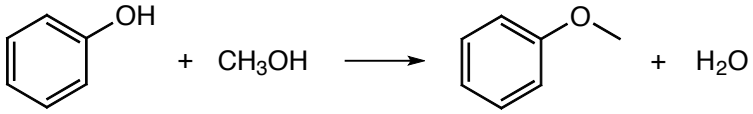
Intermediate Oxiranes in the Base-Catalyzed Depolymerisation of Lignin

T. Lankau, C.H. Yu

Supplementary Material

S.1 Method Evaluation

The well studied methoxybenzene (anisole) molecule is the smallest possible model for the βO4 link in lignin and has been used to benchmark systematically all combinations of different computational methods (HF, MP2, BLYP, OLYP, OPBE, BPBE, B3LYP, O3LYP, X3LYP, PBE1PBE, M05, M052X, M06L, M06, M062X, M06HF, B97D) with basis sets (6-31G(d,p), 6-31+G(d,p), 6-31++G(d,p), 6-311G(d,p), 6-311+G(d,p), 6-311++G(d,p), 6-311G(2d,p), 6-311+G(2d,p), 6-311++G(2d,p), cc-pVDZ, aug-cc-pVDZ, cc-pVTZ, aug-cc-pVTZ) of increasing size and complexity.



(S.1)

The geometries of H_2O, methanol, phenol and anisole have been fully optimised. Various properties (rotational constant, bond lengths, bond angles, dipole moment, frequencies, vertical and adiabatic ionisation energies)[1,2] have been calculated for the optimised geometries and were compared with their experimental counterparts. The enthalpy change for reaction S.1 in the gas phase has been calculated from listed values of the gas phase enthalpies of formation of the molecules involved and has been compared with the calculated values at the different computational levels. The unweighted geometric mean σ_{tot} of the relative differences between calculated x_i^{qm} and measured values x_i^{ref}

$$\sigma_{\mathrm{tot}} = \sqrt{\sum_{i=0}^{\text{properties}} \left(\frac{x_i^{\mathrm{ref}} - x_i^{\mathrm{qm}}}{x_i^{\mathrm{ref}}} \right)^2} \tag{S.2}$$

has been as a measure for the quality[3] of each combination of computational method with a basis set. The results for σ_{tot} are summarized in Table S.1 on page S.3. The evaluation of the resulting 221 data points shows that in average the M06 functional performs best ($\bar{\sigma}_{\mathrm{tot}} = 0.5728$) for the job at hand. The modest M06/6-31G(d,p) method offers an excellent quality to cost ratio and out-performs most methods with much bigger basis sets. The inclusion of diffuse functions into the basis set showed little influence on the acid catalysed version of reaction S.1, but a big one ($\sim$ 20 kJ mol^{-1}) on the base catalysed version independent of the chosen method (B97D, M05, M06L, M06, M06 2X). A difference of 0.3 kJ mol^{-1} in Gibbs free energy of the transition states between the M06/6-31+G(d,p) and M06/6-31++G(d,p) calculations suggests

[1] Computational Chemistry Comparison and Benchmark DataBase, NIST Standard Reference Database 101, http://cccbdb.nist.gov

[2] NIST Chemistry WebBook, NIST Standard Reference Database 69, http://webbook.nist.gov/chemistry/

[3] Timm Lankau, C. H. Yu; Phys. Chem. Chem. Phys. 16 (2014) 26658 http://dx.doi.org/10.1039/C4CP03965C

that one set of diffuse functions on the heavy atoms is sufficient to describe negatively charged transition states. Geometry optimisations with a PCM for the chemical environment and diffuse functions tend to converge badly, specially when weakly bound solvent molecules are part of the system. Hence, geometries were optimised on the M06/6-31G(d,p) level and electronic energies were calculated on the M06/6-31+G(d,p) level. This set up provides high quality data at a reasonable cost while allowing future extensions of the system.

C_6H_5OH	exp	6-31G(d,p)	6-31+G(d,p)
r_{CC} / Å	1.398	1.3914	1.3927
r_{CO} / Å	1.364	1.3581	1.3615
r_{OH} / Å	0.956	0.9633	0.9638
$r_{o\text{-}CH}$ / Å	1.084	1.0885	1.0885
$r_{m\text{-}CH}$ / Å	1.076	1.0877	1.0876
$r_{p\text{-}CH}$ / Å	1.082	1.0865	1.0866
ω_{COH} / deg	109	109.0903	109.9247
B_1 / cm^{-1}	0.18848	0.1896	0.1893
B_2 / cm^{-1}	0.08737	0.0880	0.0878
B_3 / cm^{-1}	0.0597	0.0601	0.0600
μ / D	1.224	1.3594	1.4067
vert. IE / eV	8.75	8.2766	8.4847
adj. IE / eV	8.508	8.0736	8.2817
PhO^-, H^+aff, ΔH / kJ mol^{-1}	1462	1497.2083	1449.0094
PhOH, H^+aff, ΔH / kJ mol^{-1}	817.3	849.7469	829.9270
PhO^-, H^+aff, ΔG / kJ mol^{-1}	1434	1467.6439	1419.5683
PhOH, H^+aff, ΔG / kJ mol^{-1}	786.3	819.2373	799.2126

Table S.1: Experimental reference values and their calculated [M06/6-31G(d,p) and M06/6-31+G(d,p)] counterparts for phenol. r: bond length, ω: bond angle, B_x: rotational constant, μ: dipole moment, IE: ionisation energy.

H_2O	exp	6-31G(d,p)	6-31+G(d,p)
r_{OH} / Å	0.958	0.9605	0.9612
ω_{HOH} / deg	104.4776	104.1694	105.8864
μ / D	1.85	2.0956	2.2285
ν_1 / cm^{-1}	1595	1646.5496	1588.1343
ν_2 / cm^{-1}	3657	3888.8292	3880.3979
ν_3 / cm^{-1}	3756	4021.9712	4020.5556
adj. IE / eV	12.621	12.3982	12.7118

Table S.2: Experimental reference values and their calculated [M06/6-31G(d,p) and M06/6-31+G(d,p)] counterparts for water. r_{OH}: OH bond length, ω_{HOH}: HOH bond angle, μ: dipole moment, ν_x: IR vibrational frequency, adj. IE: adiabatic ionisation energy.

CH_3OH	exp	6-31G(d,p)	6-31+G(d,p)
r_{CH} / Å	1.096	1.0989	1.0973
r_{OH} / Å	0.956	0.9612	0.9617
r_{CO} / Å	1.427	1.4036	1.4094
ω_{HOC} / deg	108.87	108.0917	109.2971
ω_{HCH} / deg	109.03	107.7087	108.261
B_1 / cm^{-1}	4.2573	4.2795	4.2775
B_2 / cm^{-1}	0.82338	0.839	0.834
B_3 / cm^{-1}	0.79273	0.8093	0.8053
μ / D	1.7	1.6861	1.8969
vert. IE / eV	10.96	10.7999	11.0002
adj. IE / eV	10.84	10.6094	10.8129
ν_1 / cm^{-1}	200	290.0193	265.5104
ν_2 / cm^{-1}	1033	1058.6564	1045.3195
ν_3 / cm^{-1}	1060	1136.1913	1114.6872
ν_4 / cm^{-1}	1165	1170.5796	1163.8221
ν_5 / cm^{-1}	1345	1361.101	1333.8811
ν_6 / cm^{-1}	1455	1470.0519	1458.1594
ν_7 / cm^{-1}	1477	1471.1825	1461.3306
ν_8 / cm^{-1}	1477	1501.127	1484.8883
ν_9 / cm^{-1}	2844	2983.3153	2997.3871
ν_{10} / cm^{-1}	2960	3043.4244	3064.1708
ν_{11} / cm^{-1}	3000	3124.3558	3138.2651
ν_{12} / cm^{-1}	3681	3916.9358	3919.1417

Table S.3: Experimental reference values and their calculated [M06/6-31G(d,p) and M06/6-31+G(d,p)] counterparts for methanol. r: bond length, ω: bond angle, B_x: rotational constant, μ: dipole moment, IE: ionisation energy, ν_x: vibrational frequency.

$C_6H_5OCH_3$	exp	6-31G(d,p)	6-31+G(d,p)
r_{CO} / Å	1.399	1.3578	1.3588
r_{O-CH3} / Å	1.433	1.405	1.4079
ω_{COC} / deg	113.8	117.8834	118.2155
B_1 / cm^{-1}	0.16774	0.1691	0.1688
B_2 / cm^{-1}	0.05235	0.0527	0.0525
B_3 / cm^{-1}	0.04022	0.0405	0.0404
μ / D	1.262	1.2804	1.3542
adj. IE / eV	8.2	7.8563	8.0333

Table S.4: Experimental reference values and their calculated [M06/6-31G(d,p) and M06/6-31+G(d,p)] counterparts for anisole. r: bond length, ω: bond angle, B_x: rotational constant, μ: dipole moment, IE: ionisation energy.

	G-31G(d,p)	G-31+G(d,p)	6-31++G(d,p)	G-311G(d,p)	G-311+G(d,p)	6-311++G(d,p)	G-311G(2d,p)	G-311+G(2d,p)	6-311++G(2d,p)
HF	1.2953	1.1147	1.1109	1.2969	1.1079	1.1139	1.2880	1.1121	1.1202
MP2	0.8393	0.8435	0.8445	0.8347	0.7785	0.8784	0.7264	0.6879	0.6603
BLYP	1.1294	0.8092	0.8083	1.2023	0.7610	0.7757	1.2089	0.7586	0.7669
OLYP	1.4249	1.0147	1.0090	1.4870	0.9819	0.9908	1.4859	0.9957	1.0041
OPBE	1.4683	1.0685	1.0590	1.5057	1.0420	1.0511	1.4929	1.0607	1.0704
BPBE	1.1628	0.8473	0.8404	1.1866	0.7794	0.7949	1.1800	0.7808	0.7901
B3LYP	1.0697	0.8054	0.8026	1.1056	0.7542	0.7671	1.0980	0.7434	0.7505
O3LYP	1.3297	0.9738	0.9686	1.3762	0.9389	0.9480	1.3697	0.9461	0.9543
X3LYP	1.0400	0.7831	0.7803	1.0794	0.7308	0.7423	1.0700	0.7161	0.7217
PBE1PBE	1.0204	0.7805	0.7730	1.0335	0.7195	0.7285	1.0102	0.6996	0.7027
M05	0.9695	0.6969	0.6901	1.0417	0.7004	0.7036	1.0190	0.6757	0.6744
M05 2X	1.1646	1.0790	1.0736	1.0124	0.9110	0.9124	0.9349	0.8150	0.8089
M06L	0.7163	0.5086	0.4946	0.8144	0.5797	0.5844	0.8146	0.5702	0.5651
M06	0.6570	0.4829	0.4768	0.7838	0.5258	0.5257	0.7490	0.4870	0.4798
M06 2X	1.0730	0.9935	0.9850	0.9945	0.8947	0.8931	0.9280	0.8069	0.8007
M06 HF	1.5668	1.4076	1.4020	1.2253	1.1741	1.1640	1.1134	1.0439	1.0266
B97D	0.8493	0.6397	0.6266	0.8600	0.5598	0.5569	0.8334	0.5140	0.5035
average	1.1045	0.8735	0.8674	1.1082	0.8200	0.8312	1.0778	0.7890	0.7882

	cc-pVDZ	aug-cc-pVDZ	cc-pVTZ	aug-cc-pVTZ	average
HF	1.3429	1.0579	1.1178	1.0347	1.1626
MP2	0.8283	0.8170	0.6532	0.6836	0.7750
BLYP	1.3776	0.6656	0.9496	0.6779	0.9147
OLYP	1.6662	0.9497	1.2512	0.9149	1.1674
OPBE	1.6698	1.0309	1.2726	0.9823	1.2134
BPBE	1.3731	0.7105	0.9307	0.7050	0.9294
B3LYP	1.2520	0.6499	0.8594	0.6557	0.8703
O3LYP	1.5388	0.8928	1.1412	0.8612	1.0953
X3LYP	1.2236	0.6284	0.8309	0.6312	0.8445
PBE1PBE	1.1638	0.6469	0.7894	0.6229	0.8224
M05	1.1306	0.5559	0.8038	0.6093	0.7901
M05 2X	1.2535	1.0200	0.6760	0.6274	0.9453
M06L	0.8176	0.3164	0.6985	0.6420	0.6248
M06	0.7905	0.2717	0.6452	0.5714	0.5728
M06 2X	1.1587	0.9131	0.7156	0.6659	0.9094
M06 HF	1.6394	1.4086	0.7413	0.9606	1.2210
B97D	0.9973	0.5223	0.6352	0.4917	0.6607
average	1.2485	0.7681	0.8654	0.7257	0.9129

Table S.5: Combined results from the quality function (Eq. S.2) obtained with different methods. The column 'average' contains the average value for all basis sets with a fixed method. The row 'average' lists the average value for all methods with a fixed basis set.

S.2 Compounds

(1) 2-Phenoxy-1-phenylethanol (β-Phenoxy-α-phenylethanol)

(2) 1-Hydroxy-2-phenoxy-1-phenylethanide (carbanion)

(3) 1-Phenylethenol (enol)

(4) Phenoxide ion

(5) 1-Phenylethanone (acetophenone)

(6) 2-Phenoxy-1-phenylethanolate (alkoxide)

(7) 2-Phenyloxirane (oxirane)

(8) 1-Phenyl-1,2-ethanediol (styrene glycol)

(9) 1-Phenylethenololate (enolate)

(10) 1-Phenoxy-1-phenylethanol (hemiketal)

(11) 6-(1-Hydroxy-1-phenylethyl)cyclohexa-2,4-dienone

(12) 2-(1-Hydroxy-1-phenylethyl)phenolate

(13) 3-Hydroxy-1,3-diphenyl-1-butanone

(14) (2E)-1,3-Diphenyl-2-buten-1-one (dypnone)

(15) 6-(2-Hydroxy-2-phenylethyl)cyclohexa-2,4-dienone

(16) 2-(2-Oxocyclohexa-3,5-dienyl)-1-phenylethanolate

(17) 2-(2-Hydroxy-2-phenylethyl)phenolate

(18) Benzaldehyde

(19) Bicyclo[4.1.0]hepta-2,4-dien-2-olate

(20) *o*-Cresolate ion

(21) Benzyl alcohol

(22) 4-Oxo-1,4-diphenyl-1-butanolate

(23) 1-Phenylcyclopropanolate

(24) 1-Phenyl-1-propanone (propiophenone)

(25) 1,2-Dihydroxy-1-phenylethanide

(26) 2-Hydroxy-2-phenylethanolate

(27) 2-(4-Hydroxybenzyl)phenol dianion (2,4'-Bisphenol dianion)

S.3 Stationary points in Figure 1

A1	±0.0 kJ mol^{-1}	Starting point for reaction analysed with either 1 or 2 molecules of **1** with the necessary number of H_2O, $(H_2O)_2$ and $H_3O_2^-$ molecules to balance the equations.	
		carbanion route:	**1** + 2 $H_3O_2^-$	Scheme 2
		alkoxide route:	**1** + 2 $H_3O_2^-$ + H_2O	Scheme 2
		H_2CO formation:	**1** + 2 $H_3O_2^-$ + 2 H_2O	Scheme 8
		8 → **5** + H_2O	**1** + 2 $H_3O_2^-$	Text
		Therm. limit:	2×**1** + 2 $H_3O_2^-$	Scheme 2
		Char formation:	2×**1** + 2 $H_3O_2^-$ + 2 H_2O	Schemes 2, 9
		Nuc. attack on C^α:	2×**1** + 2 $H_3O_2^-$	Scheme 3
		Aldol rxn:	2×**1** + 3 $H_3O_2^-$	Scheme 4
		4 exchange in **1**:	2×**1** + 2 $H_3O_2^-$ + H_2O	Scheme 5, 6
		formation of **24**:	2×**1** + 3 $H_3O_2^-$	Scheme 7
A2	+116.641 kJ mol^{-1}	TS(**1**→**2**) + $H_3O_2^-$	
A3	+95.159 kJ mol^{-1}	**2** + $(H_2O)_2$ + $H_3O_2^-$	
A4	+122.920 kJ mol^{-1}	TS(**2**→**3**+**4**) + $H_3O_2^-$ Rearrangement of H_2O molecules.	
A5	−71.034 kJ mol^{-1}	**3** + **4** + $(H_2O)_2$ + $H_3O_2^-$	
A6	−138.211 kJ mol^{-1}	**4** + **5** + $(H_2O)_2$ + $H_3O_2^-$ The base catalysed tautomerization **3**→**5** is practically barrier-free.	
A7	+18.626 kJ mol^{-1}	**6** + $(H_2O)_2$ + $H_3O_2^-$ + H_2O	
A8	+140.163 kJ mol^{-1}	TS(**6**→**7**) + $(H_2O)_2$ + $H_3O_2^-$ The H_2O molecule stabilises the leaving PhO^- ion.	
A9	−7.601 kJ mol^{-1}	**4** + **7** + $(H_2O)_2$ + $H_3O_2^-$ + H_2O	
A10	+116.609 kJ mol^{-1}	TS(**7**→**8**) + $(H_2O)_2$ + H_2O The $H_3O_2^-$ ion attacks C^β in **7**.	
A11	−37.838 kJ mol^{-1}	**4** + **8** + $(H_2O)_2$ + $H_3O_2^-$	
A12	118.866 kJ mol^{-1}	TS(**2**→**6**) H^+ transfer between **2** and **6** catalysed by a H_2O molecule.	
B1	−276.422 kJ mol^{-1}	2×**4** + 2×**5** + 2 $(H_2O)_2$ Two times the carbanion route: 2 × [**1** + $H_3O_2^-$ → **4** + **5** + $(H_2O)_2$] Thermodynamically preferred products and reference point for the analysis of follow-up reactions.	
B2	−230.275 kJ mol^{-1}	2×**5** + **4** + PhOH + $H_3O_2^-$ + $(H_2O)_2$ Starting point for the nucleophilic attack of **4** on C^α in **5** supported by a PhOH molecule generated from **4** and $(H_2O)_2$.	
B3	−86.684 kJ mol^{-1}	TS(**4**+**5**→**11**) + **5** + $H_3O_2^-$ + $(H_2O)_2$	
B4	−118.310 kJ mol^{-1}	**4** + **5** + **11** + $H_3O_2^-$ + $(H_2O)_2$	
B5	−249.914 kJ mol^{-1}	**4** + **5** + **12** + 2 $(H_2O)_2$ Base catalysed rearomatisation of **11**.	
B6	−140.084 kJ mol^{-1}	TS(**4**+**5**→**10**) + **5** + $H_3O_2^-$ + $(H_2O)_2$	
B7	−159.624 kJ mol^{-1}	**4** + **5** + **10** + $H_3O_2^-$ + $(H_2O)_2$	
C1	−252.827 kJ mol^{-1}	2×**4** + **5** + **9** + 3 $(H_2O)_2$	

		Starting point for the aldol reaction.
C2	−179.702 kJ mol^{-1}	TS(**5**+**9**→**13**)
		The deprotonated form of **13**, the direct product form the addition of **9** to **5**, is not shown in Figure 1.
C3	−217.697 kJ mol^{-1}	2×**4** + **13** + 2 $(H_2O)_2$ + $H_3O_2^-$
C4	−137.793 kJ mol^{-1}	RDS(**13**→**14**) + 2×**4** + 2 $(H_2O)_2$
		The RDS in the elimination of H_2O from **13** is the cleavage of the CO bond and the emittance of the OH^- ion stabilised by $(H_2O)_2$ yielding a cyclic $H_5O_3^-$ ion.
C5	−234.981 kJ mol^{-1}	2×**4** + **14** + 2 $(H_2O)_2$ + $H_3O_2^-$ + H_2O
D1	−138.211 kJ mol^{-1}	**1** + **4** + **5** + $(H_2O)_2$ + $H_3O_2^-$ + H_2O
		Starting point for the S_N2 exchange of **4** in **1**.
D2	+79.676 kJ mol^{-1}	TS(**1**+**4**→**15**) + **5** + $(H_2O)_2$ + $H_3O_2^-$ + H_2O
D3	−114.198 kJ mol^{-1}	**15** + **4** + **5** + $(H_2O)_2$ + $H_3O_2^-$ + H_2O
D4	−255.875 kJ mol^{-1}	**17** + **4** + **5** + 2 $(H_2O)_2$ + H_2O
		The product ion **17** is formed in a series of barrier-free steps directly from **15** when the base removes the proton form O^{α} and the C^3H group is close by.
D5	−84.825 kJ mol^{-1}	**16** + **4** + **5** + 2 $(H_2O)_2$ + H_2O
		Stable, high energy conformer of **16**. An internal rotation around the $C^{\alpha}C^{\beta}$ bond can initialize the rearomatisation of **16** yielding the diphenyl system **17** (D4).
D6	+32.291 kJ mol^{-1}	TS(**16**→**18**+**19**) + **4** + **5** + 2 $(H_2O)_2$
		The H_2O molecule from the addition E1→E2 is still attached to O^{β}.
D7	−120.077 kJ mol^{-1}	**4** + **5** + **18** + **19** + 2 $(H_2O)_2$ + H_2O
D8	−2.691 kJ mol^{-1}	TS(**19**→**20**) + **18** + **4** + **5** + 2 $(H_2O)_2$
		The H_2O molecule acts as a H^+ shuttle from C^3 to O^{β}.
D9	−175.961 kJ mol^{-1}	**4** + **5** + **18** + **20** + 2 $(H_2O)_2$ + H_2O
E1	−145.812 kJ mol^{-1}	2×**4** + **5** + **7** + 2 $(H_2O)_2$ + H_2O
		Staring from **4** and **7** to build **16**.
E2	+21.726 kJ mol^{-1}	TS(**4**+**7**→**16**) + **4** + **5** + 2 $(H_2O)_2$
		The H_2O molecule links to O^{β} to assist the cleavage of the CO bond. (Reverse alkoxide route)
F1	−122.218 kJ mol^{-1}	2×**4** + **7** +**9** + 3 $(H_2O)_2$
		Starting point for the formation of propiohenone (**24**).
F2	−11.753 kJ mol^{-1}	TS(**7**+**9**→**22**) + 2×**4** + 3 $(H_2O)_2$
F3	−191.198 kJ mol^{-1}	**22** + 2×**4** + 3 $(H_2O)_2$
F4	−60.282 kJ mol^{-1}	TS(**22**→**18**+**23**) + 2×**4** + 3 $(H_2O)_2$
F5	−134.693 kJ mol^{-1}	2×**4** + **18** + **23** + 3 $(H_2O)_2$
F6	−76.995 kJ mol^{-1}	TS(**23**→**24**) + 2×**4** + **18** + 2 $(H_2O)_2$
		One $(H_2O)_2$ molecule donates the H^+ to open the cyclopropane ring.
F7	−238.796 kJ mol^{-1}	2×**4** + **18** + **24** + 2 $(H_2O)_2$ + $H_3O_2^-$
G1	+141.820 kJ mol^{-1}	TS(**8**→**21**+H_2CO) + **4** + 2 $(H_2O)_2$

		The H_2O molecules in TS acts as H^+ shuttle.
G2	-11.771 kJ mol^{-1}	**4** + **21** + H_2CO + $(H_2O)_2$ + $H_3O_2^-$ + H_2O
G3	-149.982 kJ mol^{-1}	2×**4** + **5** + **21** + H_2CO + 2 $(H_2O)_2$
		Starting point for the formation of char generated by mixing the carbanion and the alkoxide route (Scheme 2).
G4	-205.231 kJ mol^{-1}	**5** + **21** + **27** + 2 $(H_2O)_2$ + H_2O
		Example for the first step in the formation of char.
G5	$+78.909$ kJ mol^{-1}	RDS(**8**→**5**) + **4**
G6	$+84.471$ kJ mol^{-1}	TS(**8**−$O^{\alpha-}$→**25**) + **4** + 2 $(H_2O)_2$

S.4 Molecule structures

S.4.1 2-Phenoxy-1-phenylethanol (1)

```
Cartesian coordinates of the freq job (Standard orientation)
C       2.398212     0.353994     0.178181
C       3.009694    -0.277390     1.261189
C       4.195414    -0.982994     1.088827
C       4.782986    -1.058752    -0.171107
C       4.177556    -0.429329    -1.255223
C       2.987528     0.270164    -1.083223
H       2.551972    -0.208537     2.247976
H       4.665765    -1.468896     1.940386
H       5.713900    -1.604038    -0.306858
H       4.633886    -0.484937    -2.240878
H       2.509196     0.767284    -1.923761
C       1.079529     1.052548     0.367499
H       1.012773     1.422978     1.407271
C      -0.055579     0.065989     0.160341
H       0.002629    -0.347157    -0.860184
H       0.013813    -0.762510     0.881808
O      -1.255572     0.797287     0.336101
C      -2.443908     0.165145     0.132559
C      -3.585696     0.954140     0.296111
C      -2.564690    -1.181024    -0.209628
C      -4.842108     0.396467     0.117451
H      -3.459734     2.000323     0.564252
C      -3.836158    -1.725525    -0.386412
H      -1.687622    -1.808386    -0.337478
C      -4.976502    -0.948952    -0.225763
H      -5.725021     1.017776     0.247344
H      -3.925601    -2.775980    -0.653423
H      -5.962104    -1.384976    -0.365374
O       0.963101     2.116875    -0.548740
```

```
H      0.038262     2.396872    -0.524774

Frequencies
  23.0422    38.9313    45.8071    63.8381   138.2154   140.7362   220.6407
 240.1773   248.4175   274.0936   362.3854   395.3323   412.0843   418.4783
 445.3832   512.0143   517.6122   545.7104   601.7786   619.1066   622.0005
 637.1592   696.6690   710.2226   760.3347   768.6919   804.5364   819.4909
 862.4138   877.5058   888.4142   926.7882   940.3588   959.3901   979.4683
 986.0251  1000.8842  1001.3088  1006.0378  1040.1094  1050.4375  1078.7580
1085.8011  1097.3034  1108.9231  1150.9659  1153.4212  1154.5555  1161.2902
1174.7052  1207.5979  1225.5852  1263.8567  1292.7814  1309.6412  1327.8313
1336.8630  1364.4477  1367.2344  1395.0164  1434.5882  1467.7473  1479.9738
1486.4669  1524.3419  1530.9446  1647.5482  1650.4016  1666.9681  1672.4591
2970.4424  2997.8469  3062.8014  3160.2796  3178.2062  3179.3900  3186.7881
3187.1241  3196.3896  3196.9393  3202.7748  3204.3273  3217.1920  3842.4302

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -691.892550627
SCF energy, 6-31+G(d,p)                         -691.917963694
Zero-point correction                              0.246505
Thermal correction to Energy                       0.260240
Thermal correction to Enthalpy                     0.261184
Thermal correction to Gibbs Free Energy            0.203912
Sum of electronic and zero-point Energies       -691.646046
Sum of electronic and thermal Energies          -691.632311
Sum of electronic and thermal Enthalpies        -691.631367
Sum of electronic and thermal Free Energies     -691.688638
```

S.4.2 1-Hydroxy-2-phenoxy-1-phenylethanide (2)

```
Optimized cartesian coordinates (Standard orientation)
C     -2.276190     0.271021    -0.063937
C     -2.143309    -1.147802    -0.255451
C     -3.228150    -2.001328    -0.194269
C     -4.522044    -1.540294     0.086247
C     -4.673588    -0.168045     0.318984
C     -3.605663     0.709232     0.255826
H     -1.152281    -1.566206    -0.436563
H     -3.060740    -3.068037    -0.354834
H     -5.367095    -2.222574     0.141879
H     -5.661400     0.229885     0.559655
H     -3.764756     1.768804     0.450440
C     -1.210971     1.165394    -0.196515
C      0.126182     0.808321    -0.623394
H      0.136598    -0.065905    -1.293873
```

```
H      0.620355     1.651838    -1.130225
O      1.029741     0.439432     0.515019
C      2.297509     0.095405     0.232579
C      3.111804    -0.244074     1.326436
C      2.850636     0.052783    -1.055836
C      4.433615    -0.614890     1.138755
H      2.671854    -0.207279     2.321004
C      4.182189    -0.323660    -1.227329
H      2.254873     0.309503    -1.925673
C      4.983534    -0.659093    -0.143465
H      5.042615    -0.873259     2.002968
H      4.593501    -0.351319    -2.234732
H      6.020372    -0.950387    -0.291072
O     -1.411088     2.532084     0.128150
H     -1.881727     2.943957    -0.607552

Frequencies
  20.4878    35.6851    46.3447    92.5992   127.9725   148.8915   190.4854
 228.1180   241.5434   264.4682   292.3917   368.6377   418.0367   427.8471
 442.5812   476.2190   496.9754   521.7052   544.5993   607.1375   621.3707
 622.3344   684.6407   699.5116   700.6625   742.6410   757.3205   785.8925
 794.8563   813.4326   826.8653   854.4109   875.6374   930.4426   937.0639
 946.4780   959.4731   968.3096   980.2419   995.0537  1032.6540  1049.2553
1063.4294  1083.8725  1103.4584  1134.5320  1149.1017  1169.0013  1177.4703
1185.1461  1249.8852  1266.4099  1282.3043  1319.1184  1329.9149  1364.5450
1367.0438  1387.8815  1424.0885  1446.2023  1481.6738  1489.8281  1529.2555
1551.8088  1562.6964  1635.3339  1655.5401  1664.1589  2979.6722  3048.0344
3128.9594  3132.6146  3149.5938  3166.8918  3172.3286  3173.8735  3183.1914
3187.2947  3197.9071  3218.2745  3799.9878

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                        -691.342973234
SCF energy, 6-31+G(d,p)                       -691.381882704
Zero-point correction                            0.230513
Thermal correction to Energy                     0.244660
Thermal correction to Enthalpy                   0.245604
Thermal correction to Gibbs Free Energy          0.187659
Sum of electronic and zero-point Energies    -691.112460
Sum of electronic and thermal Energies       -691.098313
Sum of electronic and thermal Enthalpies     -691.097369
Sum of electronic and thermal Free Energies  -691.155314
```

S.4.3 1-Phenylethenol (3)

```
Optimized cartesian coordinates (Standard orientation)
```

```
C     -1.344266    -0.306543     0.012717
C      0.045579    -0.337183     0.028978
C      0.773702     0.847735     0.009321
C      0.100973     2.067191    -0.033309
C     -1.286263     2.099517    -0.052169
C     -2.028655     0.913444    -0.017655
H     -1.913162    -1.231866     0.030331
H      0.561666    -1.293963     0.058290
H      1.860469     0.822578     0.019680
H      0.661537     2.998352    -0.063579
H     -1.800406     3.055995    -0.115426
C     -3.503433     0.936439    -0.013574
C     -4.252583     1.990215     0.336666
H     -3.800144     2.912917     0.680378
H     -5.338217     1.944329     0.305547
O     -4.033393    -0.257971    -0.395058
H     -4.993883    -0.218191    -0.303240

Frequencies
  59.9248   156.0054   234.5202   381.6079   400.3130   407.8291   439.0326
 492.6566   571.5384   622.3968   631.0600   695.2543   714.4547   764.1818
 774.6845   789.9976   853.5011   930.9362   975.7545   978.0897   999.4324
1005.0622  1049.6468  1094.4910  1119.2733  1151.8555  1174.0298  1225.0048
1313.2250  1362.6806  1395.0787  1435.2384  1473.6097  1530.2826  1637.8485
1670.6080  1716.6376  3166.8892  3178.2934  3183.7375  3191.9191  3199.3125
3205.2508  3270.5802  3860.9552

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                        -384.608855230
SCF energy, 6-31+G(d,p)                       -384.624438899
Zero-point correction                            0.137794
Thermal correction to Energy                     0.145420
Thermal correction to Enthalpy                   0.146364
Thermal correction to Gibbs Free Energy          0.105486
Sum of electronic and zero-point Energies    -384.471061
Sum of electronic and thermal Energies       -384.463436
Sum of electronic and thermal Enthalpies     -384.462491
Sum of electronic and thermal Free Energies  -384.503369
```

S.4.4 Phenoxide ion (4)

```
Optimized cartesian coordinates (Standard orientation)
C     -0.905993    -0.066503     0.000029
C      0.479855    -0.058264     0.000480
C      1.203846     1.138493     0.000007
```

```
C      0.479900     2.335339    -0.001015
C     -0.905895     2.343949    -0.001495
C     -1.690643     1.138703    -0.001017
H     -1.450475    -1.012987     0.000410
H      1.016327    -1.009410     0.001261
H      2.291840     1.138481     0.000332
H      1.016545     3.286393    -0.001466
H     -1.450065     3.290512    -0.002402
O     -2.960923     1.138210    -0.001091

Frequencies
 201.3487   418.6654   444.0195   509.7420   531.7829   611.8392   705.0107
 720.1531   807.9579   836.3516   839.1656   940.3121   950.2137   971.3131
1032.1258  1067.4898  1129.1159  1149.6915  1254.5996  1339.7320  1412.8323
1485.8280  1576.8176  1587.0664  1664.3382  3121.7535  3123.0067  3141.9963
3145.1400  3180.4868

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                        -306.769315460
SCF energy, 6-31+G(d,p)                       -306.800649740
Zero-point correction                            0.090899
Thermal correction to Energy                     0.096131
Thermal correction to Enthalpy                   0.097075
Thermal correction to Gibbs Free Energy          0.062079
Sum of electronic and zero-point Energies    -306.678417
Sum of electronic and thermal Energies       -306.673185
Sum of electronic and thermal Enthalpies     -306.672240
Sum of electronic and thermal Free Energies  -306.707236
```

S.4.5 1-Phenylethanone (5)

```
Optimized cartesian coordinates (Standard orientation)
C     -0.666457    -0.549409    -0.128417
C      0.723150    -0.540100    -0.110379
C      1.409252     0.666660    -0.009801
C      0.705189     1.866927     0.073400
C     -0.681188     1.856940     0.055962
C     -1.380735     0.649659    -0.045121
H     -1.192952    -1.497437    -0.208674
H      1.271939    -1.475960    -0.175941
H      2.496320     0.672933     0.003782
H      1.241982     2.808917     0.152531
H     -1.251812     2.779981     0.119793
C     -2.869344     0.691052    -0.060473
O     -3.465327     1.754459     0.023779
```

```
C     -3.621108    -0.605357    -0.184719
H     -3.363164    -1.118554    -1.118227
H     -3.370811    -1.286249     0.636614
H     -4.692894    -0.400037    -0.170383

Frequencies
  60.9310   134.5765   153.0038   217.3251   365.7080   407.3239   426.2362
 464.3818   592.8467   596.2740   620.1383   696.7043   745.8163   767.8270
 857.8881   941.0983   958.1922   985.0147  1007.1232  1007.9162  1029.6723
1046.8184  1092.8786  1096.7473  1153.0372  1173.1947  1289.8102  1315.6444
1368.1622  1372.0513  1431.5710  1437.1273  1475.0765  1520.7154  1642.9667
1663.2548  1795.8279  3049.5741  3131.0617  3173.7023  3183.2004  3189.5097
3197.4123  3202.0266  3207.8392

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -384.634774041
SCF energy, 6-31+G(d,p)                         -384.648880948
Zero-point correction                              0.137249
Thermal correction to Energy                       0.145177
Thermal correction to Enthalpy                     0.146121
Thermal correction to Gibbs Free Energy            0.104343
Sum of electronic and zero-point Energies       -384.497525
Sum of electronic and thermal Energies          -384.489597
Sum of electronic and thermal Enthalpies        -384.488653
Sum of electronic and thermal Free Energies     -384.530432
```

S.4.6 2-Phenoxy-1-phenylethanolate (6)

```
Optimized cartesian coordinates (Standard orientation)
C      2.164778     0.424196     0.259175
C      2.116549    -0.847533     0.835603
C      2.944217    -1.871243     0.382338
C      3.839408    -1.638027    -0.660674
C      3.900946    -0.371926    -1.238364
C      3.072522     0.646315    -0.774472
H      1.419450    -1.031936     1.653524
H      2.896544    -2.855206     0.846963
H      4.490212    -2.436146    -1.012915
H      4.604529    -0.179453    -2.047524
H      3.106288     1.657977    -1.176856
C      1.271574     1.595473     0.713699
C     -0.152378     1.368083     0.160926
H     -0.761926     2.234131     0.463460
H     -0.101107     1.354297    -0.941924
O     -0.753914     0.162137     0.636641
```

```
C     -2.024287    -0.117948     0.276332
C     -2.810795     0.693760    -0.546407
C     -2.560388    -1.310295     0.781016
C     -4.116143     0.307988    -0.847640
H     -2.415318     1.619971    -0.951625
C     -3.859444    -1.680443     0.470891
H     -1.930749    -1.928064     1.417661
C     -4.650787    -0.872536    -0.346757
H     -4.719503     0.948660    -1.487533
H     -4.259330    -2.609433     0.871864
H     -5.670004    -1.162913    -0.588217
O      1.685734     2.797449     0.332069
H      1.157901     1.430935     1.836122

Frequencies
  28.5706    39.0104    57.0782    84.9580   125.7650   181.3824   220.1175
 234.6028   244.5551   312.9278   377.5901   407.9708   422.1915   422.6765
 518.9624   527.5791   544.8569   594.8080   618.7278   619.4796   635.4917
 700.4848   719.5829   759.5297   763.8793   767.5107   830.5167   840.7265
 872.5129   885.8331   919.0805   963.9550   978.6855   983.7294   991.3831
 996.0310   999.3668  1005.0496  1035.1806  1038.7202  1051.3743  1065.9696
1073.4748  1088.3688  1139.3407  1149.2508  1154.4108  1159.4499  1180.3414
1209.1901  1267.1923  1288.0319  1295.7175  1309.7577  1311.0645  1333.3890
1358.8453  1370.1446  1387.7126  1455.2579  1470.7163  1484.1311  1510.9633
1528.0746  1642.0064  1643.8521  1655.7625  1666.9990  2578.4851  2976.7952
3045.5490  3148.8606  3155.1215  3164.3013  3174.1494  3180.0464  3180.5399
3184.4694  3190.6090  3199.1845  3212.7370

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                        -691.368071257
SCF energy, 6-31+G(d,p)                       -691.413863524
Zero-point correction                            0.232174
Thermal correction to Energy                     0.245446
Thermal correction to Enthalpy                   0.246390
Thermal correction to Gibbs Free Energy          0.190490
Sum of electronic and zero-point Energies    -691.135897
Sum of electronic and thermal Energies       -691.122625
Sum of electronic and thermal Enthalpies     -691.121681
Sum of electronic and thermal Free Energies  -691.177581
```

S.4.7 2-Phenyloxirane (7)

```
Optimized cartesian coordinates (Standard orientation)
C     -1.803173    -0.069800     0.378527
C     -1.898642     0.812345    -0.697656
```

```
C     -3.056878     0.861937    -1.466197
C     -4.133542     0.035762    -1.157968
C     -4.046732    -0.838606    -0.076951
C     -2.887636    -0.892072     0.688086
H     -1.057978     1.463811    -0.932821
H     -3.121029     1.551710    -2.304327
H     -5.041491     0.076706    -1.754736
H     -4.888655    -1.479798     0.173503
H     -2.815646    -1.560472     1.543814
C     -0.546268    -0.131708     1.165092
C      0.118777    -1.405429     1.456432
H      1.199782    -1.433844     1.598028
H     -0.336818    -2.327661     1.090118
O     -0.614588    -0.720327     2.456030
H      0.082856     0.760742     1.107523

Frequencies
  77.2433   158.1403   203.0639   346.1097   398.9321   414.1899   543.4810
 582.2590   624.5247   707.9766   765.5887   769.4917   859.4932   912.5477
 925.2489   945.4513   976.4757   999.5654  1006.4511  1007.3884  1050.0432
1090.3936  1097.1636  1146.6392  1155.2876  1167.6016  1172.2601  1230.6722
1287.8105  1321.5479  1362.1574  1428.0544  1479.9341  1518.9046  1536.5793
1650.2371  1671.6036  3081.1979  3112.2422  3168.3769  3176.9565  3181.6545
3185.4003  3191.6352  3202.0622

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -384.587934111
SCF energy, 6-31+G(d,p)                         -384.601566343
Zero-point correction                              0.138718
Thermal correction to Energy                       0.145872
Thermal correction to Enthalpy                     0.146817
Thermal correction to Gibbs Free Energy            0.106774
Sum of electronic and zero-point Energies       -384.449216
Sum of electronic and thermal Energies          -384.442062
Sum of electronic and thermal Enthalpies        -384.441117
Sum of electronic and thermal Free Energies     -384.481160
```

S.4.8 1-Phenyl-1,2-ethanediol (8)

```
Optimized cartesian coordinates (Standard orientation)
C     -0.458111     0.320938    -0.327266
C     -0.524589    -1.068353    -0.433136
C     -1.715784    -1.740437    -0.180452
C     -2.855564    -1.025472     0.176875
C     -2.795790     0.361462     0.283812
```

```
C     -1.602008     1.031583     0.037322
H      0.367158    -1.625325    -0.720957
H     -1.756484    -2.823444    -0.269595
H     -3.789836    -1.547914     0.368648
H     -3.684192     0.924584     0.560877
H     -1.546072     2.115050     0.113440
C      0.855253     1.023959    -0.522427
C      1.602224     1.126529     0.803790
H      0.953932     1.632395     1.531908
H      1.835589     0.124005     1.191806
O      0.654727     2.322356    -1.031588
H      1.478795     0.426947    -1.217552
O      2.754850     1.933741     0.662069
H      3.416704     1.428232     0.173828
H      1.461319     2.807139    -0.799359

Frequencies
  52.2302   105.4184   126.7534   241.4547   268.8430   334.8447   352.6580
 376.9316   413.8320   508.5969   535.9418   552.6129   625.0216   635.8450
 712.7846   768.1903   843.7703   865.9366   912.9471   925.2908   980.3353
1001.6215  1006.3162  1020.3646  1046.6022  1085.7077  1110.8636  1148.8030
1154.4700  1165.5017  1174.6583  1231.5351  1266.4588  1320.7631  1335.7893
1363.5427  1366.8093  1385.1095  1438.2716  1457.8969  1481.7893  1527.8416
1652.0531  1670.6782  2939.0986  3021.4071  3091.7859  3159.4865  3174.6538
3184.1593  3192.9214  3199.4506  3798.2812  3866.3037

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -461.019595823
SCF energy, 6-31+G(d,p)                         -461.041367478
Zero-point correction                              0.166719
Thermal correction to Energy                       0.175838
Thermal correction to Enthalpy                     0.176782
Thermal correction to Gibbs Free Energy            0.132209
Sum of electronic and zero-point Energies      -460.852877
Sum of electronic and thermal Energies         -460.843758
Sum of electronic and thermal Enthalpies       -460.842814
Sum of electronic and thermal Free Energies    -460.887387
```

S.4.9 1-Phenylethenololate (9)

```
Optimized cartesian coordinates (Standard orientation)
C     -1.334892    -0.299913     0.002687
C      0.055260    -0.332027     0.023056
C      0.782421     0.855230     0.013772
C      0.099115     2.069658    -0.020608
```

```
C     -1.291230     2.092991    -0.034891
C     -2.038668     0.908669    -0.011293
H     -1.926126    -1.213130    -0.007738
H      0.576652    -1.287985     0.042242
H      1.870151     0.835982     0.024001
H      0.655209     3.005387    -0.044879
H     -1.806723     3.050361    -0.087218
C     -3.556675     0.848083    -0.023463
C     -4.238810     2.000402     0.303534
H     -3.743349     2.916181     0.614416
H     -5.328432     1.991540     0.319880
O     -4.070498    -0.280241    -0.322361

Frequencies
  46.8356   153.4354   239.7539   379.5675   412.8047   415.5572   476.9107
 504.8462   595.5060   613.6797   624.1905   706.2204   716.5697   744.6473
 795.4582   857.7205   921.8360   969.6252   988.3349  1003.3678  1007.8715
1043.8018  1082.8462  1125.1914  1144.5654  1173.0797  1300.9981  1321.2609
1362.0484  1458.4437  1463.9996  1512.3705  1620.1947  1658.4908  1659.2213
3132.3399  3160.8485  3166.0597  3182.7226  3185.1941  3191.5793  3226.8402

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -384.109513503
SCF energy, 6-31+G(d,p)                         -384.143367170
Zero-point correction                              0.123811
Thermal correction to Energy                       0.131301
Thermal correction to Enthalpy                     0.132245
Thermal correction to Gibbs Free Energy            0.091399
Sum of electronic and zero-point Energies       -383.985702
Sum of electronic and thermal Energies          -383.978213
Sum of electronic and thermal Enthalpies        -383.977268
Sum of electronic and thermal Free Energies     -384.018115
```

S.4.10 1-Phenoxy-1-phenylethanol (10)

```
Optimized cartesian coordinates (Standard orientation)
C     -1.761693    -1.301287     0.321390
C     -1.369798    -1.442705    -1.012307
C     -2.114101    -2.222653    -1.888939
C     -3.263347    -2.869782    -1.443789
C     -3.660072    -2.733559    -0.117946
C     -2.911807    -1.956031     0.761595
H     -0.483359    -0.920558    -1.368087
H     -1.800227    -2.319129    -2.925423
H     -3.849558    -3.476401    -2.129472
```

H	-4.557816	-3.233266	0.237565
H	-3.236456	-1.858514	1.794887
C	-0.875447	-0.512165	1.272483
O	0.205912	-1.303376	1.665534
H	-2.405202	0.581130	2.376897
C	-1.524677	-0.040125	2.555956
H	-1.811303	-0.896763	3.171119
H	-0.784542	0.545599	3.108546
O	-0.266805	0.600497	0.590108
C	-0.970359	1.673735	0.131071
C	-2.355069	1.728977	-0.045018
C	-2.935424	2.895020	-0.540827
C	-2.161483	3.999982	-0.872445
C	-0.779463	3.933936	-0.703574
C	-0.187809	2.783360	-0.204605
H	-2.982912	0.873349	0.183708
H	-4.014836	2.928274	-0.670672
H	-2.627210	4.902318	-1.259585
H	-0.155542	4.787836	-0.957568
H	0.888056	2.716413	-0.061966
H	0.582456	-1.709428	0.873020

Frequencies

20.2563	30.8017	66.9372	116.1198	160.7475	196.8439	236.9104
274.5545	293.1264	300.9976	355.9513	357.3115	376.1612	407.6422
415.5389	427.9765	511.9499	530.2097	574.2648	594.0249	618.8538
621.6394	636.5917	701.1912	705.5339	725.8019	757.6443	783.7952
838.2595	845.8336	852.9100	898.0689	925.3995	937.1775	959.4475
970.6833	974.9399	986.4890	999.3710	1001.4778	1004.2562	1046.5199
1051.3983	1071.8698	1090.1664	1100.1289	1117.4411	1152.9532	1155.5972
1176.7255	1178.2659	1183.0251	1269.7065	1289.2010	1314.8739	1322.8015
1353.2338	1365.8219	1370.4506	1415.5164	1453.5107	1473.8011	1477.1773
1484.3624	1524.8506	1526.2142	1644.8285	1647.3092	1664.3663	1666.4807
3069.2509	3162.3775	3172.3728	3176.0699	3178.9984	3180.5790	3184.4971
3191.1345	3194.7080	3195.4080	3202.1594	3204.0408	3207.3564	3843.5328

Energies (Hartree/Particle):

SCF energy, 6-31G(d,p)	-691.901781343
SCF energy, 6-31+G(d,p)	-691.926081182
Zero-point correction	0.245461
Thermal correction to Energy	0.259184
Thermal correction to Enthalpy	0.260128
Thermal correction to Gibbs Free Energy	0.203875
Sum of electronic and zero-point Energies	-691.656321
Sum of electronic and thermal Energies	-691.642597

Sum of electronic and thermal Enthalpies -691.641653
Sum of electronic and thermal Free Energies -691.697907

S.4.11 6-(1-Hydroxy-1-phenylethyl)cyclohexa-2,4-dienone (11)

Optimized cartesian coordinates (Standard orientation)

C	-0.186374	-0.772803	4.027479
C	1.123992	-0.554885	4.461520
C	2.125939	-1.479933	4.194641
C	1.833184	-2.642540	3.486139
C	0.533214	-2.868951	3.049040
C	-0.468980	-1.940020	3.317158
H	1.344836	0.345689	5.029868
H	3.138995	-1.294453	4.544093
H	2.615199	-3.368713	3.277796
H	0.292132	-3.773887	2.496382
H	-1.477840	-2.135286	2.962128
C	-1.238547	0.288706	4.312499
O	-1.004266	0.746769	5.625521
H	-2.937079	-0.473003	3.159037
C	-2.666937	-0.233048	4.194222
H	-2.794030	-1.129382	4.810003
H	-3.366086	0.526825	4.559626
O	-2.122052	3.047558	4.762609
C	-2.030357	2.596114	3.614473
C	-1.029060	1.496472	3.307789
C	-0.979010	1.061530	1.885023
C	-1.800128	1.561261	0.948099
C	-2.775881	2.571461	1.293802
C	-2.888299	3.068913	2.546415
H	-0.036421	1.893350	3.581141
H	-0.238428	0.308024	1.624314
H	-1.740336	1.223249	-0.082415
H	-3.434363	2.940376	0.509966
H	-3.618183	3.832072	2.803822
H	-1.422822	1.626928	5.688076

Frequencies

49.8264	62.2297	77.6609	83.5465	183.0151	229.6167	236.4344
275.2423	292.8887	331.3324	355.9434	369.4825	411.8260	432.1711
453.7484	475.0381	496.8843	527.7178	566.1312	569.6186	596.1781
613.1716	625.7439	675.2046	709.7039	747.7306	762.4058	787.1529
799.4525	848.7406	854.3340	894.3593	929.3369	956.1245	968.1063
976.4091	991.0225	997.7457	998.5310	1005.0648	1023.5888	1051.7738
1059.9953	1080.9466	1097.9824	1119.1688	1145.4963	1150.8158	1155.2630

1175.5996 1190.7463 1217.2490 1249.1297 1259.5932 1327.3387 1335.2948
1360.4103 1391.4009 1391.9657 1432.1145 1446.7230 1470.1117 1474.7990
1486.1524 1528.7713 1632.5243 1644.5835 1667.4796 1704.4125 1737.0011
3019.5690 3042.5421 3133.8551 3140.4491 3179.4933 3180.2685 3184.1443
3186.1210 3195.0679 3200.7856 3202.0980 3206.6010 3209.0643 3648.6542

Energies (Hartree/Particle):

SCF energy, 6-31G(d,p)	-691.887332897
SCF energy, 6-31+G(d,p)	-691.912448218
Zero-point correction	0.245937
Thermal correction to Energy	0.259339
Thermal correction to Enthalpy	0.260283
Thermal correction to Gibbs Free Energy	0.205977
Sum of electronic and zero-point Energies	-691.641396
Sum of electronic and thermal Energies	-691.627994
Sum of electronic and thermal Enthalpies	-691.627049
Sum of electronic and thermal Free Energies	-691.681356

S.4.12 2-(1-Hydroxy-1-phenylethyl)phenolate (12)

Optimized cartesian coordinates (Standard orientation)

C	-0.989737	-0.220865	-2.191280
C	-0.468710	-0.442352	-3.470344
C	-1.102175	0.056199	-4.600600
C	-2.277793	0.795291	-4.476217
C	-2.805536	1.025196	-3.211948
C	-2.165454	0.519952	-2.080209
H	0.447197	-1.021820	-3.560113
H	-0.678476	-0.130940	-5.585347
H	-2.777023	1.187040	-5.359649
H	-3.722611	1.599673	-3.099226
H	-2.597889	0.713342	-1.100959
C	-0.227064	-0.769229	-0.993095
O	0.145661	-2.098717	-1.334425
H	-1.376278	0.177403	0.622003
C	-1.086171	-0.821156	0.273532
H	-1.991439	-1.419411	0.108119
H	-0.493853	-1.294716	1.063598
O	2.075035	-1.812611	0.346316
C	2.103646	-0.566509	0.009597
C	1.022526	0.067849	-0.698432
C	1.092240	1.420315	-1.012086
C	2.195069	2.210444	-0.680506
C	3.259737	1.610387	-0.008909
C	3.217288	0.264614	0.323038

```
H      0.251670     1.877652    -1.537369
H      2.219304     3.265787    -0.943894
H      4.136103     2.201563     0.259582
H      4.046982    -0.206762     0.851805
H      0.885706    -2.278263    -0.692993

Frequencies
  33.7888    54.6401    68.6930   117.6128   195.6314   237.9555   244.3280
 296.2659   319.2743   342.5743   358.6349   381.9759   409.7883   435.6794
 476.3326   512.5595   529.3623   560.2361   573.8641   592.9598   625.7833
 635.2083   698.4917   707.8578   735.2263   747.6177   771.9335   823.6067
 832.2537   851.7424   859.1204   875.1619   916.9487   920.9502   944.2286
 948.5765   967.7548   992.1490  1004.9971  1048.2299  1051.0021  1058.4091
1091.7935  1096.0358  1112.9251  1137.9503  1154.7437  1157.5456  1187.6709
1198.1236  1251.6210  1266.0405  1323.2089  1338.7853  1362.4355  1366.2614
1380.5054  1451.8852  1468.3525  1473.4586  1483.5839  1504.0111  1525.8241
1572.9873  1594.3382  1644.8497  1656.2875  1670.1536  3023.4589  3112.2825
3133.4647  3137.0103  3142.4343  3155.0997  3168.7786  3176.1995  3179.8037
3187.3657  3194.3823  3198.5144  3244.8096

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -691.426696151
SCF energy, 6-31+G(d,p)                         -691.466055067
Zero-point correction                              0.233021
Thermal correction to Energy                       0.246046
Thermal correction to Enthalpy                     0.246990
Thermal correction to Gibbs Free Energy            0.193043
Sum of electronic and zero-point Energies       -691.193675
Sum of electronic and thermal Energies          -691.180650
Sum of electronic and thermal Enthalpies        -691.179706
Sum of electronic and thermal Free Energies     -691.233654
```

S.4.13 3-Hydroxy-1,3-diphenyl-1-butanone (13)

```
Optimized cartesian coordinates (Standard orientation)
C      1.273372     2.849566    -2.186688
C      1.871669     3.838393    -2.958336
C      3.183895     4.223836    -2.702100
C      3.899178     3.627532    -1.664467
C      3.299671     2.651386    -0.886043
C      1.982330     2.245918    -1.141571
H      0.244999     2.567275    -2.398077
H      1.311598     4.307804    -3.762389
H      3.651737     4.992682    -3.311870
H      4.923786     3.929983    -1.464970
```

H	3.836278	2.179512	-0.067480
C	1.396775	1.211585	-0.257844
O	1.982123	0.873564	0.770944
C	0.068462	0.570568	-0.572631
H	0.240791	-0.511001	-0.654763
H	-0.352948	0.902929	-1.523722
C	-0.952966	0.784258	0.572903
C	-1.135845	2.274504	0.865009
H	-1.901480	2.406988	1.636264
H	-0.198754	2.704177	1.239793
H	-1.437105	2.841893	-0.023121
O	-0.491408	0.136016	1.741513
C	-2.271926	0.145373	0.167630
C	-2.747418	-0.989859	0.823030
C	-3.949345	-1.579451	0.440155
C	-4.691639	-1.045594	-0.607046
C	-4.222831	0.085183	-1.270576
C	-3.025036	0.674986	-0.885190
H	-2.165181	-1.405384	1.639580
H	-4.305570	-2.462793	0.965728
H	-5.629865	-1.506720	-0.906339
H	-4.793018	0.511644	-2.092544
H	-2.676013	1.557997	-1.419751
H	0.469699	0.283545	1.773934

Frequencies

27.5756	45.4088	49.4927	66.5129	105.8908	151.0364	198.5523
217.2640	236.5121	284.7704	306.6223	320.8042	352.5210	387.8526
410.1273	413.9836	432.3880	457.4196	463.5147	487.2085	524.6839
553.1524	592.7579	615.7360	620.4754	625.0803	692.4448	698.0155
713.0631	747.8257	756.2821	779.9999	842.3163	856.5288	863.7192
878.8184	927.5385	933.8634	950.2976	979.7008	984.3135	988.9448
1001.1879	1004.4898	1006.0228	1009.9103	1037.1147	1049.5115	1054.8637
1089.0915	1093.5958	1099.9893	1132.4038	1154.8343	1158.7118	1170.5018
1181.9350	1185.9391	1235.4006	1246.4299	1265.9422	1316.5076	1321.9397
1350.9562	1365.5458	1371.7758	1401.6272	1425.1856	1440.5924	1469.2150
1474.5144	1477.6000	1482.6264	1521.9858	1528.7247	1638.7456	1649.0394
1658.6325	1669.2622	1745.8457	3037.4075	3062.2184	3124.8622	3137.4778
3150.8380	3163.5186	3173.8291	3183.4625	3188.1443	3195.8248	3197.5735
3202.4317	3208.0871	3212.7358	3217.7873	3720.9687		

Energies (Hartree/Particle):

SCF energy, 6-31G(d,p)	-769.277254587
SCF energy, 6-31+G(d,p)	-769.303759219
Zero-point correction	0.280685

```
Thermal correction to Energy                    0.296097
Thermal correction to Enthalpy                  0.297041
Thermal correction to Gibbs Free Energy         0.237049
Sum of electronic and zero-point Energies    -768.996570
Sum of electronic and thermal Energies       -768.981158
Sum of electronic and thermal Enthalpies     -768.980214
Sum of electronic and thermal Free Energies  -769.040206
```

S.4.14 (2E)-1,3-Diphenyl-2-buten-1-one (14)

```
Optimized cartesian coordinates (Standard orientation)
C     -3.057609    -1.369138    -0.338621
C     -4.303063    -1.784261    -0.796229
C     -5.387135    -0.912648    -0.755343
C     -5.227696     0.373634    -0.243118
C     -3.988390     0.782256     0.225890
C     -2.887213    -0.079345     0.175602
H     -2.223441    -2.066771    -0.362197
H     -4.427622    -2.792026    -1.184004
H     -6.358636    -1.236978    -1.120292
H     -6.074007     1.055268    -0.209424
H     -3.845112     1.778442     0.636189
C     -1.585095     0.421493     0.713368
O     -1.572764     1.418319     1.435517
C     -0.368038    -0.295836     0.321300
H     -0.454020    -0.960871    -0.534995
C      0.848989    -0.168654     0.902682
C      1.127576     0.738827     2.060649
H      1.383786     1.746457     1.707052
H      0.246587     0.856318     2.693088
H      1.970414     0.370018     2.652478
C      1.988138    -0.949848     0.379138
C      3.282725    -0.412548     0.410139
C      4.360447    -1.122092    -0.104100
C      4.171241    -2.393579    -0.637237
C      2.894535    -2.948543    -0.656831
C      1.814258    -2.233216    -0.157132
H      3.445159     0.582366     0.818974
H      5.353720    -0.680402    -0.085463
H      5.016975    -2.953870    -1.027783
H      2.740169    -3.948720    -1.053956
H      0.825993    -2.688455    -0.148852

Frequencies
  32.2334     36.7074     62.8537     79.8839    102.7291    140.9976    162.0938
```

```
 201.9220   233.9321   249.8315   320.6483   335.5791   404.7800   412.1352
 414.6722   432.1336   490.8738   502.2870   565.9984   577.0150   619.9578
 622.4498   678.3991   697.0197   703.1412   717.1786   763.8322   770.6527
 808.6877   853.7621   858.7800   872.7499   887.8550   931.9852   948.8538
 978.3313   981.0810   984.5530  1000.6621  1002.7971  1006.4125  1009.5025
1027.0714  1049.9369  1052.1816  1077.7156  1088.6268  1106.1930  1112.7571
1154.4158  1157.0285  1181.5243  1185.8657  1239.5502  1311.7558  1313.2838
1324.7546  1354.0266  1367.3024  1371.6445  1396.7119  1441.3306  1456.7197
1472.7306  1477.6779  1522.0110  1526.0443  1632.6593  1639.6923  1658.6292
1663.5469  1666.4015  1749.1203  3040.5985  3119.0954  3173.1840  3179.4755
3180.6573  3184.1418  3186.4231  3191.6268  3192.7765  3196.5067  3197.2944
3202.7059  3206.0100  3209.6733

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                        -692.857935881
SCF energy, 6-31+G(d,p)                       -692.879650073
Zero-point correction                            0.252186
Thermal correction to Energy                     0.266657
Thermal correction to Enthalpy                   0.267601
Thermal correction to Gibbs Free Energy          0.209205
Sum of electronic and zero-point Energies    -692.605749
Sum of electronic and thermal Energies       -692.591279
Sum of electronic and thermal Enthalpies     -692.590335
Sum of electronic and thermal Free Energies  -692.648730
```

S.4.15 6-(2-Hydroxy-2-phenylethyl)cyclohexa-2,4-dienone (15)

```
Optimized cartesian coordinates (Standard orientation)
C      2.241992    -1.030312     0.397018
C      1.468502    -2.192378     0.323357
C      1.675735    -3.120017    -0.689846
C      2.664633    -2.899207    -1.647120
C      3.442073    -1.748649    -1.577805
C      3.232511    -0.820015    -0.560426
H      0.700134    -2.374869     1.075429
H      1.067611    -4.020725    -0.732015
H      2.828514    -3.624941    -2.440107
H      4.218647    -1.571112    -2.318581
H      3.841451     0.077994    -0.488913
C      1.963881    -0.005523     1.478438
H      1.867044    -0.550267     2.434942
C      0.610807     0.674273     1.240508
H      0.418853     1.375917     2.062046
H     -0.170098    -0.093322     1.297135
O      3.014022     0.918076     1.602608
```

```
H      2.685862     1.801412     1.338865
C      0.490137     1.414825    -0.110277
C     -0.789256     1.130719    -0.819007
C     -1.491317     2.084661    -1.450251
C     -1.033033     3.455385    -1.424888
C      0.081641     3.838263    -0.759277
C      0.860954     2.879636    -0.002794
H      1.277445     1.001589    -0.777629
H     -1.112256     0.090139    -0.836440
H     -2.406298     1.846023    -1.984559
H     -1.620458     4.203285    -1.954037
H      0.399362     4.876791    -0.717793
O      1.815059     3.230502     0.700262

Frequencies
  19.2442    40.2744    46.6660    76.7676   156.5473   194.7217   217.8169
 221.0074   267.9915   348.8002   389.4618   405.3189   413.5331   465.2571
 469.8861   507.3124   519.1980   536.9547   568.7880   582.0651   623.4462
 669.3366   687.9618   714.6012   735.8521   760.2889   792.1025   813.0298
 856.1991   860.7629   879.6312   921.6164   949.9372   974.4275   975.6706
 992.8136  1000.2920  1002.0722  1005.7475  1022.7557  1049.0325  1061.8350
1085.1711  1096.1590  1145.6753  1151.6736  1154.0977  1165.4033  1173.6339
1182.3675  1207.1818  1237.1402  1252.4098  1282.0201  1312.9351  1342.4550
1356.6668  1359.0507  1389.4496  1396.4382  1437.8860  1446.0787  1462.8254
1477.9498  1521.8936  1627.8085  1644.9179  1668.8453  1705.6788  1738.7344
2928.4010  2973.5725  3056.2455  3112.1919  3156.6375  3171.6834  3176.8821
3184.7448  3187.4505  3198.6300  3203.3622  3204.4524  3208.8482  3585.3593

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -691.883766183
SCF energy, 6-31+G(d,p)                         -691.909399185
Zero-point correction                              0.246425
Thermal correction to Energy                       0.259879
Thermal correction to Enthalpy                     0.260823
Thermal correction to Gibbs Free Energy            0.204494
Sum of electronic and zero-point Energies       -691.637341
Sum of electronic and thermal Energies          -691.623887
Sum of electronic and thermal Enthalpies        -691.622943
Sum of electronic and thermal Free Energies     -691.679272
```

S.4.16 2-(2-Oxocyclohexa-3,5-dienyl)-1-phenylethanolate (16)

```
Optimized cartesian coordinates (Standard orientation)
C     -2.002205     0.178703     0.486246
C     -1.919904     1.085073    -0.574966
```

C	-2.987790	1.257256	-1.453483
C	-4.159573	0.523113	-1.284779
C	-4.254246	-0.379798	-0.226562
C	-3.186148	-0.540295	0.650206
H	-0.998793	1.656093	-0.703341
H	-2.909225	1.972714	-2.270948
H	-4.995782	0.658591	-1.968094
H	-5.170625	-0.951193	-0.083127
H	-3.232965	-1.210275	1.507781
C	-0.856462	-0.048944	1.488361
C	0.135864	-1.087260	0.852645
H	0.916659	-1.277058	1.604334
H	-0.437751	-2.021707	0.751163
O	1.471734	1.508984	-0.390872
C	1.821994	0.328686	-0.363637
C	3.214963	-0.044418	-0.144546
C	0.832023	-0.800410	-0.523706
C	3.644510	-1.304206	-0.394068
H	3.901640	0.750990	0.137051
C	1.431115	-2.094485	-0.942717
H	0.043393	-0.478442	-1.218568
C	2.749172	-2.347730	-0.835845
H	4.701234	-1.542396	-0.281589
H	0.738938	-2.876481	-1.253682
H	3.155615	-3.326793	-1.074965
O	-1.239737	-0.509703	2.673010
H	-0.294677	0.932073	1.501985

Frequencies

26.9722	36.1119	55.8112	87.6417	127.3000	166.6873	187.1227
228.6628	258.5861	323.3002	352.1624	393.9828	416.7032	449.4460
471.7648	502.1008	534.6351	559.0824	591.3319	619.9607	626.4887
701.1645	715.1725	736.9821	756.8715	767.4541	787.3991	836.2234
871.6363	895.1185	916.0129	933.1124	973.0990	977.7550	979.3256
987.9149	992.6856	1002.7352	1007.5429	1012.5501	1036.9919	1047.1360
1066.0747	1105.7829	1142.2950	1146.0878	1151.7768	1167.4798	1183.5533
1219.9869	1245.2887	1261.5185	1273.3441	1287.5477	1308.0192	1355.6214
1363.3826	1388.3411	1392.8063	1427.8494	1445.1838	1472.2518	1507.1677
1610.4112	1640.9317	1656.8978	1699.7916	1749.6015	2687.0423	3011.4127
3055.5697	3076.9744	3137.9882	3155.0439	3163.1739	3165.5050	3168.2803
3175.9333	3182.9477	3192.3380	3200.1387			

Energies (Hartree/Particle):

SCF energy, 6-31G(d,p)	-691.352313660
SCF energy, 6-31+G(d,p)	-691.399771602

Zero-point correction	0.231444
Thermal correction to Energy	0.244940
Thermal correction to Enthalpy	0.245885
Thermal correction to Gibbs Free Energy	0.189638
Sum of electronic and zero-point Energies	-691.120870
Sum of electronic and thermal Energies	-691.107373
Sum of electronic and thermal Enthalpies	-691.106429
Sum of electronic and thermal Free Energies	-691.162676

S.4.17 2-(2-Hydroxy-2-phenylethyl)phenolate (17)

Optimized cartesian coordinates (Standard orientation)

C	1.600103	0.592542	0.157655
C	2.400568	-0.124742	1.048480
C	3.138380	-1.222612	0.618173
C	3.086179	-1.617570	-0.716736
C	2.292804	-0.905633	-1.612124
C	1.556193	0.192003	-1.176242
H	2.444563	0.185014	2.093777
H	3.760144	-1.769357	1.324168
H	3.664552	-2.473766	-1.056677
H	2.248773	-1.207072	-2.656939
H	0.930934	0.758038	-1.863878
C	0.752184	1.746827	0.650819
H	1.364633	2.315851	1.375274
C	-0.471240	1.219961	1.430601
H	-1.083485	2.105928	1.665462
H	-0.114261	0.818113	2.389896
O	0.382301	2.628051	-0.371840
C	-1.306554	0.169708	0.746722
C	-1.399193	-1.108034	1.288978
C	-2.201004	-2.106540	0.732099
C	-2.940401	-1.793529	-0.408006
C	-2.861981	-0.530680	-0.977944
C	-2.029727	0.497188	-0.449594
H	-0.524578	2.330691	-0.678816
H	-0.819158	-1.327450	2.189209
H	-2.251680	-3.095635	1.182281
H	-3.584409	-2.547284	-0.862693
H	-3.433647	-0.289036	-1.874990
O	-1.939981	1.650349	-1.022450

Frequencies

36.2367	44.5260	69.6058	108.6029	172.0593	218.9495	256.7584
264.9685	282.4586	359.3839	405.3842	416.4115	449.6557	478.4414

```
 508.4011   540.3458   553.9594   582.1357   592.7862   625.1499   683.1399
 713.9439   725.5921   735.8643   755.1009   765.0268   829.7360   832.0007
 843.3867   861.2896   883.1252   902.2288   918.3356   939.5903   943.6199
 973.4790   984.0162   994.5988  1006.1480  1051.8522  1056.9158  1093.9772
1106.8169  1136.2170  1140.3435  1154.3213  1176.7902  1179.0186  1203.8808
1244.5040  1254.7897  1270.0592  1316.1978  1351.2141  1352.3287  1360.2179
1385.0963  1388.2273  1441.7065  1478.3870  1492.2201  1523.6663  1535.8188
1568.8626  1598.8442  1647.4663  1652.5469  1669.1818  2952.1559  3000.1257
3063.0504  3098.0820  3121.5294  3137.5317  3146.8508  3155.8924  3168.0823
3179.6816  3180.2221  3192.1631  3197.7662

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -691.429234475
SCF energy, 6-31+G(d,p)                         -691.469141784
Zero-point correction                              0.233925
Thermal correction to Energy                       0.246684
Thermal correction to Enthalpy                     0.247628
Thermal correction to Gibbs Free Energy            0.193858
Sum of electronic and zero-point Energies       -691.195310
Sum of electronic and thermal Energies          -691.182551
Sum of electronic and thermal Enthalpies        -691.181607
Sum of electronic and thermal Free Energies     -691.235376
```

S.4.18 Benzaldehyde (18)

```
Optimized cartesian coordinates (Standard orientation)
C      2.938222     0.779720     0.117962
C      2.973012    -0.084212     1.214362
C      3.968202    -1.049040     1.307447
C      4.927003    -1.147448     0.302525
C      4.895569    -0.286329    -0.795755
C      3.903188     0.676320    -0.889485
H      2.214729     0.008410     1.990904
H      3.999126    -1.722650     2.159486
H      5.707162    -1.901336     0.374373
H      5.648975    -0.373197    -1.574274
H      3.855114     1.359816    -1.733709
C      1.880649     1.796275     0.036513
O      1.755015     2.596843    -0.869533
H      1.171020     1.787173     0.895940

Frequencies
 125.8167   230.0712   246.9164   417.4655   449.5742   459.7489   623.7602
 658.2954   699.1890   763.6838   843.5905   867.9221   946.7148   991.1636
1007.6628  1016.6658  1039.8082  1040.6934  1092.3199  1160.0553  1168.2998
```

```
1239.9389  1313.2979  1374.9252  1435.2414  1485.7365  1521.8921  1648.2123
1664.7425  1814.9118  2886.7897  3170.6786  3183.8336  3193.0560  3201.5676
3206.3974

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                        -345.340958443
SCF energy, 6-31+G(d,p)                       -345.354769175
Zero-point correction                            0.109786
Thermal correction to Energy                     0.116069
Thermal correction to Enthalpy                   0.117013
Thermal correction to Gibbs Free Energy          0.079308
Sum of electronic and zero-point Energies    -345.231172
Sum of electronic and thermal Energies       -345.224890
Sum of electronic and thermal Enthalpies     -345.223946
Sum of electronic and thermal Free Energies  -345.261650
```

S.4.19 Bicyclo[4.1.0]hepta-2,4-dien-2-olate (19)

```
Optimized cartesian coordinates (Standard orientation)
C      0.989539    -1.861296     0.474448
H      1.452788    -1.632075     1.433324
H      0.048645    -2.403241     0.535860
O      1.201113     1.518523    -0.485143
C      1.867562     0.448542    -0.378611
C      3.230206     0.346412    -0.069801
C      1.136625    -0.845555    -0.624065
C      3.939349    -0.892568    -0.169993
H      3.776910     1.268262     0.134098
C      1.908715    -2.164412    -0.679155
H      0.269658    -0.728039    -1.276303
C      3.371983    -2.079953    -0.507698
H      5.018452    -0.867705     0.008142
H      1.531655    -2.916953    -1.374752
H      3.969750    -2.981115    -0.634700

Frequencies
 152.2091   252.0101   319.9366   418.2060   492.2926   527.0789   569.4846
 618.8984   674.7904   746.2118   759.1347   781.6909   813.7004   881.1806
 933.1244   948.6200   998.4266  1007.8571  1034.1511  1050.4633  1087.2194
1107.8630  1149.4553  1200.4591  1255.5176  1353.6314  1373.1039  1398.0381
1451.8929  1467.8978  1614.3898  1664.9965  3104.3282  3108.5405  3111.8588
3126.3813  3143.2251  3166.9521  3208.3974

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                        -346.005383123
```

```
SCF energy, 6-31+G(d,p)                          -346.036588933
Zero-point correction                               0.118632
Thermal correction to Energy                        0.124935
Thermal correction to Enthalpy                      0.125879
Thermal correction to Gibbs Free Energy             0.088489
Sum of electronic and zero-point Energies        -345.886751
Sum of electronic and thermal Energies           -345.880448
Sum of electronic and thermal Enthalpies         -345.879504
Sum of electronic and thermal Free Energies      -345.916894
```

S.4.20 *o*-Cresolate ion (20)

```
Optimized cartesian coordinates (Standard orientation)
C     -1.018234     1.847820    -0.481836
H     -1.313882     1.872423    -1.540514
H     -0.721946     2.862467    -0.188733
O     -1.301713    -0.898094    -1.051444
C     -0.186116    -0.523685    -0.566812
C      0.899020    -1.424337    -0.308472
C      0.077606     0.858135    -0.235117
C      2.113625    -1.005989     0.218120
H      0.733835    -2.476983    -0.547678
C      1.301864     1.246050     0.289681
C      2.339818     0.336135     0.526817
H      2.901900    -1.741297     0.391628
H      1.453074     2.303670     0.524287
H      3.290211     0.667905     0.940501
H     -1.933324     1.586769     0.068827

Frequencies
 168.7067   191.6018   265.5102   313.4992   445.4155   454.9920   543.5346
 553.7718   584.8264   721.8415   729.1265   752.8674   822.6824   862.3809
 902.7735   940.7018   980.5137  1034.4903  1050.6202  1110.6268  1133.0440
1182.5804  1259.7604  1342.7847  1390.5151  1396.5931  1441.6608  1461.9190
1506.4865  1581.5714  1589.4992  1659.8370  3002.8015  3062.1423  3102.6165
3113.6043  3120.8714  3143.6343  3172.3299

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                           -346.057450675
SCF energy, 6-31G(d,p)                           -346.057462754
Zero-point correction                               0.118681
Thermal correction to Energy                        0.125407
Thermal correction to Enthalpy                      0.126351
Thermal correction to Gibbs Free Energy             0.088078
Sum of electronic and zero-point Energies        -345.938770
```

```
Sum of electronic and thermal Energies       -345.932044
Sum of electronic and thermal Enthalpies     -345.931100
Sum of electronic and thermal Free Energies  -345.969373
```

S.4.21 Benzyl alcohol (21)

```
Optimized cartesian coordinates (Standard orientation)
C      0.199142    -0.305789    -0.191696
C      1.030741     0.289469    -1.141894
C      2.410044     0.301465    -0.969068
C      2.975887    -0.274558     0.165642
C      2.152103    -0.863428     1.119865
C      0.771553    -0.882001     0.941240
H      0.589102     0.750244    -2.025285
H      3.045370     0.770220    -1.717113
H      4.054047    -0.260668     0.306689
H      2.585869    -1.312367     2.010762
H      0.123809    -1.338933     1.684752
C     -1.283699    -0.348985    -0.427232
O     -1.963618    -0.511219     0.796627
H     -1.593723     0.574365    -0.946231
H     -2.887413    -0.695618     0.598077
H     -1.512141    -1.179577    -1.117576

Frequencies
  59.4796   177.4336   220.8836   251.2928   411.4984   415.1812   467.8815
 586.5999   625.8248   706.1530   742.4249   802.2782   859.9419   912.8010
 976.3153   998.7566  1005.6593  1024.2832  1047.0874  1080.8917  1126.6371
1153.0537  1164.5405  1198.2867  1239.1823  1256.8584  1319.6414  1363.8839
1444.4706  1480.1632  1490.2144  1529.8185  1650.0325  1672.6688  2968.1869
3002.6613  3161.3468  3175.0304  3183.9283  3194.5420  3200.1434  3901.5882

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                        -346.538861774
SCF energy, 6-31+G(d,p)                       -346.555069388
Zero-point correction                            0.132702
Thermal correction to Energy                     0.139871
Thermal correction to Enthalpy                   0.140815
Thermal correction to Gibbs Free Energy          0.100966
Sum of electronic and zero-point Energies    -346.406160
Sum of electronic and thermal Energies       -346.398991
Sum of electronic and thermal Enthalpies     -346.398046
Sum of electronic and thermal Free Energies  -346.437895
```

S.4.22 4-Oxo-1,4-diphenyl-1-butanolate (22)

Cartesian coordinates of the freq job (Standard orientation)

C	-2.664635	0.255881	-0.611593
C	-2.914081	-1.110756	-0.753425
C	-4.076001	-1.688552	-0.244186
C	-5.013678	-0.902685	0.420564
C	-4.781582	0.465306	0.561126
C	-3.622846	1.032164	0.042188
H	-2.191322	-1.729465	-1.288746
H	-4.254536	-2.755008	-0.374057
H	-5.923499	-1.349972	0.815995
H	-5.515175	1.089212	1.070195
H	-3.427155	2.102247	0.099225
C	-1.398353	0.955609	-1.145517
C	-0.279099	0.812330	-0.059496
H	0.569121	1.395826	-0.445975
H	-0.621270	1.323298	0.854742
O	-1.576067	2.222372	-1.479580
H	-1.030384	0.261416	-1.979423
C	3.874527	-0.296891	1.244570
C	5.123784	-0.106767	0.672302
C	5.242211	0.017122	-0.710662
C	4.108438	-0.050562	-1.515331
C	2.857517	-0.242940	-0.940878
C	2.727584	-0.368257	0.447023
H	3.758578	-0.395623	2.320896
H	6.009137	-0.053801	1.301207
H	6.220368	0.167000	-1.161496
H	4.198428	0.047324	-2.594218
H	1.978528	-0.288394	-1.580910
C	1.409912	-0.581772	1.119790
C	0.167532	-0.614991	0.281946
H	0.325277	-1.180115	-0.647739
H	-0.611329	-1.130105	0.856034
O	1.350398	-0.675880	2.340681

Frequencies

24.5075	32.6760	52.9806	58.8418	71.4523	113.1766	157.3393
175.8670	204.7666	230.0998	258.0397	333.5280	373.8874	394.7461
413.0180	414.3963	439.5999	479.8828	490.9650	549.3975	607.0287
621.0185	626.1614	636.0061	693.4485	708.6504	712.9777	730.7247
752.7275	768.1995	805.1408	835.4294	862.6744	863.4350	910.2905
946.8455	955.3809	968.5022	985.0581	987.0413	1002.9738	1006.2237
1011.4242	1021.9951	1025.4530	1039.7919	1047.1402	1060.0825	1071.6109

```
1105.8935  1126.0151  1144.9532  1151.2470  1156.8544  1175.3390  1189.3022
1202.7177  1244.5758  1278.4225  1284.0750  1285.2958  1308.5379  1313.4747
1329.8885  1354.4716  1372.3149  1395.2483  1441.5209  1467.6095  1470.3461
1478.6514  1505.8874  1526.9105  1639.2569  1642.9137  1653.7670  1665.4614
1770.1754  2520.5682  3008.7679  3034.4484  3071.5022  3105.8500  3138.9760
3158.0434  3166.7553  3175.4060  3178.7948  3185.9149  3187.8825  3193.9547
3201.3101  3206.2027

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                        -768.744266540
SCF energy, 6-31+G(d,p)                       -768.794074630
Zero-point correction                            0.265972
Thermal correction to Energy                     0.281382
Thermal correction to Enthalpy                   0.282326
Thermal correction to Gibbs Free Energy          0.221040
Sum of electronic and zero-point Energies    -768.478295
Sum of electronic and thermal Energies       -768.462884
Sum of electronic and thermal Enthalpies     -768.461940
Sum of electronic and thermal Free Energies  -768.523226
```

S.4.23 1-Phenylcyclopropanolate (23)

```
Optimized cartesian coordinates (Standard orientation)
C     -0.260137    -0.405737    -0.748235
H     -0.321763     0.674872    -0.886554
H      0.415729    -0.911944    -1.436303
C     -3.965337    -0.996978    -0.354322
C     -5.161207    -0.317379    -0.144684
C     -5.151814     0.982557     0.352731
C     -3.927387     1.587979     0.635127
C     -2.735613     0.903523     0.423646
C     -2.727802    -0.407815    -0.076643
H     -3.934395    -2.013832    -0.740274
H     -6.109147    -0.804718    -0.370644
H     -6.083469     1.519686     0.518730
H     -3.901198     2.604964     1.023994
H     -1.796313     1.405844     0.656096
C     -1.492959    -1.241791    -0.338512
C     -0.340137    -0.947672     0.650829
H     -0.459419    -0.238935     1.472130
H      0.281777    -1.811100     0.884080
O     -1.664744    -2.450735    -0.818020

Frequencies
  81.0993   164.0747   222.2001   332.9155   347.4394   425.0894   438.8423
```

```
 450.7216   493.2267   558.0362   622.8781   674.0304   703.1774   719.1669
 783.4630   785.2768   855.0217   867.0959   871.4550   917.6618   949.4336
 969.7543   983.5987   991.4047   998.4999  1035.2071  1046.4069  1074.4376
1107.7105  1141.0155  1169.5716  1178.1164  1250.6286  1301.1515  1355.4191
1402.5474  1428.1035  1455.5770  1473.6028  1508.3249  1629.7971  1654.3594
3086.9157  3093.5768  3155.1379  3159.7583  3170.4139  3181.1347  3185.0272
3189.9843  3197.2845

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -423.358335215
SCF energy, 6-31+G(d,p)                         -423.395620192
Zero-point correction                              0.152265
Thermal correction to Energy                       0.160329
Thermal correction to Enthalpy                     0.161273
Thermal correction to Gibbs Free Energy            0.119568
Sum of electronic and zero-point Energies      -423.206070
Sum of electronic and thermal Energies         -423.198006
Sum of electronic and thermal Enthalpies       -423.197062
Sum of electronic and thermal Free Energies    -423.238767
```

S.4.24 1-Phenyl-1-propanone (24)

```
Optimized cartesian coordinates (Standard orientation)
C      1.505820    -1.504006    -0.058379
H      0.715428    -1.916599     0.578412
H      2.439476    -1.526413     0.513422
C     -0.356953     1.728474    -1.035167
C     -1.633896     2.198943    -1.299164
C     -2.723339     1.332662    -1.219270
C     -2.530098    -0.001388    -0.874265
C     -1.250179    -0.471170    -0.604349
C     -0.149980     0.389606    -0.682703
H      0.507272     2.385180    -1.092571
H     -1.785526     3.241142    -1.568484
H     -3.725410     1.700188    -1.426378
H     -3.378743    -0.677480    -0.812916
H     -1.116348    -1.515473    -0.332819
C      1.243889    -0.058323    -0.406841
C      1.657989    -2.333558    -1.333410
H      0.739077    -2.334406    -1.930403
H      1.904167    -3.371730    -1.092741
O      2.180143     0.722077    -0.507575
H      2.462195    -1.929027    -1.957771

Frequencies
```

```
  43.4505    80.2277   144.0481   200.2935   238.0065   257.0696   385.6075
 412.7178   445.0162   478.1533   583.0670   622.3454   694.8709   710.1641
 734.4165   791.6854   805.3832   859.2869   943.9474   947.8975   987.8282
1006.4491  1009.1833  1028.3669  1047.3157  1068.5893  1096.8442  1114.1794
1157.2034  1175.1149  1233.4105  1290.6469  1311.3245  1335.8867  1367.7483
1390.0488  1456.7467  1466.6945  1474.4872  1482.1602  1520.2799  1641.7809
1660.6295  1788.2137  3039.6989  3067.9732  3116.5307  3132.7562  3140.8014
3184.3170  3190.7743  3197.1463  3202.7111  3208.3961

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -423.916032796
SCF energy, 6-31+G(d,p)                         -423.930680148
Zero-point correction                              0.166238
Thermal correction to Energy                       0.175353
Thermal correction to Enthalpy                     0.176298
Thermal correction to Gibbs Free Energy            0.131394
Sum of electronic and zero-point Energies       -423.749795
Sum of electronic and thermal Energies          -423.740679
Sum of electronic and thermal Enthalpies        -423.739735
Sum of electronic and thermal Free Energies     -423.784639
```

S.4.25 1,2-Dihydroxy-1-phenylethanide (25)

```
Optimized cartesian coordinates (Standard orientation)
C      0.812850    -0.225276    -0.609483
C      1.232877    -1.062811     0.481362
C      2.313614    -0.744023     1.277468
C      3.053387     0.434921     1.091467
C      2.643286     1.290639     0.067857
C      1.563146     0.991168    -0.750012
H      0.675275    -1.975743     0.693114
H      2.584667    -1.426227     2.084893
H      3.896716     0.679281     1.732993
H      3.179921     2.226227    -0.098964
H      1.284326     1.675048    -1.549812
C     -0.257371    -0.538009    -1.461457
C     -1.249421    -1.560397    -1.161771
H     -1.845652    -1.799960    -2.053518
H     -0.795364    -2.489256    -0.787656
O     -0.695431     0.459201    -2.373632
H     -2.031205     0.738555     0.027597
O     -1.550441    -0.203653     2.512175
H     -3.007253    -1.665699    -0.152980
O     -2.218456    -1.108091    -0.118957
H     -0.697229     1.421905     0.236705
```

```
H     -1.117179     1.161133    -1.849686
H     -1.647271    -0.755128     1.717314
O     -1.647145     1.621222     0.204439
H     -1.628970     0.679831     2.128436

Frequencies
  45.2933    52.9885    76.7366   105.6702   152.4870   159.8145   182.0121
 201.8253   230.8583   244.9485   253.2125   278.9413   322.0793   374.0150
 392.0264   425.3853   440.0873   448.9306   473.6170   492.9263   522.3562
 589.3904   623.6062   689.9291   704.3843   709.9017   740.9498   791.1661
 809.8938   817.7520   821.6607   886.6563   924.3975   947.6752   956.9587
 970.3333  1032.7069  1049.6064  1080.6447  1139.6879  1152.3092  1171.4935
1206.4498  1249.8410  1294.9716  1329.9156  1364.4821  1378.7475  1424.2183
1459.4485  1485.3937  1536.7288  1564.0768  1648.1991  1659.9511  1726.4457
3010.1745  3068.6519  3130.4858  3135.3818  3154.5793  3171.5440  3182.9305
3632.5194  3711.5152  3740.7408  3779.1820  3835.7512  3858.5190

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                        -613.286312700
SCF energy, 6-31+G(d,p)                       -613.336544500
Zero-point correction                            0.203277
Thermal correction to Energy                     0.217723
Thermal correction to Enthalpy                   0.218667
Thermal correction to Gibbs Free Energy          0.162668
Sum of electronic and zero-point Energies    -613.083036
Sum of electronic and thermal Energies       -613.068590
Sum of electronic and thermal Enthalpies     -613.067646
Sum of electronic and thermal Free Energies  -613.123644
```

S.4.26 2-Hydroxy-2-phenylethanolate (26)

The free anion is stabilized by an internal hydrogen bond ($\Delta E = -43$ kJ mol^{-1}). The is the open conformer used for the calculations.

```
Optimized cartesian coordinates (Standard orientation)
C      0.510946    -0.812129    -1.680939
C      0.169426    -2.164946    -1.561837
C     -0.563977    -2.801396    -2.555661
C     -0.966559    -2.100366    -3.692347
C     -0.640230    -0.753674    -3.815037
C      0.087240    -0.113997    -2.813081
H      0.460514    -2.682560    -0.651629
H     -0.823702    -3.853160    -2.447819
H     -1.531346    -2.602005    -4.475396
H     -0.953893    -0.195026    -4.695028
H      0.331377     0.943065    -2.902544
```

```
C      1.249173    -0.141593    -0.562413
C      0.330405     0.018338     0.691678
H      0.937272     0.728831     1.343054
H     -0.498329     0.705350     0.303010
O      1.738841     1.143041    -0.919907
H      2.080954    -0.796776    -0.240924
O     -0.047072    -1.116869     1.246737
H      2.299860     1.039218    -1.697074

Frequencies
  70.0692   118.0025   170.2043   239.4735   259.7077   324.4925   369.9679
 391.7083   421.8635   489.9417   562.1330   618.9361   624.7490   710.9099
 756.6727   781.7372   847.9101   897.7649   935.2542   961.6031   982.7354
1002.4926  1037.3102  1050.8337  1081.0911  1114.1554  1151.8292  1172.8410
1197.0921  1221.6749  1255.0345  1282.9364  1312.2232  1328.6219  1348.1775
1378.5528  1410.9627  1474.8993  1507.3211  1521.4981  1637.9272  1663.1526
2535.9387  2595.3622  2951.4302  3165.2752  3171.8672  3180.6302  3191.1859
3211.3740  3871.2847

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -460.488473804
SCF energy, 6-31+G(d,p)                         -460.531647186
Zero-point correction                              0.151637
Thermal correction to Energy                       0.160438
Thermal correction to Enthalpy                     0.161382
Thermal correction to Gibbs Free Energy            0.117738
Sum of electronic and zero-point Energies       -460.336837
Sum of electronic and thermal Energies          -460.328036
Sum of electronic and thermal Enthalpies        -460.327092
Sum of electronic and thermal Free Energies     -460.370736
```

S.4.27 2-(4-Hydroxybenzyl)phenol dianion (27)

Intermediate carbanion stabilised by H_2O molecules.

```
Optimized cartesian coordinates (Standard orientation)
C     -1.025561     0.024149    -0.150266
C      0.406595     0.150218     0.001141
C      1.002256     1.396920     0.128392
C      0.270725     2.590234     0.113329
C     -1.113087     2.500945    -0.043042
C     -1.738351     1.268045    -0.173107
H      2.089959     1.433829     0.249617
H      0.766877     3.553866     0.213527
H     -1.716161     3.410909    -0.063886
H     -2.822102     1.210520    -0.295461
```

```
C      1.240936    -1.106062     0.053170
H      0.722312    -1.870714    -0.543427
H      2.215369    -0.919230    -0.425720
C      1.486390    -1.624071     1.451042
C      2.733641    -1.519546     2.074795
C      0.450548    -2.190393     2.208790
C      2.951319    -1.958823     3.375241
H      3.563282    -1.078251     1.513029
C      0.647712    -2.634792     3.506754
H     -0.533437    -2.260958     1.738981
C      1.916274    -2.544358     4.178863
H      3.941185    -1.864680     3.827550
H     -0.180050    -3.073533     4.069774
O      2.102469    -2.947256     5.372913
O     -1.612084    -1.103307    -0.260116

Frequencies
  47.7150    57.6636    76.7353   133.1918   173.9219   213.6225   275.2071
 327.8421   371.6374   439.1313   443.0046   458.4261   475.3019   508.3003
 532.6459   548.2371   572.6902   606.6402   639.7512   719.0697   721.8311
 730.6925   777.8135   795.0755   807.3247   830.2818   838.0736   846.4070
 864.8585   903.4772   909.6369   928.2720   932.9352   981.5711   990.2356
1048.1851  1076.0736  1100.0739  1131.6856  1151.0575  1162.5582  1183.3639
1216.7705  1252.4254  1254.6756  1306.0480  1332.2938  1345.5916  1398.7661
1419.9867  1435.8450  1456.1033  1496.3244  1566.0998  1574.2073  1584.1374
1591.4655  1652.3508  1669.7629  2997.8231  3059.2188  3100.0826  3101.9563
3118.4617  3120.8407  3131.7656  3137.7777  3140.6314  3172.2919

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -651.633989194
SCF energy, 6-31+G(d,p)                         -651.692964017
Zero-point correction                              0.191288
Thermal correction to Energy                       0.203059
Thermal correction to Enthalpy                     0.204003
Thermal correction to Gibbs Free Energy            0.152502
Sum of electronic and zero-point Energies       -651.442701
Sum of electronic and thermal Energies          -651.430931
Sum of electronic and thermal Enthalpies        -651.429986
Sum of electronic and thermal Free Energies     -651.481487
```

S.5 Transition states

S.5.1 Carbanion route, A2

```
Cartesian coordinates of the freq job (Standard orientation)
C      2.163860     0.126080    -0.373500
```

C	1.759117	-1.219496	-0.264310
C	2.685314	-2.254331	-0.228487
C	4.052194	-1.991051	-0.299979
C	4.472375	-0.667367	-0.410392
C	3.548683	0.370148	-0.447493
H	0.696978	-1.455894	-0.212545
H	2.334340	-3.282269	-0.150007
H	4.775557	-2.802745	-0.272517
H	5.535488	-0.438822	-0.472195
H	3.889177	1.399728	-0.535809
C	1.197156	1.236555	-0.361563
H	0.977896	1.636068	0.934802
C	-0.162416	0.901882	-0.931150
H	-0.636757	1.835202	-1.270746
H	-0.140290	0.198780	-1.788048
O	-0.963839	0.314314	0.103678
C	-2.253855	-0.003233	-0.157736
C	-2.972086	-0.528547	0.923765
C	-2.877672	0.165534	-1.394856
C	-4.300262	-0.888374	0.763454
H	-2.450533	-0.627917	1.874683
C	-4.216014	-0.201278	-1.536887
H	-2.335647	0.576656	-2.241152
C	-4.933024	-0.729145	-0.470684
H	-4.849166	-1.295940	1.609614
H	-4.697889	-0.069749	-2.503440
H	-5.975077	-1.011972	-0.595322
O	1.710157	2.418194	-0.992177
H	2.025079	2.174165	-1.874027
O	0.757724	2.064063	2.100166
H	-0.136682	2.403214	1.982715
H	0.286275	0.518734	2.656591
O	-0.014133	-0.420077	2.801598
H	-0.198249	-0.673448	1.890186

Frequencies

-1389.9275	16.0998	37.1810	52.6812	56.0828	83.0706	88.9276
115.6580	131.8026	152.9399	171.0617	208.8658	240.8892	246.8108
285.3615	304.2391	324.9504	385.4933	411.3877	417.5967	420.3619
427.1472	481.1280	494.3386	505.3199	518.7333	544.0446	560.5290
599.8777	618.7428	625.4386	645.0327	662.8101	703.2637	714.9793
759.9443	763.1645	796.9586	833.0924	851.7430	854.8414	897.3316
902.6828	949.8548	967.2838	974.3077	980.9723	987.3552	993.4799
998.6257	1001.6692	1042.0430	1045.3182	1056.9829	1064.9070	1088.8642
1104.6894	1132.6198	1148.2521	1152.4704	1178.5280	1182.0191	1235.8458

```
 1269.4718  1286.8433  1305.1785  1317.3170  1326.2100  1359.9049  1367.1892
 1376.2987  1449.6512  1462.8027  1474.4600  1485.1454  1520.9278  1529.7690
 1619.5472  1645.8148  1648.0904  1660.0706  1664.6682  1722.7802  2925.5914
 3040.5314  3159.1876  3163.4343  3172.1690  3175.8919  3175.9527  3185.9361
 3186.8078  3193.5093  3201.5226  3219.8577  3293.7775  3790.1181  3896.9052
 3914.5866

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                        -844.157225225
SCF energy, 6-31+G(d,p)                       -844.214964611
Zero-point correction                            0.278817
Thermal correction to Energy                     0.297000
Thermal correction to Enthalpy                   0.297944
Thermal correction to Gibbs Free Energy          0.231189
Sum of electronic and zero-point Energies    -843.878408
Sum of electronic and thermal Energies       -843.860225
Sum of electronic and thermal Enthalpies     -843.859281
Sum of electronic and thermal Free Energies  -843.926036
```

S.5.2 Carbanion route, A4

```
Cartesian coordinates of the freq job (Standard orientation)
C      2.233557     0.385865    -0.383536
C      2.032047    -0.891710    -1.000519
C      3.080670    -1.760425    -1.239977
C      4.394963    -1.450095    -0.868730
C      4.612842    -0.222783    -0.235166
C      3.580747     0.668147     0.005768
H      1.020381    -1.189792    -1.280472
H      2.868143    -2.717027    -1.719497
H      5.211080    -2.145297    -1.050885
H      5.621822     0.047801     0.080021
H      3.787707     1.613218     0.504733
C      1.187566     1.302054    -0.175432
H      1.049228     0.801192     1.942520
C     -0.157166     1.146130    -0.690717
H     -0.640776     2.125073    -0.809020
H     -0.218980     0.589952    -1.640956
O     -1.039820     0.353869     0.247043
C     -2.327905     0.119763    -0.099656
C     -3.025704    -0.787787     0.710581
C     -2.982145     0.720779    -1.179523
C     -4.356377    -1.075810     0.452849
H     -2.478556    -1.265141     1.522563
C     -4.321127     0.417368    -1.425436
```

```
H     -2.464399     1.422856    -1.825473
C     -5.017886    -0.472683    -0.617979
H     -4.883403    -1.781697     1.091504
H     -4.821486     0.892908    -2.266708
H     -6.061579    -0.699416    -0.820205
O      1.467910     2.532538     0.477970
H      1.952435     3.094750    -0.141152
O      0.434960     0.662531     2.688264
H     -0.402266     0.750158     2.206047
H      0.241854    -1.221211     2.327593
O     -0.010701    -1.974462     1.764726
H     -0.204492    -1.507020     0.940198

Frequencies
-138.1725    17.2556    29.8406    41.8663    67.0670    88.4512    89.4710
 103.3628   134.1746   158.4992   165.8096   184.4018   214.5790   240.5955
 244.8424   257.9984   301.7559   308.1903   350.9046   363.1620   379.9660
 419.2886   424.2210   444.4354   480.3828   500.3369   523.1115   542.9749
 550.1003   609.3800   620.2602   622.4288   662.1797   702.2824   703.3733
 704.1394   721.2354   746.9974   760.6798   799.6693   806.3522   810.1326
 834.5489   854.0662   897.2163   934.0933   944.2550   954.2921   967.8191
 972.5897   987.6625  1000.0865  1037.5963  1054.9725  1068.3144  1092.8114
1107.9908  1140.0351  1151.9843  1175.0754  1179.0898  1185.5256  1240.8560
1253.1200  1288.0908  1320.4660  1330.3260  1365.4440  1367.1521  1378.5854
1427.2440  1455.0577  1485.1195  1487.7868  1526.1785  1535.9967  1575.0432
1639.2297  1641.3784  1660.8324  1675.2364  1708.9519  2984.4816  3072.6652
3135.3975  3139.9558  3153.3579  3169.2990  3174.8473  3179.0910  3184.5206
3185.9345  3198.1200  3222.2244  3687.0657  3726.1341  3792.5763  3817.9431
3855.7941

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -844.161359269
SCF energy, 6-31+G(d,p)                         -844.214156975
Zero-point correction                              0.281303
Thermal correction to Energy                       0.300371
Thermal correction to Enthalpy                     0.301315
Thermal correction to Gibbs Free Energy            0.232774
Sum of electronic and zero-point Energies       -843.880056
Sum of electronic and thermal Energies          -843.860988
Sum of electronic and thermal Enthalpies        -843.860044
Sum of electronic and thermal Free Energies     -843.928586
```

S.5.3 Alkoxide route, A8

```
Optimized cartesian coordinates (Standard orientation)
```

C	-2.328687	0.412168	-0.312969
C	-2.394626	-0.812369	-0.981071
C	-3.320044	-1.775102	-0.592576
C	-4.195797	-1.521304	0.462380
C	-4.135607	-0.300480	1.128352
C	-3.204301	0.659676	0.741405
H	-1.703565	-1.002326	-1.804318
H	-3.364728	-2.727971	-1.116801
H	-4.922991	-2.273177	0.761842
H	-4.819574	-0.095228	1.949923
H	-3.137093	1.626360	1.236453
C	-1.318765	1.464178	-0.707497
C	-0.039339	1.409970	-0.002005
H	0.767502	2.041821	-0.354297
H	-0.100148	1.203536	1.060422
O	0.920002	-0.214230	-0.451556
C	2.216732	-0.195115	-0.224491
C	3.117160	-0.811849	-1.126790
C	2.779814	0.422518	0.916804
C	4.484316	-0.818648	-0.890494
H	2.700814	-1.274425	-2.020897
C	4.152326	0.413944	1.136998
H	2.118657	0.897635	1.639599
C	5.021733	-0.205307	0.241876
H	5.144546	-1.306255	-1.607154
H	4.548932	0.898329	2.028766
H	6.094344	-0.209810	0.420828
O	-1.422944	2.685646	-0.101464
H	-1.212418	1.464797	-1.815226
O	0.345070	-1.118822	-2.982849
H	0.524426	-0.759702	-2.081750
H	0.242645	-2.061862	-2.822345

Frequencies

-558.4654	29.2255	45.7004	49.0248	64.3313	88.9574	93.3497
141.2853	169.5345	177.9465	208.7191	230.7305	263.4395	293.1967
302.1938	365.6408	394.0607	418.8292	424.3279	425.1489	502.8166
535.2170	545.3359	557.8937	607.6048	620.7161	626.7433	706.9336
716.0031	753.9506	760.8501	770.5405	828.8118	840.9092	853.4969
875.0603	879.2168	922.5905	951.7068	959.7038	974.1677	986.9810
988.4585	1004.0877	1012.0813	1022.9704	1036.3309	1048.5245	1072.0928
1082.0872	1096.0146	1138.1449	1144.1516	1150.5182	1165.5730	1175.2421
1197.4917	1254.8207	1275.0627	1303.6208	1308.5198	1345.6490	1357.7247
1361.0141	1378.1471	1430.8949	1479.3246	1480.6344	1519.2525	1527.2646
1616.0124	1645.1518	1652.5224	1656.2706	1666.4340	2870.5554	3152.8210

```
3156.4064  3162.8928  3169.2602  3170.2727  3176.0017  3176.3837  3179.9658
3187.1681  3190.6835  3194.7751  3300.0797  3472.6712  3936.8425

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                        -767.742616483
SCF energy, 6-31+G(d,p)                       -767.790066345
Zero-point correction                            0.255273
Thermal correction to Energy                     0.271535
Thermal correction to Enthalpy                   0.272479
Thermal correction to Gibbs Free Energy          0.210135
Sum of electronic and zero-point Energies    -767.487344
Sum of electronic and thermal Energies       -767.471081
Sum of electronic and thermal Enthalpies     -767.470137
Sum of electronic and thermal Free Energies  -767.532482
```

S.5.4 Alkoxide route, A10

```
Optimized cartesian coordinates (Standard orientation)
C     -0.467108     0.451499    -0.187130
C     -0.745877    -0.899696    -0.412726
C     -1.977652    -1.430382    -0.046187
C     -2.944658    -0.617127     0.544030
C     -2.669367     0.728855     0.769078
C     -1.433197     1.258628     0.407731
H      0.029067    -1.516014    -0.872054
H     -2.189401    -2.483368    -0.222503
H     -3.909919    -1.032750     0.825526
H     -3.421980     1.367338     1.228084
H     -1.189930     2.306432     0.572564
C      0.878129     1.012186    -0.546405
C      1.886204     1.029050     0.493335
H      2.925148     1.163933     0.229170
H      1.568933     1.189141     1.514761
O      1.098085     2.360542    -0.331153
H      1.217950     0.602286    -1.515397
O      2.363548    -1.903028    -1.383033
H      2.097473    -2.815898    -1.244861
O      2.371904    -0.929598     1.023970
H      2.389956    -1.520747    -0.435316
H      1.471605    -1.172457     1.267915

Frequencies
-605.5725    55.6824    62.0704    83.0706   122.5996   173.8081   191.9628
 218.7678   268.7693   300.2906   325.3867   368.0094   388.0993   418.7568
 431.8210   544.3892   568.4759   596.5831   624.0105   661.8998   718.0720
```

```
 762.9252   774.1467   878.1019   923.5568   954.5921   990.2939  1003.3084
1006.5918  1008.0180  1045.7057  1054.5046  1077.8028  1086.7874  1124.4129
1153.4350  1167.3257  1198.8585  1245.0864  1280.8063  1316.8713  1361.3306
1381.1629  1453.7794  1483.8934  1522.7630  1646.3384  1666.5384  1698.6293
2736.0605  2973.4133  3155.9249  3165.0966  3173.3771  3188.2495  3193.7058
3194.1432  3326.3468  3882.6630  3941.3075

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                        -536.844990567
SCF energy, 6-31+G(d,p)                       -536.897548891
Zero-point correction                            0.173871
Thermal correction to Energy                     0.185666
Thermal correction to Enthalpy                   0.186611
Thermal correction to Gibbs Free Energy          0.135915
Sum of electronic and zero-point Energies    -536.671120
Sum of electronic and thermal Energies       -536.659324
Sum of electronic and thermal Enthalpies     -536.658380
Sum of electronic and thermal Free Energies  -536.709075
```

S.5.5 Tautomerisation, A12

```
Optimized cartesian coordinates (Standard orientation)
C      1.989206    -0.087908    -0.029393
C      1.734761    -1.131440     0.881460
C      2.585956    -2.224301     0.991764
C      3.723703    -2.326816     0.193350
C      3.988847    -1.308766    -0.720987
C      3.140203    -0.214601    -0.830400
H      0.846571    -1.092703     1.511028
H      2.350845    -3.013340     1.704898
H      4.385869    -3.185597     0.277352
H      4.868748    -1.369097    -1.360513
H      3.346269     0.572068    -1.553404
C      1.177625     1.142273    -0.097043
C     -0.228445     1.042706     0.376112
H     -0.280308     0.728151     1.430931
H     -0.711171     2.029115     0.297288
O     -0.989292     0.101777    -0.417158
C     -2.290971    -0.088318    -0.116672
C     -2.976394    -1.016418    -0.913452
C     -2.975235     0.566981     0.912265
C     -4.316501    -1.283483    -0.684455
H     -2.426734    -1.515321    -1.708616
C     -4.323840     0.286513     1.129717
H     -2.470185     1.291651     1.543241
```

```
C     -5.003768    -0.633139     0.341449
H     -4.831299    -2.006928    -1.313128
H     -4.844155     0.802851     1.933924
H     -6.055029    -0.842981     0.521078
O      1.232828     1.766109    -1.390536
H      1.823996     2.143551     0.511500
O      2.471421     3.264557     0.463880
H      1.720384     2.584896    -1.160286
H      3.365521     2.928149     0.336888

Frequencies
-1611.6824    25.0817    43.0840    48.2873    52.0594    75.7492   123.8244
  163.1687   188.6653   230.4389   242.0498   253.7580   317.5638   327.9940
  369.4225   416.0505   420.7297   435.5579   454.2028   500.3911   523.0100
  531.1342   587.4735   618.3905   620.5192   621.5557   701.1026   706.7099
  722.5971   741.4386   757.6327   759.6025   802.1376   830.2399   842.9619
  864.9872   882.2797   898.6984   919.6333   957.7046   965.6664   975.4872
  983.5335   992.0353   995.1868   999.1410  1045.4621  1049.6821  1065.1780
 1093.6911  1098.7248  1141.7507  1148.8056  1163.0031  1176.3104  1184.8427
 1239.8169  1283.9868  1304.8012  1320.9433  1326.9094  1359.4967  1367.9715
 1376.9594  1428.7672  1450.6258  1473.1788  1485.0203  1521.1090  1531.4271
 1604.9318  1622.4380  1644.0306  1656.8824  1665.6435  1679.4552  2994.5251
 3048.1412  3154.1109  3158.8551  3172.0725  3173.1377  3179.4791  3185.3469
 3190.7446  3191.7874  3201.4101  3220.3970  3569.6413  3891.3491

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -767.744875620
SCF energy, 6-31+G(d,p)                         -767.797024872
Zero-point correction                              0.253632
Thermal correction to Energy                       0.269221
Thermal correction to Enthalpy                     0.270166
Thermal correction to Gibbs Free Energy            0.208981
Sum of electronic and zero-point Energies       -767.491243
Sum of electronic and thermal Energies          -767.475654
Sum of electronic and thermal Enthalpies        -767.474710
Sum of electronic and thermal Free Energies     -767.535894
```

S.5.6 Scheme 3, B3

```
Optimized cartesian coordinates (Standard orientation)
C      2.118046    -1.218283     0.061891
C      2.524097    -1.883592     1.221013
C      3.673000    -2.665752     1.236318
C      4.438906    -2.808181     0.081584
C      4.042689    -2.157553    -1.082273
```

C	2.894601	-1.368480	-1.089489
H	1.901918	-1.781741	2.107238
H	3.969610	-3.173933	2.151964
H	5.335199	-3.424375	0.088164
H	4.627564	-2.265290	-1.993506
H	2.606285	-0.864471	-2.009841
C	0.837963	-0.375951	0.115740
O	0.000507	-0.783029	1.057432
H	0.807917	0.280838	-1.996915
C	0.183804	-0.231455	-1.258271
H	-0.052828	-1.232365	-1.641094
H	-0.756455	0.320954	-1.160089
O	-0.361211	1.957339	1.941367
C	0.276055	2.053236	0.886578
C	1.457692	1.199348	0.603504
C	2.399874	1.730165	-0.383131
C	2.053778	2.713715	-1.245340
C	0.755643	3.329070	-1.142429
C	-0.111700	2.998558	-0.152909
H	1.929083	0.883456	1.540502
H	3.381656	1.263541	-0.453519
H	2.745254	3.058125	-2.010254
H	0.484972	4.098149	-1.864909
H	-1.068698	3.504353	-0.032408
H	-1.147590	-1.355785	0.612376
C	-2.998130	0.319962	0.509461
C	-4.085511	1.161114	0.303898
C	-5.250051	0.701422	-0.309037
C	-5.309769	-0.630212	-0.717590
C	-4.230779	-1.483245	-0.522824
C	-3.052864	-1.024412	0.093672
H	-2.092440	0.677628	0.997833
H	-4.019160	2.197810	0.633864
H	-6.095991	1.366820	-0.464896
H	-6.210158	-1.011198	-1.197523
H	-4.271980	-2.522677	-0.844790
O	-2.040389	-1.865660	0.265593

Frequencies

-440.4723	35.6635	42.6947	48.4208	55.2922	60.1780	85.8772
103.8421	110.8480	140.1996	184.5638	200.8415	230.1402	237.4964
241.3455	263.4920	283.7184	317.8536	361.0890	375.3997	413.4496
429.5782	432.5961	461.3491	470.4261	490.7123	496.3424	532.1406
535.1464	561.9273	568.4911	598.0711	607.4908	619.2627	621.1887
709.3853	713.5637	726.2886	746.6954	764.4805	770.6683	783.0024

```
 807.8619   835.8153   848.9603   856.4962   864.2888   909.1372   910.7755
 922.8290   969.3195   973.2655   978.2643   985.7928   991.9002   994.0980
1001.9924  1003.4979  1006.7443  1009.5127  1030.7707  1043.6651  1047.9615
1058.7567  1067.8689  1089.7863  1095.5591  1123.8056  1136.4358  1145.4195
1148.3245  1150.0419  1176.4218  1181.6493  1184.2675  1237.3275  1260.6550
1293.7733  1310.8214  1335.8556  1353.2028  1357.2475  1359.9591  1365.1753
1373.3739  1400.0640  1431.1537  1450.4843  1457.2749  1463.3095  1467.8156
1496.5665  1517.0163  1554.4000  1577.7732  1599.8156  1640.9631  1645.3650
1660.0646  1685.9549  1695.3147  1729.0563  3039.5483  3097.5641  3126.3168
3146.6916  3153.9686  3159.1791  3161.1601  3168.6593  3174.4683  3175.9181
3176.9556  3181.5577  3188.6608  3189.0047  3195.2032  3197.5654  3198.6899
3199.4318

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                        -998.670977413
SCF energy, 6-31+G(d,p)                       -998.718024083
Zero-point correction                            0.334054
Thermal correction to Energy                     0.353870
Thermal correction to Enthalpy                   0.354815
Thermal correction to Gibbs Free Energy          0.285029
Sum of electronic and zero-point Energies    -998.336923
Sum of electronic and thermal Energies       -998.317107
Sum of electronic and thermal Enthalpies     -998.316163
Sum of electronic and thermal Free Energies  -998.385949
```

S.5.7 Scheme 3, B6

```
Optimized cartesian coordinates (Standard orientation)
C     -1.745758    -1.487030     0.378196
C     -1.326207    -1.775699    -0.923333
C     -2.204425    -2.331163    -1.843284
C     -3.516126    -2.628358    -1.473173
C     -3.936867    -2.363835    -0.175477
C     -3.056204    -1.795403     0.743673
H     -0.304566    -1.534538    -1.209033
H     -1.868200    -2.533978    -2.858078
H     -4.204138    -3.063057    -2.194633
H     -4.955685    -2.596992     0.126436
H     -3.404422    -1.582754     1.753084
C     -0.759065    -0.924488     1.374596
O      0.330245    -1.548520     1.519010
H     -2.134892     0.447747     2.388283
C     -1.328065    -0.258907     2.606964
H     -1.710184    -1.024893     3.294429
H     -0.513081     0.268298     3.109858
```

O	-0.202128	0.599605	0.477434
C	-0.892304	1.646192	0.097429
C	-2.300559	1.686226	-0.054046
C	-2.945004	2.844713	-0.475975
C	-2.237044	4.006954	-0.771155
C	-0.847787	3.986385	-0.633332
C	-0.191506	2.842245	-0.208034
H	-2.883923	0.789949	0.143744
H	-4.029787	2.833028	-0.580997
H	-2.751805	4.905934	-1.102052
H	-0.266615	4.880157	-0.859377
H	0.892826	2.828414	-0.099516
H	1.358331	-1.708547	0.274031
C	4.154755	-1.117206	-1.179488
C	5.256050	-0.280163	-1.049335
C	5.304850	0.678588	-0.039376
C	4.228415	0.789633	0.838541
C	3.118737	-0.039417	0.720142
C	3.075647	-1.004477	-0.294705
H	4.107589	-1.871494	-1.962470
H	6.086663	-0.380596	-1.745412
H	6.168528	1.331341	0.060153
H	4.250526	1.536401	1.630434
H	2.260308	0.051556	1.382384
O	2.035070	-1.839459	-0.453987

Frequencies

-213.8795	21.5753	27.5340	30.1222	44.7800	47.8757	64.5410
79.6191	98.0322	99.9243	144.2017	174.6930	193.9256	214.1287
238.0600	254.6830	280.4765	295.0135	351.6607	380.5741	411.3542
419.0391	421.2248	464.7576	477.3931	508.7708	518.4507	530.5231
536.7103	562.5559	577.2758	598.3388	623.4707	624.6027	626.2563
698.6738	705.1518	712.5616	739.7113	753.9827	756.3654	779.3437
825.4567	830.3777	840.9658	848.6646	862.6160	863.4243	878.3072
924.2693	942.3906	955.2024	958.3649	968.2705	974.0587	975.7887
982.9695	984.6652	1000.9840	1001.5138	1004.1451	1014.4305	1044.4667
1047.3327	1047.5804	1088.6500	1090.0526	1094.3923	1103.6111	1142.0097
1150.0318	1154.2791	1165.4868	1175.4413	1175.9190	1278.3429	1284.1074
1292.3814	1314.8377	1333.9966	1340.3766	1355.7075	1358.5259	1367.1216
1372.0944	1427.0051	1438.2363	1448.3827	1470.6202	1478.6074	1509.4851
1518.0023	1523.3075	1545.6381	1576.2131	1611.1563	1645.2302	1651.6802
1653.2325	1667.5744	1671.5746	3034.7485	3121.8533	3139.5020	3148.4564
3153.8612	3154.1729	3167.8353	3170.4570	3170.5521	3172.6030	3177.3819
3184.6025	3185.1015	3188.3241	3193.3622	3195.0063	3195.5555	3199.0521
3199.1350						

```
Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -998.691845434
SCF energy, 6-31+G(d,p)                         -998.737419313
Zero-point correction                              0.336005
Thermal correction to Energy                       0.356458
Thermal correction to Enthalpy                     0.357402
Thermal correction to Gibbs Free Energy            0.284085
Sum of electronic and zero-point Energies       -998.355841
Sum of electronic and thermal Energies          -998.335387
Sum of electronic and thermal Enthalpies        -998.334443
Sum of electronic and thermal Free Energies     -998.407761
```

S.5.8 Scheme 4, C2

```
Optimized cartesian coordinates (Standard orientation)
C      2.294216    -1.096032    -0.118209
C      3.447751    -1.825027     0.157114
C      4.696462    -1.209666     0.119313
C      4.785264     0.148416    -0.179630
C      3.632131     0.877183    -0.440058
C      2.373449     0.267180    -0.425475
H      1.317896    -1.570239    -0.048639
H      3.371698    -2.882017     0.405321
H      5.596305    -1.784908     0.326723
H      5.757152     0.637557    -0.204917
H      3.675104     1.941534    -0.659433
C      1.168337     1.117453    -0.726607
O      1.308521     2.363870    -0.687797
C     -0.069619     0.474937    -0.968262
H     -0.082503    -0.554870    -1.323359
H     -0.833188     1.120209    -1.404140
C     -0.953871    -0.017673     0.963364
C     -0.648556     1.285513     1.678308
H     -1.289888     1.370024     2.568332
H      0.393673     1.257979     2.011600
H     -0.784010     2.179252     1.062519
O     -0.415331    -1.066839     1.392089
C     -2.328025    -0.132008     0.340049
C     -2.767477    -1.395470    -0.063211
C     -4.024773    -1.571703    -0.627022
C     -4.880120    -0.482642    -0.783272
C     -4.460547     0.779648    -0.371654
C     -3.197077     0.953000     0.184421
H     -2.089223    -2.233528     0.081680
```

```
H     -4.345458    -2.563272    -0.941166
H     -5.867130    -0.617197    -1.220268
H     -5.122447     1.636345    -0.482456
H     -2.882439     1.948131     0.493451

Frequencies
-294.2282    28.0970    44.3367    64.6818    80.9834    96.8854   148.2429
 166.3177   226.2523   229.4110   244.7884   270.4592   328.7721   375.6823
 389.9924   415.4020   417.6368   419.4684   437.9504   479.1870   497.7569
 545.7843   595.6411   608.2053   622.5284   626.5455   689.0127   706.0280
 710.6532   731.1317   746.8131   771.1725   794.7480   806.2274   847.7237
 856.9622   860.6786   925.2181   930.4086   964.5483   974.9221   977.4531
 990.0054   997.2876  1004.4814  1006.4648  1017.1221  1037.9282  1043.7860
1049.8988  1081.6123  1086.7752  1100.4130  1124.8678  1149.4393  1153.7073
1177.7199  1180.0021  1266.2519  1315.9723  1317.0405  1322.7636  1360.4613
1365.2800  1372.1986  1449.1408  1455.3047  1462.0754  1469.9791  1473.3371
1517.8869  1520.8918  1593.3694  1628.1597  1648.9337  1656.9419  1663.4328
1669.8416  3016.4822  3114.4844  3118.1199  3152.3806  3164.8175  3167.6981
3171.7235  3174.7027  3182.7831  3188.6426  3189.1980  3194.2275  3195.7060
3205.9243  3212.2714

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -768.747159569
SCF energy, 6-31+G(d,p)                         -768.789118209
Zero-point correction                              0.263891
Thermal correction to Energy                       0.279244
Thermal correction to Enthalpy                     0.280189
Thermal correction to Gibbs Free Energy            0.220463
Sum of electronic and zero-point Energies       -768.483269
Sum of electronic and thermal Energies          -768.467915
Sum of electronic and thermal Enthalpies        -768.466971
Sum of electronic and thermal Free Energies     -768.526697
```

S.5.9 Scheme 4, C4

```
Optimized cartesian coordinates (Standard orientation)
C      2.969663    -1.574320    -1.275861
C      4.136878    -2.323808    -1.377700
C      5.365042    -1.751434    -1.058862
C      5.422193    -0.420392    -0.651311
C      4.256722     0.329359    -0.566277
C      3.014718    -0.239048    -0.863349
H      2.016902    -2.026508    -1.544261
H      4.087943    -3.357873    -1.711182
H      6.276380    -2.340363    -1.132757
```

H	6.379248	0.033029	-0.403268
H	4.282171	1.374317	-0.266388
C	1.792332	0.636264	-0.766935
O	1.958343	1.866058	-0.842767
C	0.536796	-0.029159	-0.567996
H	-1.689924	0.651023	2.764266
H	0.590055	-1.081038	-0.296381
C	-0.709080	0.568198	-0.514427
C	-0.966265	1.939010	-1.064681
H	-1.919911	2.337237	-0.711041
H	-0.155365	2.619500	-0.809748
H	-1.014047	1.869473	-2.162298
O	-0.869296	1.368165	1.548100
C	-1.903654	-0.317909	-0.417892
C	-3.091572	0.117659	0.188045
C	-4.209934	-0.705507	0.229925
C	-4.178953	-1.975571	-0.344336
C	-3.015038	-2.411744	-0.964504
C	-1.891851	-1.589391	-1.002165
H	-3.120922	1.094652	0.667053
H	-5.116818	-0.352280	0.717125
H	-5.058395	-2.614543	-0.313537
H	-2.977713	-3.393520	-1.431140
H	-0.995568	-1.931940	-1.515044
H	0.070710	1.562916	1.616591
O	-2.895802	2.938182	2.161609
H	-3.123893	2.226126	2.778801
H	-2.032359	2.559249	1.841563
O	-2.398435	0.333885	3.403325
H	-2.945133	-0.221591	2.837705

Frequencies

-146.7409	27.5280	38.7478	50.7171	54.4823	59.1603	83.9630
106.2879	113.7081	128.4135	149.9436	166.1659	175.4801	204.4886
222.7381	260.7500	267.9470	305.7183	307.1285	323.1550	338.5514
345.7460	362.9642	398.9955	417.4782	422.6380	429.7917	493.3476
523.8405	537.0217	550.7569	562.2931	575.1039	583.0508	622.5858
626.3880	633.9673	681.1348	702.1349	716.6850	724.4132	764.2619
769.0775	809.1700	836.0622	866.0263	870.1255	878.6276	942.0783
943.9259	955.6745	969.3723	984.7285	989.6990	1004.6183	1005.3644
1006.9168	1023.8479	1039.9977	1042.8545	1052.5622	1053.1810	1087.8700
1096.9883	1105.0397	1125.4629	1154.4423	1155.3716	1180.9792	1185.1052
1247.8544	1304.7608	1314.2064	1317.0780	1354.1584	1363.4456	1367.2534
1415.0168	1439.1326	1455.0873	1469.9575	1474.8405	1516.5410	1521.8268
1568.9665	1634.5682	1639.8790	1660.7506	1664.5418	1697.5223	1715.6417

```
1744.3277  3018.9847  3075.6659  3127.4988  3171.2585  3173.4627  3177.2974
3179.7718  3184.4993  3186.3383  3190.2126  3191.4262  3192.2628  3196.8833
3198.3231  3201.9220  3300.9997  3807.2371  3908.7501  3911.2899

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                        -921.554770244
SCF energy, 6-31+G(d,p)                       -921.615690432
Zero-point correction                            0.315472
Thermal correction to Energy                     0.336302
Thermal correction to Enthalpy                   0.337246
Thermal correction to Gibbs Free Energy          0.265264
Sum of electronic and zero-point Energies    -921.239298
Sum of electronic and thermal Energies       -921.218469
Sum of electronic and thermal Enthalpies     -921.217524
Sum of electronic and thermal Free Energies  -921.289507
```

S.5.10 Scheme 5, D2

```
Cartesian coordinates of the freq job (Standard orientation)
C      2.489526     0.280029    -0.284569
C      3.002824     1.492268    -0.738340
C      4.055001     2.112176    -0.070057
C      4.603463     1.524057     1.065494
C      4.094632     0.312563     1.528327
C      3.048410    -0.305415     0.853209
H      2.561606     1.956296    -1.618312
H      4.446794     3.058156    -0.437622
H      5.424529     2.008092     1.589412
H      4.518246    -0.152917     2.415619
H      2.657608    -1.257979     1.211262
C      1.380418    -0.433183    -1.020650
H      1.086815     0.179472    -1.888506
C      0.114508    -0.477645    -0.152237
H     -0.869707    -0.530774    -0.596090
H      0.171169    -0.216471     0.894571
O     -0.115671     1.581312    -0.476793
C     -1.301875     2.051877    -0.225282
C     -1.762992     3.215070    -0.903087
C     -2.203108     1.484744     0.717083
C     -3.009260     3.766277    -0.649688
H     -1.091098     3.667263    -1.632416
C     -3.453985     2.043568     0.951325
H     -1.904576     0.595662     1.271383
C     -3.877694     3.188359     0.278977
H     -3.313428     4.662207    -1.191153
```

H	-4.111760	1.573793	1.682933
H	-4.856912	3.620260	0.472080
O	1.899968	-1.669484	-1.439107
H	1.158430	-2.242010	-1.763404
C	-0.071313	-2.570735	0.388970
C	-0.735275	-2.452103	1.639335
C	-2.099923	-2.541976	1.737964
C	-2.842775	-2.857475	0.571453
C	-2.233959	-3.077305	-0.636626
C	-0.806562	-2.978115	-0.792857
H	1.005721	-2.725630	0.378833
H	-0.135817	-2.225854	2.522025
H	-2.607451	-2.398090	2.688017
H	-3.926984	-2.938377	0.642966
H	-2.813130	-3.339834	-1.520398
O	-0.251850	-3.156264	-1.918309

Frequencies

-653.3072	8.5671	34.9149	43.9263	47.8704	63.6701	64.7223
82.9045	96.5671	160.7692	162.5781	177.9277	186.3072	225.5334
238.7677	252.4155	272.2726	356.3496	372.1158	413.4492	423.1425
425.0668	475.4015	485.5724	516.4944	526.7113	527.3269	540.7107
553.2665	572.8471	613.1210	618.7634	621.7048	637.3242	707.5964
711.1985	734.6913	752.7842	767.0709	770.2179	780.8619	821.7934
823.1666	840.2701	849.5264	854.7205	856.5447	857.0312	890.0470
923.2392	952.3365	961.2669	964.4404	967.0897	969.7808	982.1447
983.6439	990.8984	996.1565	1002.7609	1008.0757	1025.8585	1038.3643
1042.0664	1054.3916	1074.9865	1082.0301	1095.5882	1105.7463	1142.4657
1144.3364	1148.5540	1153.8187	1160.6540	1162.3660	1184.0815	1230.1422
1275.6749	1280.7374	1291.3369	1321.6231	1344.9860	1348.9650	1361.5973
1372.4341	1374.2154	1411.3953	1414.0469	1473.5647	1475.3307	1480.2305
1490.8921	1525.1807	1532.8666	1573.2576	1600.4001	1603.7083	1649.6623
1650.8251	1668.2988	1674.2028	3004.6310	3145.0767	3147.1256	3148.4007
3156.4978	3162.4850	3165.8307	3167.3862	3171.9085	3177.2057	3181.2397
3186.1425	3187.8926	3188.8349	3196.4873	3196.7407	3208.5835	3322.2937
3338.9836						

Energies (Hartree/Particle):

SCF energy, 6-31G(d,p)	-998.606014540
SCF energy, 6-31+G(d,p)	-998.655604299
Zero-point correction	0.337199
Thermal correction to Energy	0.357053
Thermal correction to Enthalpy	0.357997
Thermal correction to Gibbs Free Energy	0.285971
Sum of electronic and zero-point Energies	-998.268816

```
Sum of electronic and thermal Energies       -998.248962
Sum of electronic and thermal Enthalpies     -998.248018
Sum of electronic and thermal Free Energies  -998.320043
```

S.5.11 Scheme 5, D6

```
Optimized cartesian coordinates (Standard orientation)
C     -2.056788    -0.300363     0.517974
C     -2.032424     0.727582    -0.430268
C     -3.004012     0.785863    -1.425435
C     -4.007621    -0.178218    -1.484070
C     -4.037923    -1.202899    -0.538123
C     -3.071711    -1.259326     0.457949
H     -1.229833     1.465558    -0.382964
H     -2.980380     1.589108    -2.159489
H     -4.765313    -0.131551    -2.263264
H     -4.823257    -1.955346    -0.578554
H     -3.083328    -2.042795     1.213465
C     -1.035469    -0.369451     1.604921
C      0.495640    -1.308317     0.501886
H      1.158913    -1.381924     1.361039
H     -0.095870    -2.195895     0.285634
O      1.107193     1.868771    -0.180193
C      1.733807     0.772703    -0.230596
C      3.090964     0.605605     0.116070
C      0.984623    -0.453458    -0.667789
C      3.754492    -0.611248    -0.083395
H      3.623985     1.482321     0.479761
C      1.766158    -1.661811    -0.927027
H      0.161018    -0.214575    -1.350516
C      3.133314    -1.734676    -0.606589
H      4.812000    -0.669041     0.176731
H      1.284413    -2.467228    -1.475199
H      3.680524    -2.661226    -0.756589
O     -1.189004    -1.107740     2.601781
H     -0.421702     0.557020     1.667325
O      2.722759     3.815741     0.934649
H      2.117201     3.168896     0.506900
H      2.744537     3.517573     1.848249

Frequencies
-738.0943    20.9189    35.7541    54.6712    77.5485    92.4074   102.8413
 130.8573   146.4743   174.0980   189.7633   200.1925   232.4227   252.9460
 277.8064   349.2039   402.1657   412.7492   424.9898   461.8637   479.3318
 522.2882   533.7565   560.1107   578.9286   620.7481   643.5964   686.2305
```

```
 712.8899   717.8390   747.0778   768.5740   794.6305   812.6132   837.9002
 847.7057   870.0292   872.6008   895.6979   936.6152   961.2848   970.9520
 984.3927   988.2753  1002.8970  1008.3002  1025.1994  1041.4732  1046.0824
1064.2603  1074.8342  1086.9209  1146.5490  1153.3735  1161.6131  1167.7085
1199.8996  1218.8432  1280.3336  1313.1319  1361.1508  1365.3597  1385.1786
1393.0565  1414.0054  1430.0045  1474.9771  1517.3885  1528.4478  1566.4215
1618.4788  1633.4361  1657.9109  1660.7938  1669.5093  2890.7423  3076.1137
3131.8957  3147.8723  3154.7727  3165.5529  3171.7179  3182.0867  3184.4494
3188.8412  3190.8278  3203.2314  3249.0510  3508.4528  3946.4897

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -767.728754231
SCF energy, 6-31+G(d,p)                         -767.776540479
Zero-point correction                              0.253887
Thermal correction to Energy                       0.270519
Thermal correction to Enthalpy                     0.271463
Thermal correction to Gibbs Free Energy            0.208164
Sum of electronic and zero-point Energies       -767.474868
Sum of electronic and thermal Energies          -767.458235
Sum of electronic and thermal Enthalpies        -767.457291
Sum of electronic and thermal Free Energies     -767.520590
```

S.5.12 Scheme 5, D8

```
Optimized cartesian coordinates (Standard orientation)
C      0.996186    -1.559539     1.341157
H      0.923493    -0.737566     2.072423
H      2.033714    -1.929139     1.372392
O     -1.662969    -0.751340     0.017023
C     -0.559757    -0.195559    -0.015374
C     -0.428837     1.248101     0.075204
C      0.713771    -0.995876    -0.091926
C      0.765026     1.862002    -0.143417
H     -1.339153     1.817466     0.252955
C      1.922423    -0.224885    -0.455951
H      0.542170    -1.870193    -0.737228
C      1.965885     1.127546    -0.424653
H      0.817259     2.950010    -0.111793
H      2.824707    -0.801377    -0.660557
H      2.893157     1.667589    -0.597999
O     -0.726754    -3.518257     1.203509
H     -1.335513    -2.930015     0.742321
H      0.142021    -2.551413     1.425024

Frequencies
```

```
-1599.3837    53.8781   121.5734   134.2524   198.6799   235.2833   331.9947
  381.7064   423.9817   464.4263   496.7964   521.3793   581.8024   602.4957
  694.0178   726.4402   757.9333   782.4818   842.0451   912.8367   958.3914
  962.5680   991.5915  1003.9707  1028.9439  1035.5106  1058.9727  1141.7447
 1162.1549  1193.5048  1257.6056  1357.7647  1388.6658  1432.6349  1450.2024
 1478.0026  1581.8988  1674.6413  1693.6355  1733.9834  2996.1447  3032.5247
 3061.4037  3159.3082  3162.9836  3186.0790  3192.6011  3881.7198
```

```
Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -422.362927359
SCF energy, 6-31+G(d,p)                         -422.410121081
Zero-point correction                              0.137882
Thermal correction to Energy                       0.146870
Thermal correction to Enthalpy                     0.147814
Thermal correction to Gibbs Free Energy            0.103881
Sum of electronic and zero-point Energies       -422.225045
Sum of electronic and thermal Energies          -422.216058
Sum of electronic and thermal Enthalpies        -422.215113
Sum of electronic and thermal Free Energies     -422.259046
```

S.5.13 Scheme 6, E2

```
Optimized cartesian coordinates (Standard orientation)
C     -1.900614    -0.051699     0.364504
C     -1.968270     0.823246    -0.722845
C     -3.087750     0.830246    -1.549213
C     -4.153179    -0.032459    -1.295978
C     -4.089415    -0.904986    -0.213019
C     -2.967809    -0.912473     0.611799
H     -1.115843     1.476089    -0.917488
H     -3.133697     1.513973    -2.395090
H     -5.029966    -0.022662    -1.940163
H     -4.919551    -1.578945    -0.008916
H     -2.893275    -1.576376     1.470825
C     -0.687694    -0.091131     1.268910
C      0.367295    -1.050604     0.850434
H      1.300298    -1.029324     1.406524
H     -0.000980    -2.029991     0.555229
O      1.177392     1.756888    -0.759742
C      1.824575     0.671631    -0.645879
C      3.147333     0.625311    -0.085684
C      1.259125    -0.611597    -1.004970
C      3.879186    -0.539605    -0.060885
H      3.569013     1.561691     0.278848
C      2.083389    -1.762691    -1.074058
```

```
H      0.318358    -0.590923    -1.556963
C      3.364037    -1.752739    -0.568796
H      4.889292    -0.523460     0.348024
H      1.658432    -2.685756    -1.468264
H      3.974348    -2.651976    -0.567385
O     -0.792835    -0.839807     2.398198
H     -0.286726     0.937314     1.395248
O      1.527522     2.859992     1.717036
H      1.401928     2.592160     0.778699
H      1.822986     2.040317     2.125341

Frequencies
-624.3250    37.8949    42.2233    55.4601    74.9891    78.9765    98.7890
 137.5315   169.6390   187.2236   214.6480   248.3889   265.0421   271.3754
 299.8028   359.9455   415.0750   418.8470   442.2013   465.1418   477.8430
 515.7845   545.1791   548.5557   601.6407   611.7809   621.2588   715.0265
 723.3440   748.5801   760.2079   767.7680   768.5642   829.9365   842.6846
 873.0383   883.0518   920.2206   942.8926   971.9928   976.1463   986.4020
 988.5060  1000.4964  1002.2426  1010.8359  1032.3040  1037.5191  1067.3706
1074.5003  1076.3971  1119.7876  1143.4480  1146.9575  1157.8522  1162.1741
1194.2455  1267.9541  1276.1873  1296.3262  1303.2560  1355.4828  1358.1689
1390.2962  1406.6341  1411.3461  1471.5902  1476.3787  1516.9389  1571.8329
1593.1696  1643.3530  1654.2500  1662.4178  1711.1311  2913.5519  3147.9539
3151.2498  3155.0195  3157.7612  3161.3804  3167.1814  3172.5219  3173.4924
3187.5139  3192.8217  3194.5867  3278.6220  3519.5917  3935.0146

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -767.733820912
SCF energy, 6-31+G(d,p)                         -767.782986169
Zero-point correction                              0.255165
Thermal correction to Energy                       0.271391
Thermal correction to Enthalpy                     0.272335
Thermal correction to Gibbs Free Energy            0.210586
Sum of electronic and zero-point Energies       -767.478655
Sum of electronic and thermal Energies          -767.462430
Sum of electronic and thermal Enthalpies        -767.461486
Sum of electronic and thermal Free Energies     -767.523235
```

S.5.14 Scheme 7, F2

```
Cartesian coordinates of the freq job (Standard orientation)
C      2.826983     0.641907     0.016186
C      3.186292     0.335363     1.328803
C      4.267580    -0.500193     1.590171
C      5.007434    -1.032113     0.536542
```

```
C      4.658402    -0.723625    -0.776198
C      3.573689     0.108758    -1.033003
H      2.608808     0.760103     2.150925
H      4.538204    -0.732754     2.618032
H      5.856887    -1.680570     0.739177
H      5.237267    -1.132339    -1.602087
H      3.288533     0.374047    -2.049360
C      1.637107     1.512337    -0.274997
C      0.440831     0.861195    -0.797498
H     -0.494719     1.405605    -0.793219
H      0.555749     0.012268    -1.462218
O      1.539332     2.056609    -1.535240
H      1.451041     2.198456     0.576036
C     -3.838088    -1.116395    -0.494116
C     -5.122876    -0.594469    -0.402568
C     -5.348524     0.582953     0.305813
C     -4.277200     1.226717     0.920272
C     -2.995134     0.694282     0.832993
C     -2.753029    -0.490321     0.126705
H     -3.635166    -2.027514    -1.052148
H     -5.952523    -1.104024    -0.889166
H     -6.351105     0.999073     0.376461
H     -4.440423     2.152964     1.467684
H     -2.171013     1.219061     1.312450
C     -1.388705    -1.126815    -0.020694
C     -0.333338    -0.620374     0.746555
H     -0.509917     0.017887     1.610404
H      0.591217    -1.196943     0.761195
O     -1.267003    -2.034178    -0.889005

Frequencies
-711.4269    17.8435    29.5332    44.5178    50.3556    61.5210   100.1162
 150.9109   170.0634   204.9376   238.7411   276.7500   286.0459   373.4999
 396.0176   412.3675   416.3085   420.2220   435.5576   485.7670   547.9201
 595.0238   602.7953   621.9423   622.6414   668.1601   695.6361   711.5545
 711.9101   744.2847   751.5134   765.1126   778.5509   803.9864   862.0872
 862.5226   913.6459   930.2662   935.5247   975.0445   977.7601   993.8626
 996.8479  1000.5344  1003.0993  1005.2161  1025.0248  1042.4318  1046.2369
1048.2317  1088.6590  1090.8193  1115.1906  1126.5580  1150.9238  1151.8291
1167.1701  1176.9660  1201.3368  1222.7091  1272.4292  1308.4388  1314.5310
1324.4649  1358.4794  1363.0773  1385.8229  1441.2854  1464.3774  1473.1680
1483.3169  1516.3413  1522.8032  1620.8185  1649.4076  1655.9785  1663.3549
1666.8662  2918.3551  3130.0196  3156.4093  3165.9307  3171.0511  3172.9637
3174.3099  3178.2593  3182.8664  3187.1257  3192.0062  3194.8998  3199.6793
3222.4802  3308.2060
```

Energies (Hartree/Particle):

SCF energy, 6-31G(d,p)	-768.675777535
SCF energy, 6-31+G(d,p)	-768.721484616
Zero-point correction	0.262769
Thermal correction to Energy	0.278536
Thermal correction to Enthalpy	0.279480
Thermal correction to Gibbs Free Energy	0.216798
Sum of electronic and zero-point Energies	-768.413009
Sum of electronic and thermal Energies	-768.397241
Sum of electronic and thermal Enthalpies	-768.396297
Sum of electronic and thermal Free Energies	-768.458980

S.5.15 Scheme 7, F4

Optimized cartesian coordinates (Standard orientation)

C	-2.831868	0.412670	-0.779233
C	-2.990185	-0.974438	-0.856321
C	-3.947135	-1.617499	-0.078784
C	-4.757124	-0.878622	0.780267
C	-4.611074	0.507879	0.854069
C	-3.660254	1.149864	0.074638
H	-2.356979	-1.542795	-1.537548
H	-4.065914	-2.696663	-0.145560
H	-5.506553	-1.380546	1.387846
H	-5.247799	1.084996	1.521209
H	-3.535259	2.230306	0.110337
C	-1.849255	1.104531	-1.637843
C	0.062753	0.574634	-0.038789
H	0.613938	1.174805	-0.752894
H	-0.482914	1.078642	0.751164
O	-1.823464	2.324004	-1.798509
H	-1.261518	0.417481	-2.287127
C	3.672486	-0.179172	1.310731
C	4.984031	0.013456	0.892442
C	5.291853	0.037507	-0.464964
C	4.266289	-0.132764	-1.394741
C	2.955887	-0.318704	-0.974290
C	2.628568	-0.340070	0.391200
H	3.412367	-0.214437	2.365996
H	5.773858	0.140946	1.631097
H	6.316991	0.184622	-0.797455
H	4.491248	-0.119468	-2.459707
H	2.176299	-0.437364	-1.725464
C	1.258363	-0.598322	0.941599

```
C      0.176720    -0.910445    -0.020554
H      0.443851    -1.367372    -0.980462
H     -0.672987    -1.427388     0.438547
O      1.095109    -0.675704     2.194357

Frequencies
-529.6658    14.4602    20.3091    48.0915    55.1664    70.4517    99.8670
 120.9918   165.0277   196.0036   228.0592   237.0272   287.2896   350.5375
 372.5768   418.4468   420.0475   429.0095   450.1166   469.1467   497.0305
 527.3359   585.3453   601.0022   621.2597   621.9560   653.0931   671.1894
 702.3830   707.2071   739.2963   753.8192   770.6957   835.1099   846.5178
 855.3388   857.7635   913.1553   919.9281   956.4875   969.6674   973.9844
 978.6937   993.7471   994.7034   999.0147  1002.5702  1042.5415  1043.0966
1058.2203  1088.8468  1091.5213  1114.7636  1146.9930  1155.0014  1163.3432
1166.5450  1179.1568  1190.6934  1230.7900  1298.7904  1311.1424  1311.7781
1363.6226  1364.2342  1402.9597  1423.0044  1440.3744  1467.3701  1476.5182
1516.4646  1516.9746  1572.3980  1636.0942  1637.4936  1654.3017  1658.4000
1731.0585  2892.8692  3040.1671  3120.9820  3160.5061  3162.1332  3164.8978
3172.7161  3175.9247  3179.7581  3182.4748  3189.4850  3192.3029  3197.8988
3198.7225  3294.9062

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -768.693498349
SCF energy, 6-31+G(d,p)                         -768.738004290
Zero-point correction                              0.261491
Thermal correction to Energy                       0.277631
Thermal correction to Enthalpy                     0.278575
Thermal correction to Gibbs Free Energy            0.214833
Sum of electronic and zero-point Energies       -768.432008
Sum of electronic and thermal Energies          -768.415867
Sum of electronic and thermal Enthalpies        -768.414923
Sum of electronic and thermal Free Energies     -768.478665
```

S.5.16 Scheme 7, F6

```
Optimized cartesian coordinates (Standard orientation)
C     -1.685599    -1.695083     0.502799
H     -1.235445    -2.701017     0.543155
H     -2.731949    -1.811040     0.195971
C      1.040521     0.549506    -0.934316
C      2.420723     0.700480    -0.938400
C      3.238099    -0.298804    -0.412749
C      2.662512    -1.442797     0.131436
C      1.278965    -1.586237     0.151884
C      0.450649    -0.593468    -0.382575
```

```
H      0.389902     1.335577    -1.313250
H      2.865817     1.602524    -1.353225
H      4.319544    -0.182887    -0.422331
H      3.293082    -2.227080     0.544381
H      0.842002    -2.482279     0.586601
C     -1.036125    -0.758675    -0.459262
C     -1.532549    -0.800540     1.733614
H     -0.689974    -1.132254     2.356201
H     -2.452846    -0.799696     2.334410
O     -1.690293    -0.090308    -1.272377
O     -1.544873     2.711156    -1.050977
H     -1.668102     1.804268    -1.374255
H     -1.371923     2.524244    -0.099535
O     -1.120143     1.909049     1.564312
H     -1.260550     0.842997     1.546344
H     -1.911754     2.219758     2.015127

Frequencies
-165.4469    51.2212    70.3639    89.8504   114.1475   129.4686   180.0641
 208.4068   243.1225   255.9654   265.1034   310.6791   356.6479   380.4116
 415.9387   425.9773   490.4172   515.1554   558.7607   585.4996   623.5765
 625.5801   649.5629   712.6583   728.3069   759.7861   791.0908   840.6978
 868.8330   899.0654   942.0086   984.8775   987.3388  1003.2690  1024.8117
1044.2984  1062.2921  1115.5499  1124.4938  1154.3796  1179.0910  1193.5287
1206.7327  1262.1845  1310.2961  1334.4902  1363.2889  1425.8830  1462.9658
1471.9760  1526.8899  1594.6364  1635.6177  1660.2067  1686.6178  1727.3710
1780.4859  2971.9527  3010.6725  3074.6128  3093.9042  3173.2647  3181.0988
3191.2837  3195.1996  3201.3028  3532.9570  3778.1423  3916.0892

Energies (Hartree/Particle):
SCF energy, 6-31G(d,p)                          -576.165889260
SCF energy, 6-31+G(d,p)                         -576.212502238
Zero-point correction                              0.199869
Thermal correction to Energy                       0.212957
Thermal correction to Enthalpy                     0.213901
Thermal correction to Gibbs Free Energy            0.160693
Sum of electronic and zero-point Energies       -575.966020
Sum of electronic and thermal Energies          -575.952932
Sum of electronic and thermal Enthalpies        -575.951988
Sum of electronic and thermal Free Energies     -576.005197
```

S.5.17 Scheme 8, G1

```
Optimized cartesian coordinates (Standard orientation)
C     -0.287824     0.550213    -0.618329
```

C	-0.812745	-0.697459	-1.008895
C	-2.071897	-1.114831	-0.601337
C	-2.856909	-0.307793	0.224319
C	-2.347771	0.923841	0.632811
C	-1.088660	1.346247	0.221817
H	-0.204765	-1.346149	-1.642272
H	-2.444120	-2.087433	-0.921090
H	-3.841834	-0.637046	0.547689
H	-2.941099	1.564753	1.284458
H	-0.690394	2.304847	0.550301
C	0.992802	1.032592	-1.137466
C	2.292442	-0.661030	0.850048
H	3.172319	-0.092313	0.481770
H	1.524759	-0.036461	1.351789
O	1.645762	1.983176	-0.291232
H	1.670771	0.201860	-1.404836
O	2.194314	-1.861146	0.740318
H	1.634780	2.769790	-0.875314
O	0.903206	3.091946	-2.625059
H	0.823675	1.903305	-2.146672
H	0.054608	3.439948	-2.328720

Frequencies

-1541.2636	37.7690	44.6661	65.9050	79.6668	97.6996	115.9062
195.4153	216.1841	238.3136	283.8973	313.4371	404.3745	414.7437
417.4132	487.9717	549.1335	619.4334	624.3567	638.3325	709.8271
743.3766	753.5056	832.0625	842.2582	865.2974	916.5573	954.5934
971.9821	995.3061	1041.0275	1053.8308	1093.5491	1143.0674	1163.7341
1199.7015	1244.5054	1261.5337	1301.1129	1349.4304	1371.7204	1414.1681
1475.5580	1515.8876	1521.9150	1599.8282	1619.2038	1651.3150	1673.9949
1836.0446	2901.0164	2973.6699	2986.3062	3143.4665	3156.9052	3167.1673
3179.2211	3189.7852	3574.5964	3886.3306			

Energies (Hartree/Particle):

SCF energy, 6-31G(d,p)	-536.840397063
SCF energy, 6-31+G(d,p)	-536.888489541
Zero-point correction	0.168855
Thermal correction to Energy	0.181522
Thermal correction to Enthalpy	0.182467
Thermal correction to Gibbs Free Energy	0.128493
Sum of electronic and zero-point Energies	-536.671542
Sum of electronic and thermal Energies	-536.658875
Sum of electronic and thermal Enthalpies	-536.657930
Sum of electronic and thermal Free Energies	-536.711904

S.5.18 Scheme 8, G5

Optimized cartesian coordinates (Standard orientation)

C	-0.675610	-0.588523	-0.425670
C	-1.102840	0.573944	-1.126160
C	-2.344555	1.143654	-0.905539
C	-3.233348	0.611589	0.034135
C	-2.827878	-0.511411	0.753019
C	-1.586519	-1.095365	0.538384
H	-0.431392	1.040119	-1.846544
H	-2.624105	2.032917	-1.470411
H	-4.204966	1.068699	0.206207
H	-3.492652	-0.943929	1.500852
H	-1.295001	-1.975482	1.106882
C	0.588798	-1.223242	-0.653529
C	1.609992	-0.689846	-1.435132
H	2.439088	-1.364204	-1.651217
H	1.324617	-0.068331	-2.282383
O	0.951978	-2.261945	0.232547
H	2.157190	0.113117	1.039890
O	1.573087	2.714610	0.778188
H	3.494866	0.440046	-0.810571
O	2.571784	0.555048	-0.553809
H	0.774212	0.179685	1.652921
H	1.263538	-1.814492	1.040298
H	1.968445	2.085662	0.135522
O	1.682282	-0.038587	1.902755
H	1.678922	2.218612	1.598197

Frequencies

-423.7067	47.6535	69.0284	78.1827	108.2924	135.7918	177.7910
213.1227	218.5450	235.5901	245.0975	260.9403	310.2177	352.8015
383.2019	421.6301	443.0070	466.7343	473.2327	531.0350	543.7969
561.2616	585.6775	624.7501	709.0669	725.4976	739.3387	752.9073
833.3034	843.6351	863.5625	911.3156	954.8741	962.9512	974.3977
982.5436	989.5843	1034.4437	1043.9789	1083.9359	1125.1137	1147.3195
1165.0118	1174.7366	1275.8798	1312.6045	1357.8859	1376.1359	1392.2695
1467.1594	1507.0030	1521.7690	1596.6083	1654.2245	1676.5105	1736.5687
3109.3015	3145.2556	3152.3620	3163.5562	3184.8899	3190.9284	3201.0151
3281.0169	3551.6449	3689.2808	3869.9066	3873.8947	3895.6321	

Energies (Hartree/Particle):

SCF energy, 6-31G(d,p)	-613.280207416
SCF energy, 6-31+G(d,p)	-613.332927307
Zero-point correction	0.202047

```
Thermal correction to Energy                    0.215959
Thermal correction to Enthalpy                  0.216903
Thermal correction to Gibbs Free Energy         0.162051
Sum of electronic and zero-point Energies    -613.078161
Sum of electronic and thermal Energies       -613.064248
Sum of electronic and thermal Enthalpies     -613.063304
Sum of electronic and thermal Free Energies  -613.118157
```

S.5.19 Scheme 8 (Text), G6

```
Optimized cartesian coordinates (Standard orientation)
C     -0.461186     0.030322     0.233886
C     -1.271185     1.116778    -0.159660
C     -2.646755     0.990954    -0.299127
C     -3.282922    -0.224888    -0.049210
C     -2.503075    -1.310273     0.344255
C     -1.125440    -1.187299     0.480796
H     -0.811760     2.086356    -0.351123
H     -3.232175     1.856256    -0.607992
H     -4.360731    -0.321756    -0.158069
H     -2.974784    -2.272128     0.543471
H     -0.526111    -2.043892     0.778906
C      0.983069     0.178499     0.463058
C      1.744340     0.998015    -0.545922
H      1.242749     1.946760    -0.778883
H      2.731161     1.256570    -0.113726
O      1.646771    -1.107995     0.514994
H      1.383561     0.528861     1.715144
O      2.093429     0.335563     2.742056
H      2.889117     0.829307     2.516376
O      1.930911     0.301028    -1.775987
H      2.113718    -1.023858     1.372176
H      2.103691    -0.602899    -1.471458

Frequencies
-1432.3659    54.5897    68.8953    92.1775   135.6567   207.7880   228.3594
  281.6391   310.3562   351.4211   371.6291   416.3710   445.6041   506.3086
  524.3584   578.7176   619.9383   623.8898   707.6144   715.2552   732.6702
  754.1039   821.7155   844.9458   885.6436   921.2979   958.2345   976.7795
  991.3380  1028.7562  1040.3285  1051.9865  1074.3447  1123.9107  1140.2824
 1168.9598  1194.2977  1294.8315  1299.8105  1338.2261  1356.5024  1406.6917
 1410.3699  1467.8634  1475.8716  1517.4198  1613.6526  1616.4557  1633.2285
 1662.2278  2932.2997  3069.8807  3154.2838  3160.1473  3170.0245  3188.6954
 3197.7963  3588.5536  3784.6622  3899.0956
```

Energies (Hartree/Particle):	
SCF energy, 6-31G(d,p)	-536.870100066
SCF energy, 6-31+G(d,p)	-536.918436413
Zero-point correction	0.173571
Thermal correction to Energy	0.184575
Thermal correction to Enthalpy	0.185519
Thermal correction to Gibbs Free Energy	0.136597
Sum of electronic and zero-point Energies	-536.696529
Sum of electronic and thermal Energies	-536.685525
Sum of electronic and thermal Enthalpies	-536.684581
Sum of electronic and thermal Free Energies	-536.733503