241	-0.926915	
H	-2.805667	2.239141	-1.471347	
H	-3.493866	1.662028	0.944965	
H	0.681500	2.285098	1.637074	
H	0.753093	2.880605	4.044695	
H	-0.073995	5.379061	-2.688581	
H	-5.895974	1.181958	0.491031	
H	-2.382055	4.385599	-2.644124	
C	-1.255272	-3.383539	0.904862	
C	0.161895	-3.035789	0.480671	
H	-1.275096	-4.249569	1.607547	
H	-1.780452	-2.541764	1.399150	
H	0.610565	-3.808575	-0.170311	
C	1.132556	-2.527343	1.420728	
H	-1.872359	-3.669432	0.029050	
O	2.384873	-2.519710	1.141362	
C	4.439340	2.759050	-0.559153	
C	3.962896	1.940563	0.397302	
H	4.511705	3.848143	-0.406036	
H	4.790184	2.366920	-1.530026	
H	3.621020	2.356825	1.364143	
C	3.909223	0.433331	0.307151	
H	4.113521	0.138919	-0.752609	
O	2.608489	-0.017999	0.706415	
H	2.690238	-0.993960	0.992538	
C	4.993011	-0.199851	1.200160	
H	4.862552	0.116090	2.256490	
H	4.926102	-1.306618	1.161320	
H	6.004690	0.107280	0.864702	
C	0.740665	-2.002205	2.793476	
H	-0.345792	-1.996270	2.989134	
H	1.232188	-2.659207	3.542764	
H	1.140264	-0.978837	2.946175	
H	3.240527	-1.353240	-2.211022	
H	-0.849635	-2.925977	-2.676943	
H	1.772625	-3.611247	-2.168258	

K				E _g (BP86/SVP) = -1788.143544 G _g (BP86/SVP) = -1787.652275 E _s (M06//TZVP//BP86/SVP) = -1788.4669051
Ru	1.160849	-0.576336	-0.872163	
P	-0.831290	0.251717	0.031675	
C	2.799195	-0.001465	-2.305937	
C	0.547433	0.060074	-2.855564	
C	-2.454759	-1.787715	-1.057017	
C	-1.145384	3.943107	-1.859893	
C	-0.700953	2.840768	-1.112433	
C	-0.453950	0.906126	4.139833	
C	-0.334267	0.374801	2.843010	
C	2.389045	-1.342180	-2.578863	
C	-1.501215	1.680353	-0.986971	
C	0.971869	-1.318011	-2.909223	
C	-1.196640	2.076946	4.367878	
C	-3.547965	-2.667846	-1.126702	
C	1.677834	0.886364	-2.488983	
C	-2.314132	-0.891899	0.027910	
C	-4.507528	-2.682970	-0.097376	
C	-2.756509	1.653589	-1.631030	
C	-3.286835	-0.909019	1.051548	
C	-0.963006	1.007790	1.746254	
C	-1.713717	2.183722	1.987432	
C	-1.827386	2.713139	3.285366	
C	-2.393997	3.901478	-2.508897	
C	-4.370832	-1.804519	0.990993	
C	-3.195282	2.754350	-2.393059	
H	-0.455049	0.429532	-3.107750	
H	-1.683841	-1.793648	-1.844242	
H	-0.512054	4.841556	-1.938158	
H	0.279211	2.877685	-0.611026	
H	0.046848	0.394956	4.977971	
H	0.265962	-0.535818	2.701740	
H	-1.283916	2.492564	5.384726	
H	-3.644529	-3.354398	-1.983256	
H	1.699044	1.979298	-2.419682	
H	-5.357825	-3.382104	-0.142546	
H	-3.404191	0.768889	-1.536307	
H	-3.198318	-0.221581	1.906593	
H	-2.223562	2.695470	1.157950	
H	-2.418173	3.629267	3.447578	
H	-2.740389	4.763470	-3.101080	
H	-5.115123	-1.812386	1.803646	
H	-4.176378	2.712132	-2.893116	
C	0.766364	-3.829461	-0.887883	
C	1.368844	-2.719950	-0.029667	
H	0.914624	-4.834673	-0.427034	
H	-0.323971	-3.703260	-1.045839	
H	2.477221	-2.713094	-0.069466	
C	0.946344	-2.651248	1.352059	
H	1.238498	-3.873199	-1.889080	
O	1.644125	-2.056710	2.245000	
C	4.199399	2.734702	-0.146802	
C	3.329270	2.068266	0.633489	
H	4.069870	3.804510	-0.376887	
H	5.086210	2.237560	-0.578392	
H	2.451631	2.585357	1.064339	
C	3.475781	0.628900	1.067840	
H	4.214545	0.117065	0.401894	
O	2.196525	-0.016891	0.977015	
H	2.148074	-0.881957	1.587636	
C	3.980198	0.540017	2.518985	
H	4.055409	-0.518374	2.842890	
H	4.982583	1.005858	2.604382	
H	3.286749	1.066148	3.206730	
C	-0.331731	-3.335127	1.802205	
H	-0.177454	-4.437041	1.792232	
H	-0.590042	-3.027750	2.832921	
H	-1.181489	-3.126675	1.122621	
H	3.805573	0.308050	-1.995507	
H	3.030935	-2.231744	-2.536318	
H	0.367163	-2.168323	-3.247237	

KL				E _g (BP86/SVP) = -1788.1338677 G _g (BP86/SVP) = -1787.649532 E _s (M06//TZVP//BP86/SVP) = -1788.4525456
Ru	-1.415561	-0.002284	-0.618651	
P	0.860172	-0.086847	0.040729	
C	-3.119810	0.203832	-2.010127	
C	-1.441116	-1.407645	-2.234219	
C	1.262100	2.536734	-0.933287	
C	2.077338	-3.542202	-1.901673	
C	1.443144	-2.624410	-1.048883	
C	1.234442	-0.454146	4.155005	
C	0.825068	-0.075391	2.865081	
C	-1.924226	0.849813	-2.546561	
C	1.786300	-1.251444	-1.082890	
C	-0.913788	-0.152204	-2.738718	
C	2.238462	-1.422627	4.330281	
C	1.962877	3.740426	-1.125461	
C	-2.813017	-1.179982	-1.815948	
C	1.814788	1.502653	-0.147911	
C	3.219717	3.927036	-0.523934	
C	2.769585	-0.818932	-1.997257	
C	3.076380	1.699246	0.458151	
C	1.422393	-0.662722	1.726075	
C	2.437299	-1.630263	1.909307	
C	2.839740	-2.007800	3.203272	
C	3.053550	-3.100503	-2.815153	
C	3.772646	2.905446	0.269788	
C	3.394114	-1.738815	-2.861796	
H	-0.925035	-2.375272	-2.250757	
H	0.264407	2.386587	-1.376781	
H	1.805803	-4.609143	-1.855271	
H	0.671528	-2.971810	-0.342035	
H	0.756341	0.013725	5.030520	
H	0.034556	0.682935	2.755329	
H	2.553049	-1.720205	5.343562	
H	1.519204	4.539866	-1.740265	
H	-3.479843	-1.944308	-1.395871	
H	3.766942	4.872617	-0.666991	
H	3.053702	0.244063	-2.034558	
H	3.515054	0.907976	1.086228	
H	2.926318	-2.093159	1.039278	
H	3.633275	-2.762544	3.326716	
H	3.546767	-3.818972	-3.488998	
H	4.753606	3.049433	0.750597	
H	4.157094	-1.384016	-3.573232	
C	-2.287397	3.982673	-0.521017	
C	-2.364819	2.804838	0.414757	
H	-3.280697	4.469300	-0.652831	
H	-1.587331	4.755718	-0.139925	
H	-3.089136	2.003264	0.183832	
C	-1.730083	2.791625	1.625985	
H	-1.942000	3.705857	-1.541713	
O	-1.780512	1.832091	2.559715	
H	-1.095994	3.653814	1.920641	
C	-3.849130	-3.462186	1.072467	
C	-2.987495	-2.565537	1.588686	
H	-3.656790	-4.546500	1.119784	
H	-4.795680	-3.145799	0.598243	
H	-2.050048	-2.907489	2.065829	
C	-3.196237	-1.070794	1.617671	
H	-4.050907	-0.791600	0.950262	
O	-2.011010	-0.358192	1.309115	
H	-1.968361	0.916722	2.090022	
H	-3.502477	-0.785090	2.657006	
H	-4.076323	0.695746	-1.789481	
H	0.082158	0.001937	-3.172503	
H	-1.841851	1.908050	-2.827736	

L				E _g (BP86/SVP) = -1788.1344193 G _g (BP86/SVP) = -1787.652087 E _s (M06//TZVP//BP86/SVP) = -1788.4525618
Ru	-0.920748	-1.048468	-0.603327	
P	1.000000	0.156512	0.066866	
C	-2.366895	-1.951962	-1.997127	
C	-0.198666	-2.769900	-1.688946	
C	0.144584	2.360125	-1.482590	
C	3.957151	-2.621668	-0.798567	
C	2.826213	-1.971900	-0.277061	
C	0.713505	1.326990	4.024232	
C	0.496386	1.154295	2.647541	
C	-1.430014	-1.075712	-2.695395	
C	2.542729	-0.627479	-0.619893	
C	-0.105340	-1.628336	-2.562088	
C	1.820632	0.729099	4.653274	
C	0.187945	3.681852	-1.960641	
C	-1.604506	-2.980942	-1.363353	
C	1.089010	1.911937	-0.535995	
C	1.172949	4.567637	-1.492153	
C	3.408994	0.040674	-1.512000	
C	2.070616	2.811430	-0.059460	
C	1.393686	0.376029	1.876974	
C	2.509353	-0.212621	2.512031	
C	2.719020	-0.036810	3.892329	
C	4.813998	-1.946628	-1.687604	
C	2.112369	4.130849	-0.539172	
C	4.533423	-0.617711	-2.044882	
H	0.634946	-3.414704	-1.383237	
H	-0.641400	1.663767	-1.819020	
H	4.167887	-3.664664	-0.512281	
H	2.150723	-2.514340	0.404181	
H	0.006467	1.937315	4.608637	
H	-0.369613	1.642024	2.174027	
H	1.985431	0.865276	5.734191	
H	-0.562200	4.022799	-2.691605	
H	-1.996198	-3.779870	-0.719794	
H	1.203921	5.605423	-1.861036	
H	3.205976	1.084127	-1.797116	
H	2.800436	2.479937	0.696360	
H	3.232421	-0.803834	1.930682	
H	3.597245	-0.499374	4.371056	
H	5.696818	-2.458602	-2.102297	
H	2.879630	4.825465	-0.161059	
H	5.195412	-0.081331	-2.743551	
C	-4.857863	2.612723	-1.560439	
C	-3.892328	1.928101	-0.630002	
H	-5.872976	2.154288	-1.526056	
H	-4.975213	3.687220	-1.304618	
H	-3.693268	0.852693	-0.794283	
C	-3.265671	2.558462	0.394233	
H	-4.531709	2.561150	-2.624725	
O	-2.400927	2.037221	1.295591	
H	-3.442716	3.635496	0.581542	
C	-3.209438	-3.635768	2.300773	
C	-2.654741	-2.413997	2.409003	
H	-2.927143	-4.462138	2.973429	
H	-3.982821	-3.852845	1.542464	
H	-1.883500	-2.219372	3.177290	
C	-3.015225	-1.222666	1.557728	
H	-3.690923	-1.538304	0.726315	
O	-1.849220	-0.552822	1.083180	
H	-2.212578	1.056819	1.126086	
H	-3.588931	-0.494139	2.183801	
H	-3.455668	-1.819358	-1.946749	
H	0.814409	-1.223448	-3.002096	
H	-1.702042	-0.194373	-3.291814	

LF				E _g (BP86/SVP) = -1555.825559 G _g (BP86/SVP) = -1555.441226 E _s (M06//TZVP//BP86/SVP) = -1556.0463736
Ru	1.434261	-0.699973	0.074179	
P	-0.761881	0.063535	-0.035769	
C	3.189398	-1.978148	0.539431	
C	1.217824	-2.869088	-0.406903	
C	-0.658369	0.677089	2.723218	
C	-2.767219	-2.912066	-2.103736	
C	-1.891874	-1.876146	-1.739646	
C	-0.523766	3.689534	-1.976886	
C	-0.313020	2.591121	-1.128544	
C	2.181247	-2.038099	1.570112	
C	-1.997992	-1.252274	-0.473046	
C	0.968401	-2.592753	0.987054	
C	-1.545433	3.653076	-2.944697	
C	-1.138549	1.209594	3.933376	
C	2.558706	-2.425856	-0.683874	
C	-1.422452	0.793710	1.543372	
C	-2.380707	1.865311	3.973842	
C	-2.986094	-1.706723	0.426717	
C	-2.662458	1.471773	1.585537	
C	-1.132545	1.441521	-1.234304	
C	-2.161681	1.412563	-2.199804	
C	-2.361525	2.514580	-3.052814	
C	-3.749466	-3.358165	-1.199309	
C	-3.140511	1.999054	2.796512	
C	-3.851229	-2.757332	0.065921	
H	0.514498	-3.317538	-1.118102	
H	0.330069	0.193500	2.670524	
H	-2.678189	-3.378666	-3.098013	
H	-1.109947	-1.546663	-2.443259	
H	0.117375	4.580832	-1.883596	
H	0.485389	2.597431	-0.365918	
H	-1.705631	4.513867	-3.613541	
H	-0.530311	1.120567	4.847762	
H	3.041694	-2.450738	-1.670736	
H	-2.754632	2.284371	4.921896	
H	-3.082805	-1.238385	1.418175	
H	-3.255861	1.596804	0.665204	
H	-2.816786	0.532329	-2.288012	
H	-3.166885	2.481124	-3.804333	
H	-4.431492	-4.175888	-1.481678	
H	-4.108888	2.524396	2.819792	
H	-4.613328	-3.103372	0.782552	
C	4.189933	0.535499	-1.940482	
C	3.092691	0.906936	-1.241818	
H	4.104621	-0.014790	-2.891459	
H	5.208580	0.770872	-1.590165	
H	2.086204	0.720214	-1.703863	
C	3.009639	1.669932	0.076848	
O	1.898997	1.195246	0.802738	
H	2.802123	2.745223	-0.194078	
C	4.311541	1.671808	0.893222	
H	4.615700	0.636632	1.151943	
H	5.146181	2.159089	0.344900	
H	4.148058	2.230068	1.836613	
H	4.225503	-1.638101	0.650416	
H	0.037195	-2.806097	1.529276	
H	2.313389	-1.751968	2.622643	

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