

Computational Supporting Information for:

Understanding Electronic Effects on Carboxylate-Assisted C–H Activation at Ruthenium: The Importance of Kinetic and Thermodynamic Control.

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1. Computational details

DFT calculations were run with Gaussian 09 (Revision D.01).¹ Geometry optimisations were performed with the BP86 functional^{2, 3} and employed a smaller basis set, BS1, in which Ru and Cl centres were described with the Stuttgart RECPs and associated basis sets,⁴ with additional d-orbital polarisation on Cl ($\zeta = 0.640$)⁵ and 6-31G** basis sets were used for all other atoms.^{6, 7} The 'grid=ultrafine' option was used throughout. All stationary points were fully characterized via analytical frequency calculations as either minima (all positive eigenvalues) or transition states (one negative eigenvalue). IRC calculations and subsequent geometry optimizations were used to confirm the minima linked by each transition state. All energies were recomputed with a larger basis set, BS2, featuring cc-pVTZ-PP⁸ on Ru and 6-311++g** on all other atoms.⁹ Dispersion corrections were included using Grimme's D3 parameter set.¹⁰ The final energies reported in the main text are free energies (298.15 K, 1 atm) based on the gas-phase BS1-optimised geometry, subsequently corrected for either methanol ($\epsilon = 32.6$) or dichloromethane solvent ($\epsilon = 8.93$) (PCM approach,¹¹ calculated with BS1), dispersion (D3 parameter set) and basis sets effects (BS2). This protocol has previously been shown to reproduce trends in the kinetic and thermodynamic selectivity of similar cyclometalation reactions.¹² For key stationary points (including all transition states, **TS(E-F)**, and the adjacent intermediates, **E** and **F**, as well as all product species **6** with R = H) two different orientations of the *p*-cymene ring were assessed and the lower energy structures and energies are reported. For R = OMe two orientations of the OMe group were assessed in all stationary points. The free energy difference between the *ortho*- and *para*-isomers of the cyclometalated products formed with **L2-NMe₂**, **L2-OMe**, **L2-Me** and **L2-F** was also re-computed at 323 K and 363 K (see Table S5). The data show the *para*-isomers do become relatively more favoured at elevated temperatures, although no change in the overall *ortho/para* preference is predicted.

Table S5. Free energy differences between **G_p** and **G_o** ($\Delta G^{para-ortho}$, kcal/mol) for R = NMe₂, OMe, Me and F computed at different temperatures.

R	$\Delta G^{para-ortho}$ (298 K)	$\Delta G^{para-ortho}$ (323 K)	$\Delta G^{para-ortho}$ (363 K)
NMe ₂	+1.56	+1.72	+1.96
OMe	-1.29	-1.02	-0.97
Me	+2.26	+2.38	+2.57
F	-3.09	-3.13	-3.19

Quantum Theory of Atoms in Molecules (QTAIM)¹³ analyses were performed with the AIMALL program,¹⁴ Natural Bond Orbital (NBO) calculations were run with NBO 6.0¹⁵ and NCI (Non-Covalent Interaction) calculations were performed using the PLOT program.¹⁶⁻¹⁷ QTAIM, NBO and NCI analyses were performed on partially optimised structures based on the experimental heavy atom positions with fully optimised H atoms positions. Orbital plots were created with Chemcraft¹⁸ with an outer contour value of 0.0622. All

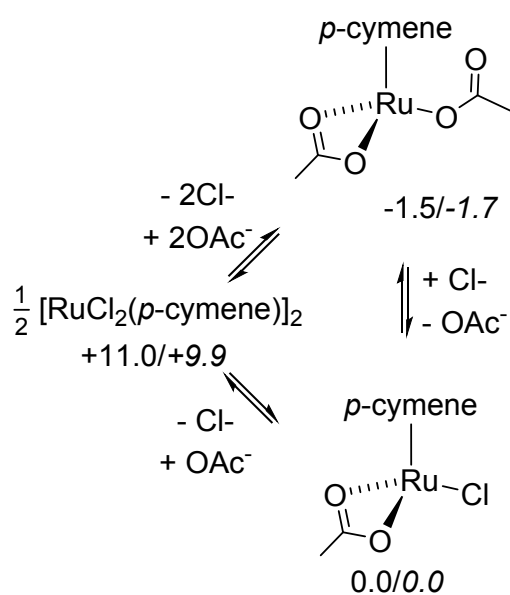
geometries are provided as sets of Cartesian coordinates as well as the separate xyz file readable by Chemcraft and Mercury.¹⁹

For NBO calculations a common Lewis structure was imposed on all species via the CHOOSE option: see Section 5.

2. References

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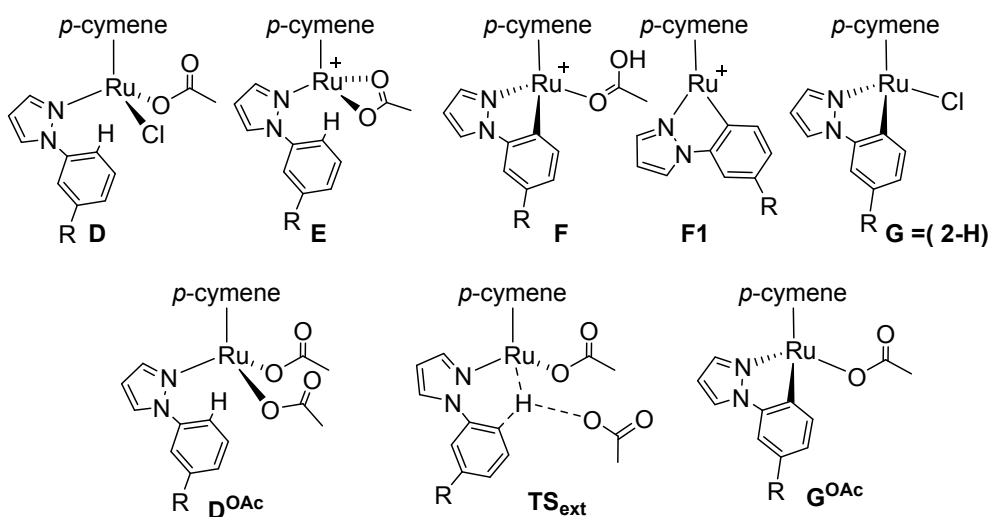
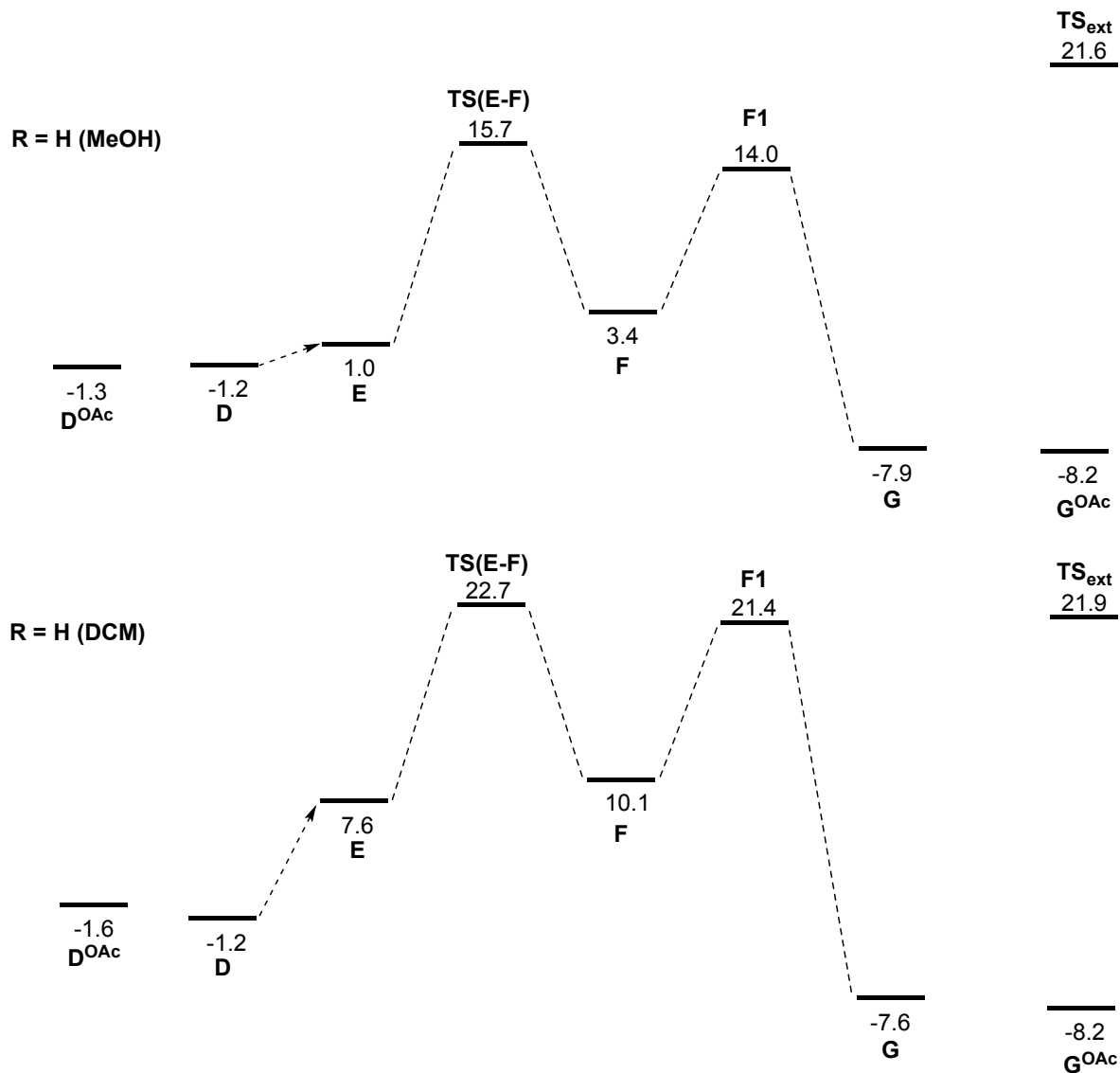
3. Energetics of $[\text{RuCl}_2(p\text{-cymene})]_2$ Dimer Opening.^a



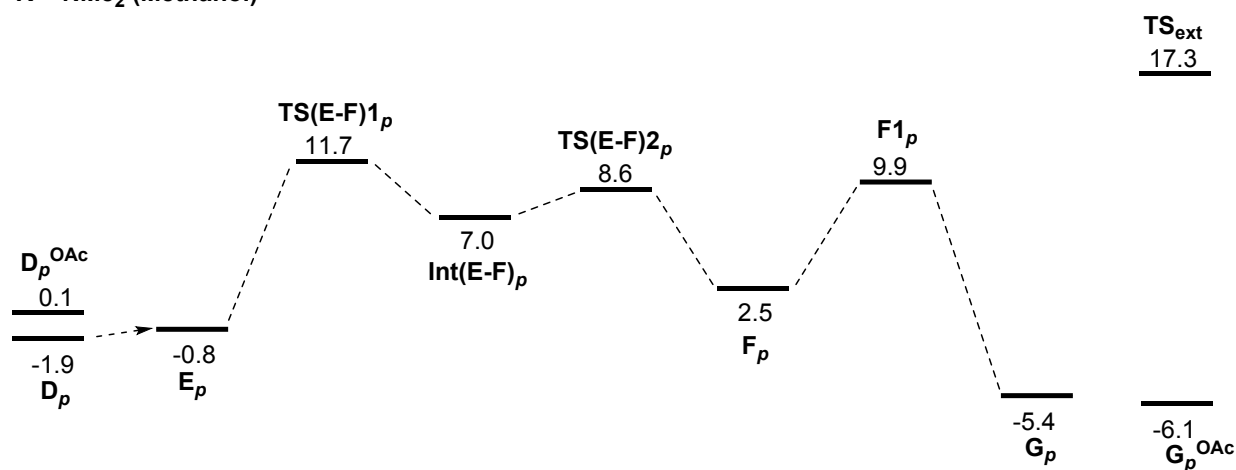
^aRelative free energies are given in kcal/mol corrected for methanol and (in italics) dichloromethane solvent

4. Computed Pathways

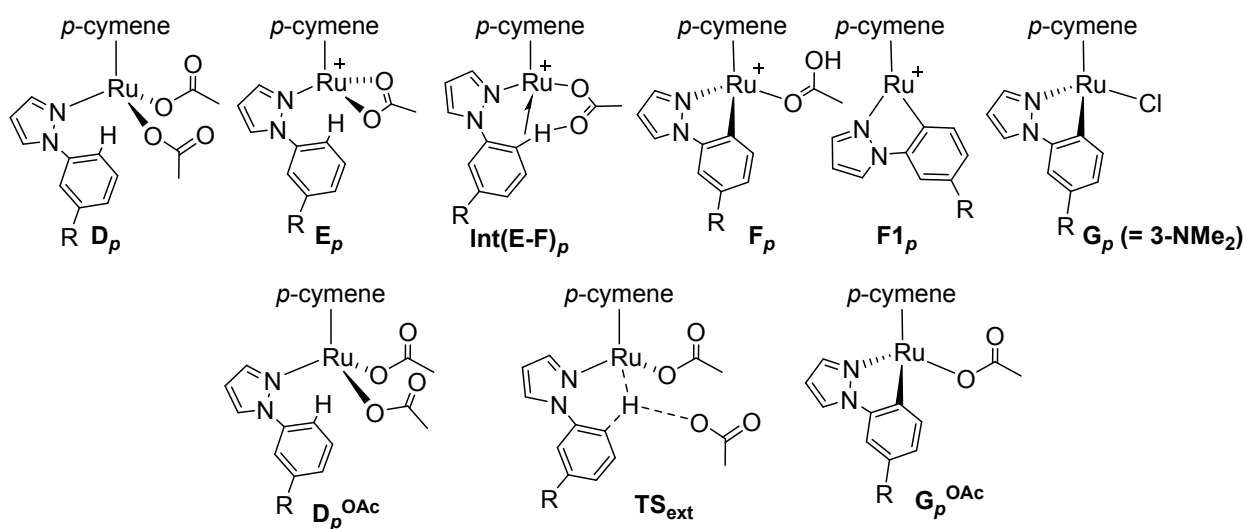
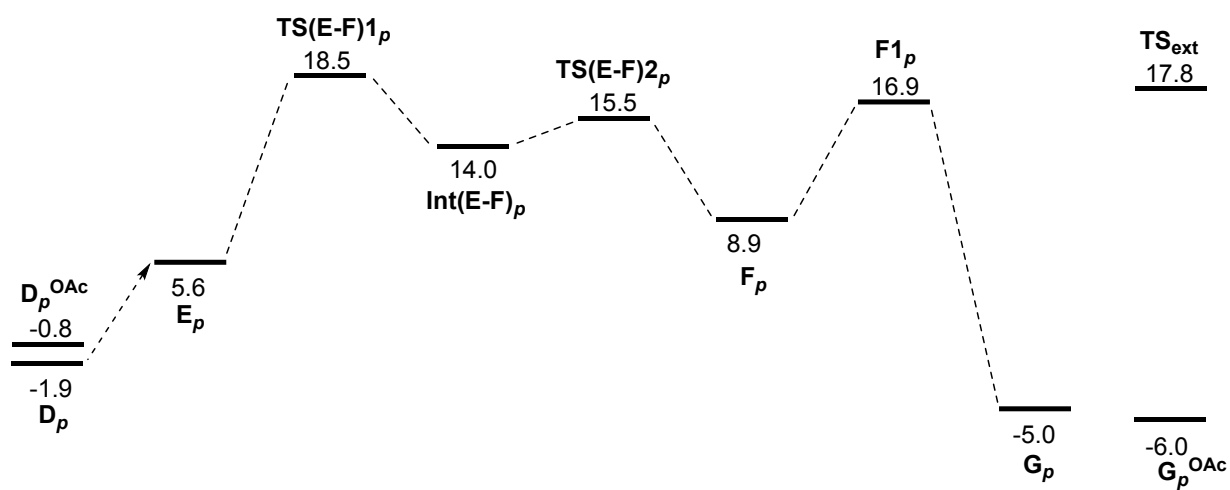
(i) Computed profiles (G, kcal/mol) for cyclometallation of **L2-R** to give *para*-substituted complexes **3-R**.

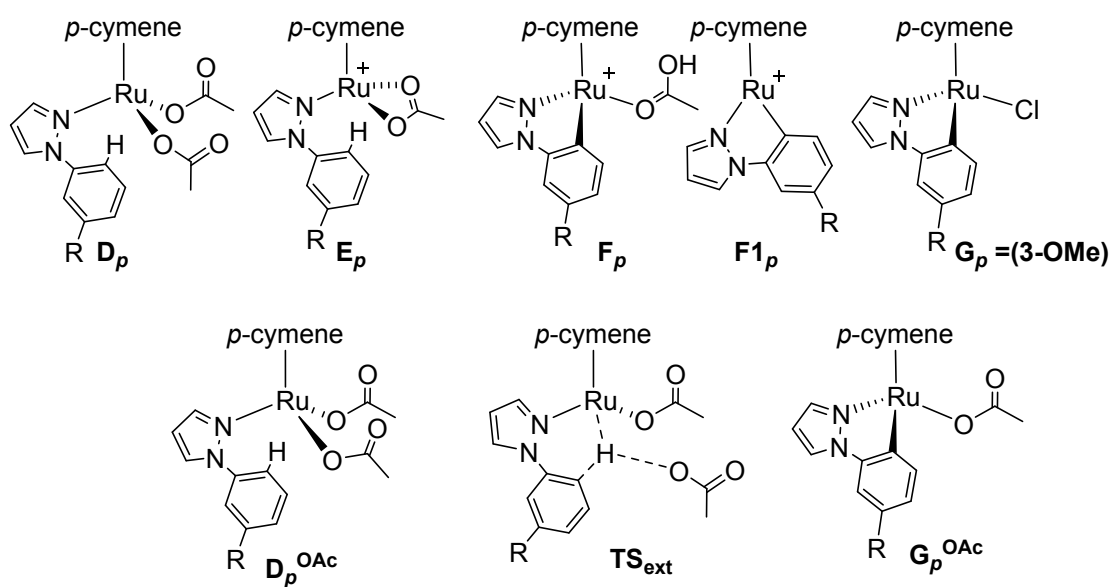
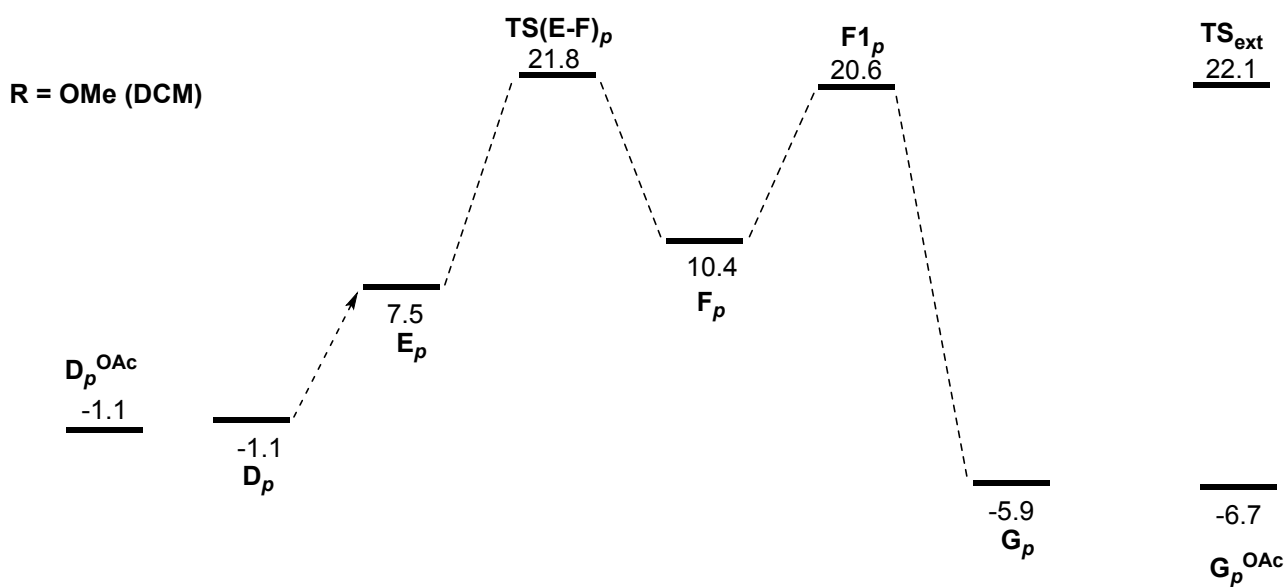
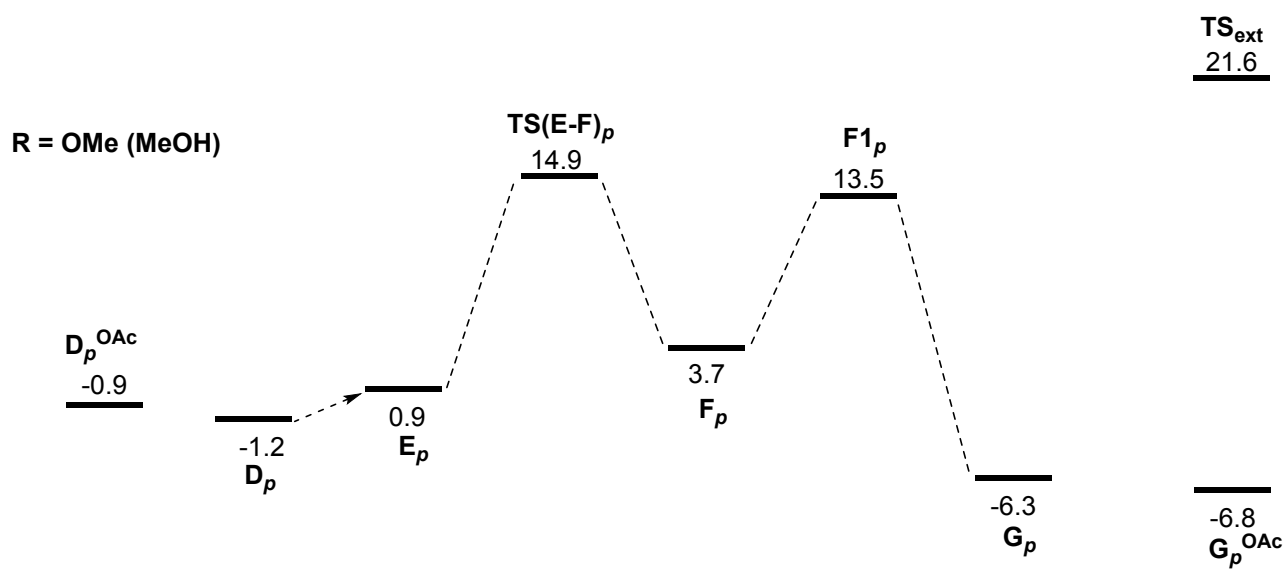


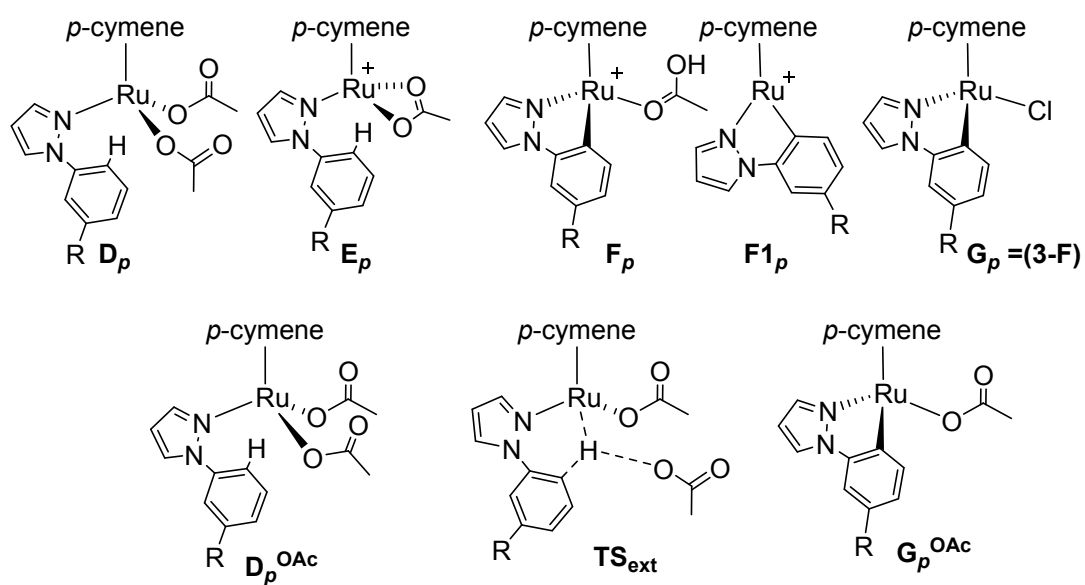
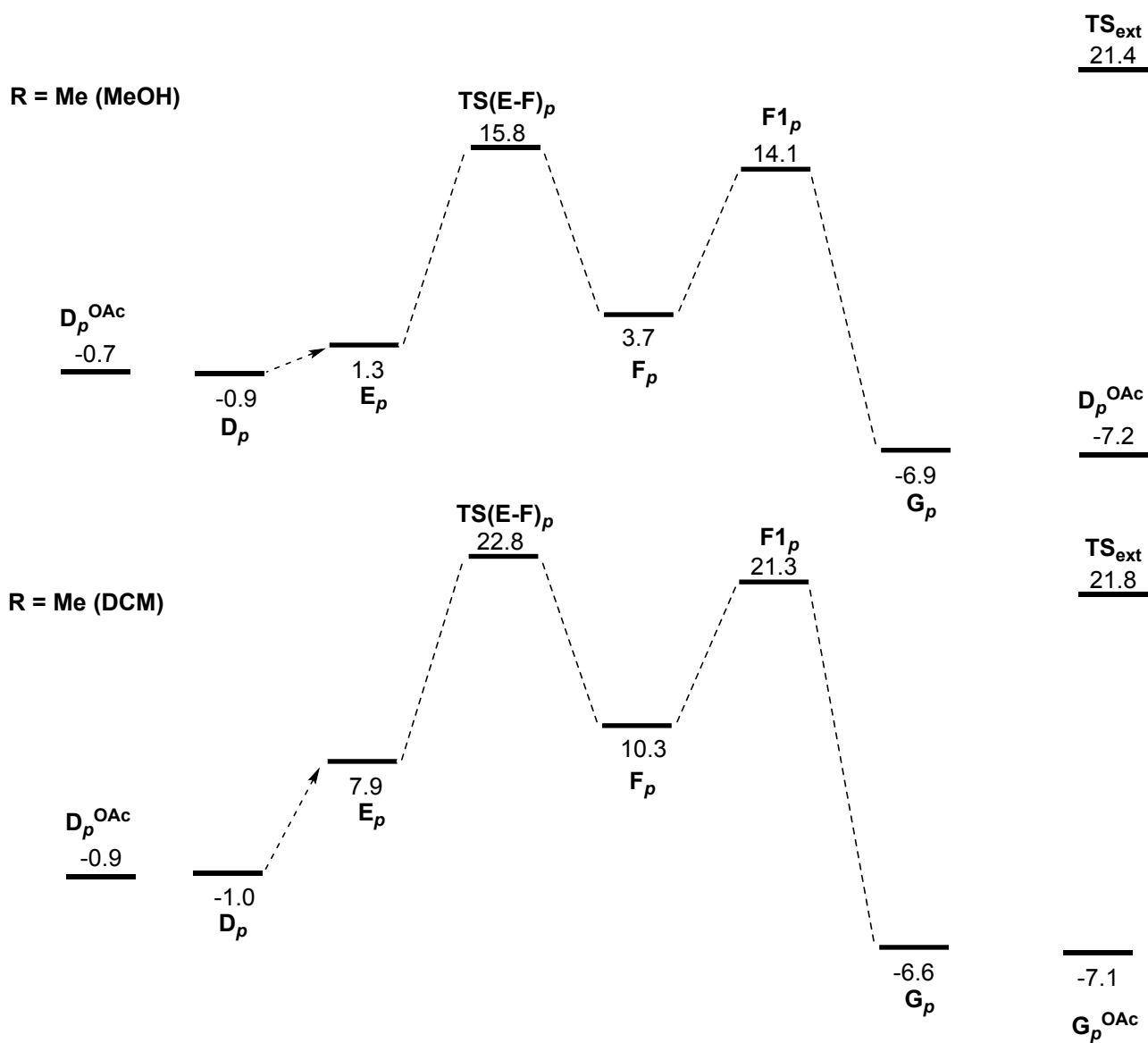
R = NMe₂ (Methanol)



R = NMe₂ (DCM)

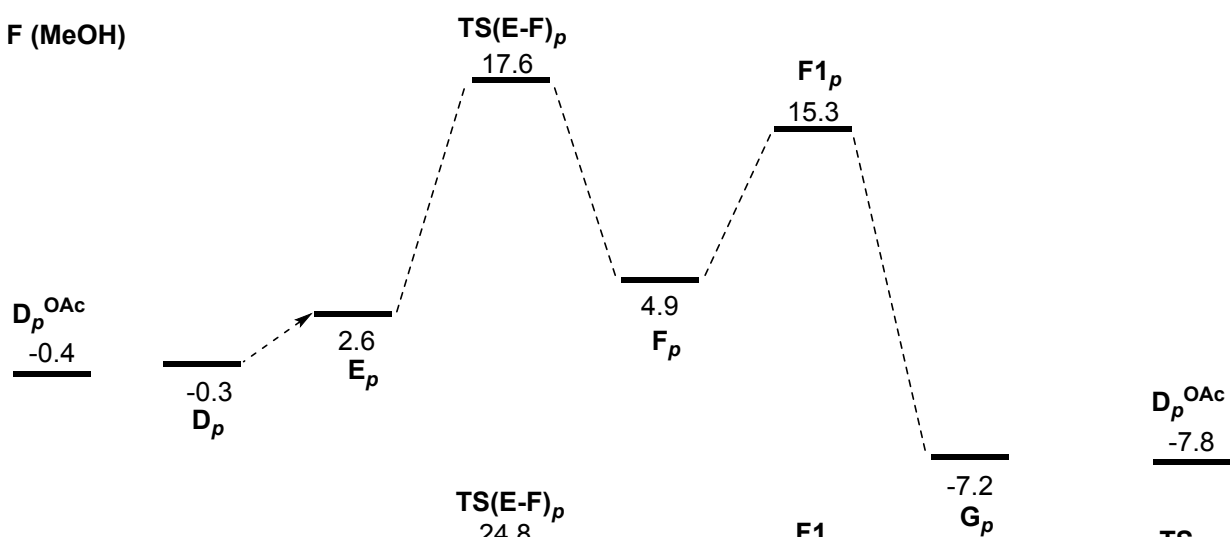




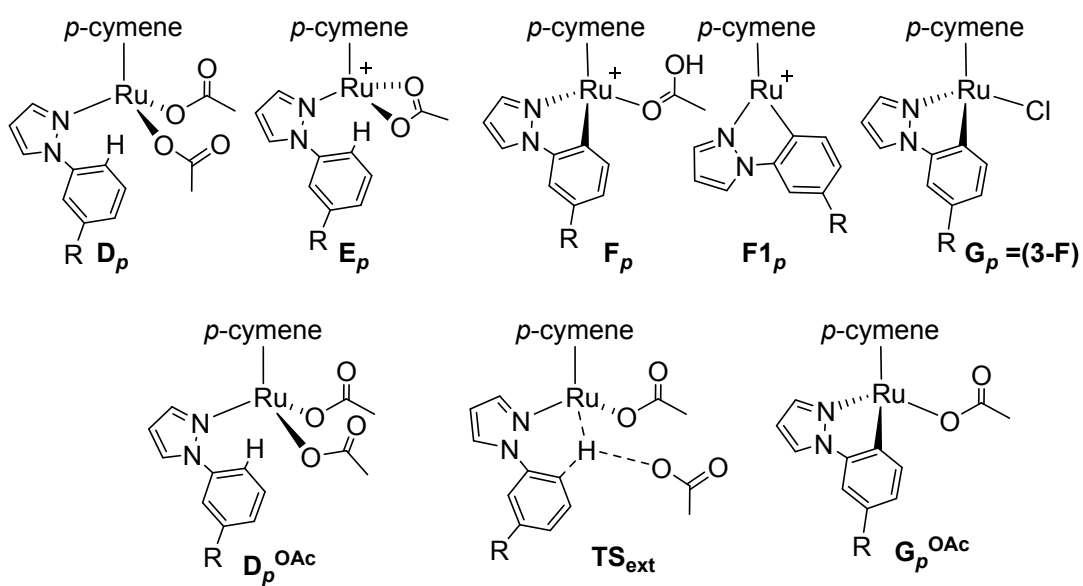
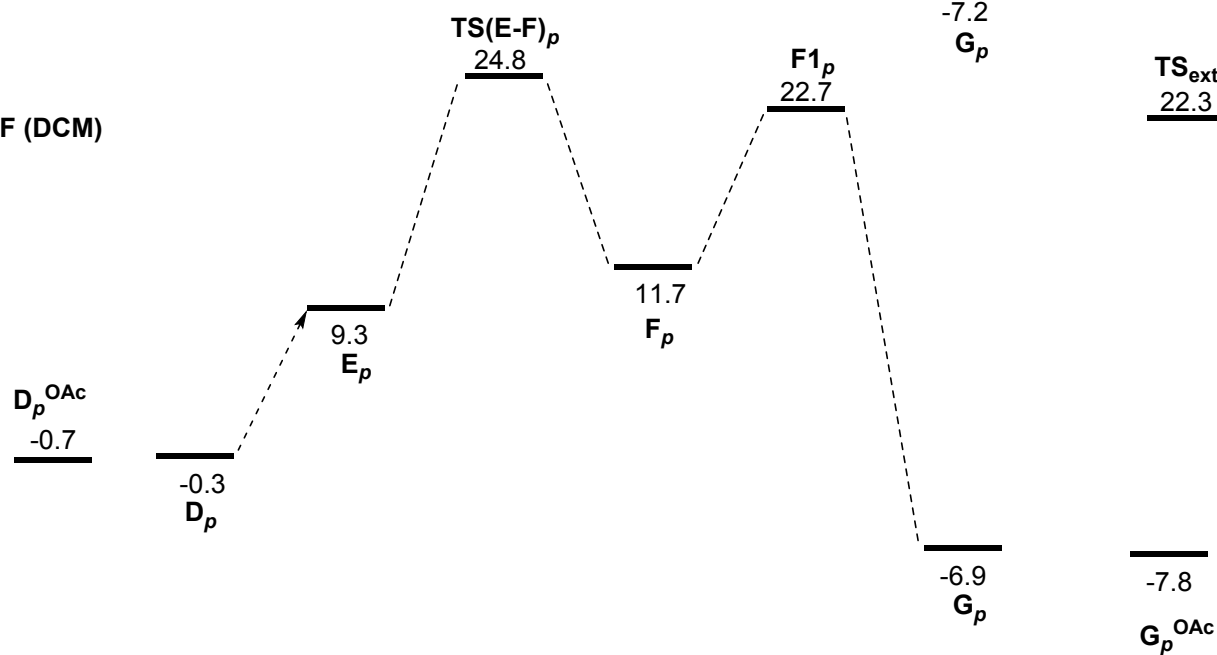


TS_{ext}
24.2

R = F (MeOH)

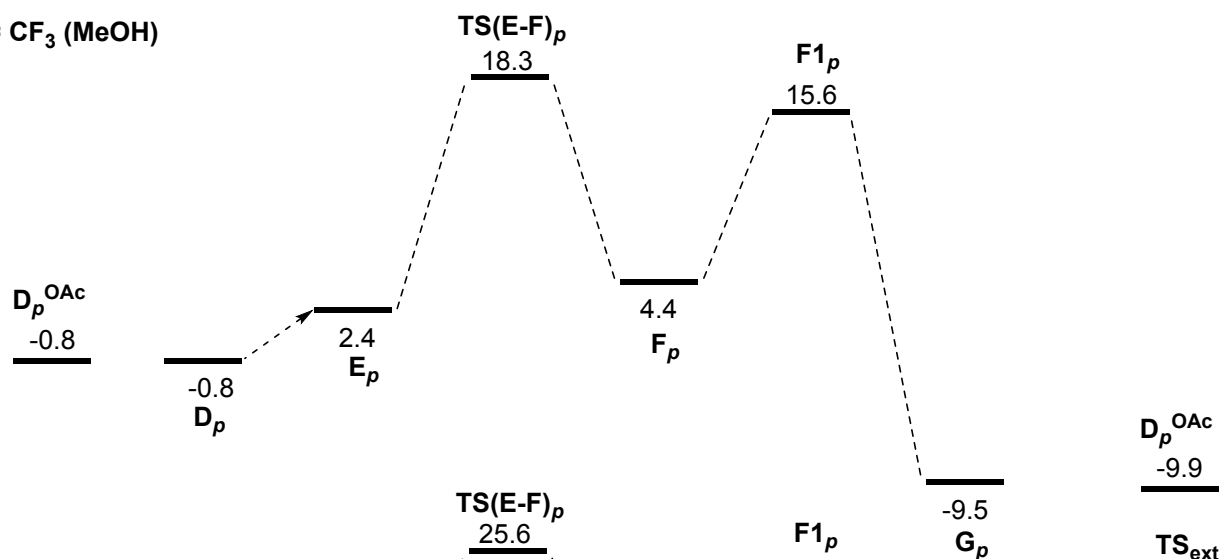


R = F (DCM)

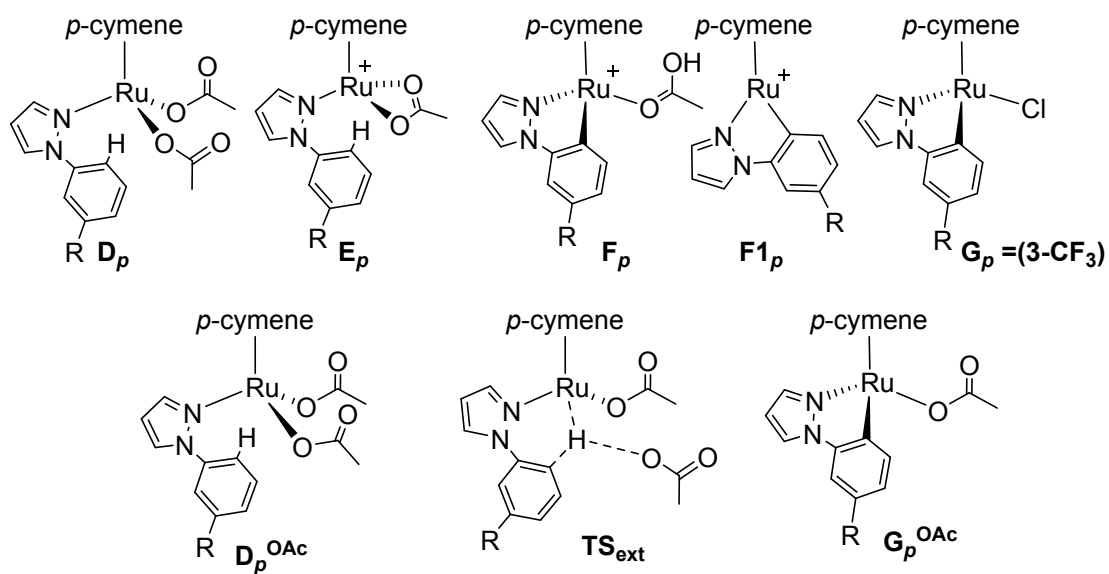
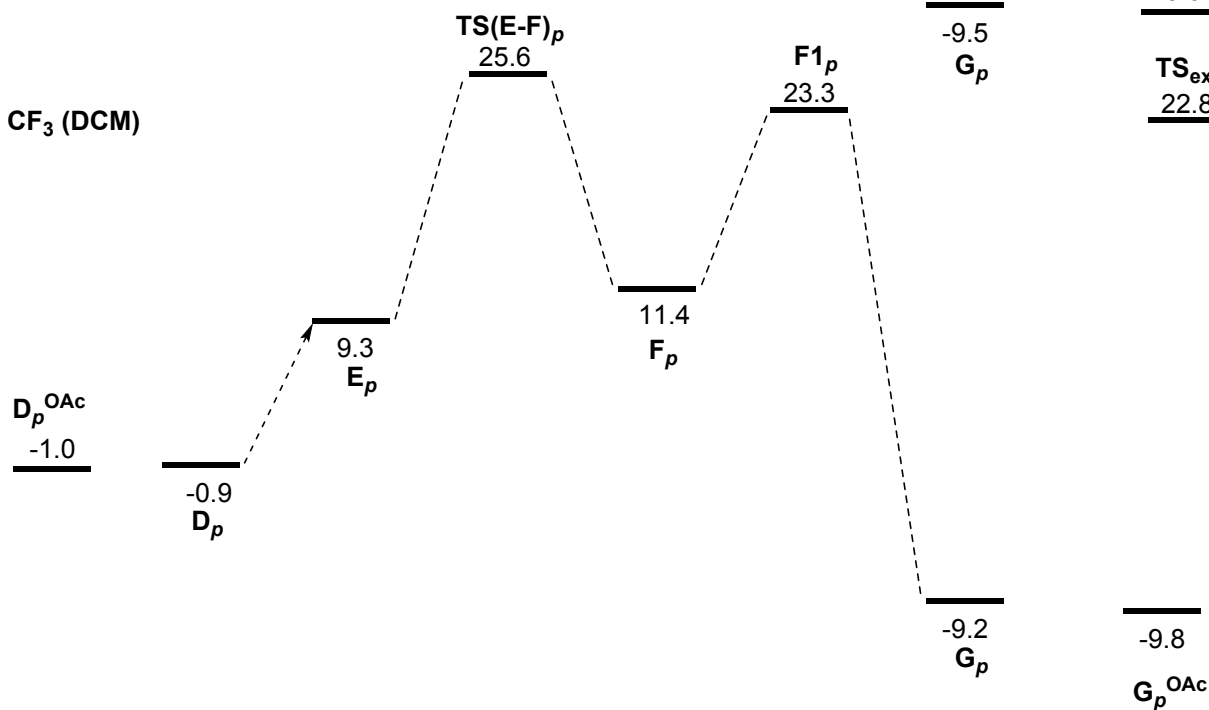


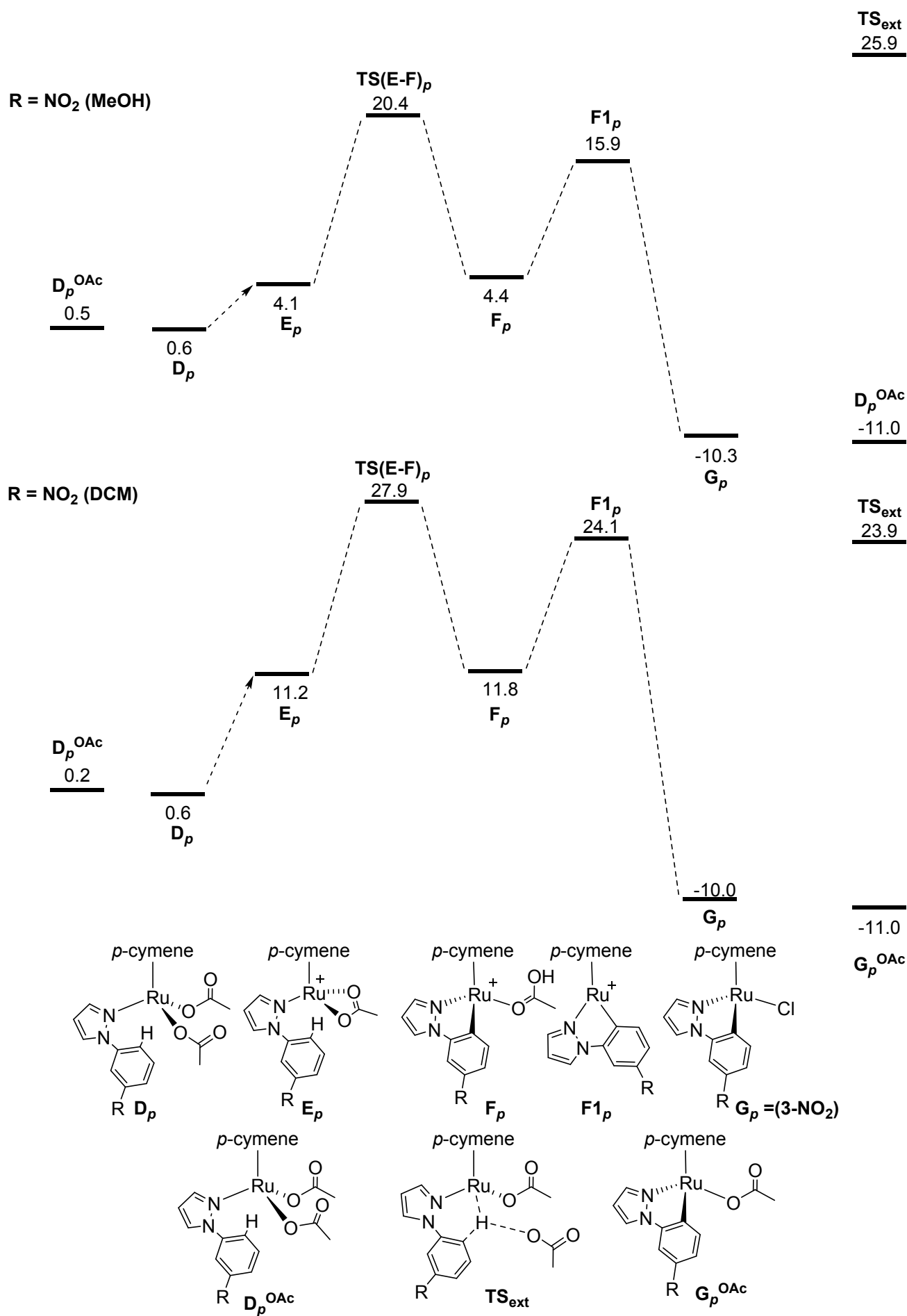
TS_{ext}
24.6

R = CF₃ (MeOH)



R = CF₃ (DCM)

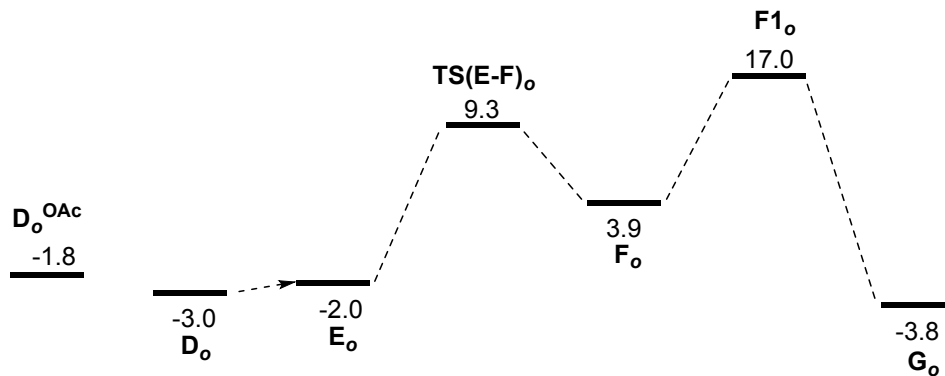




(ii) Computed profiles (G, kcal/mol) for cyclometallation of **L2-R** to give *ortho*-substituted complexes **2-R**.

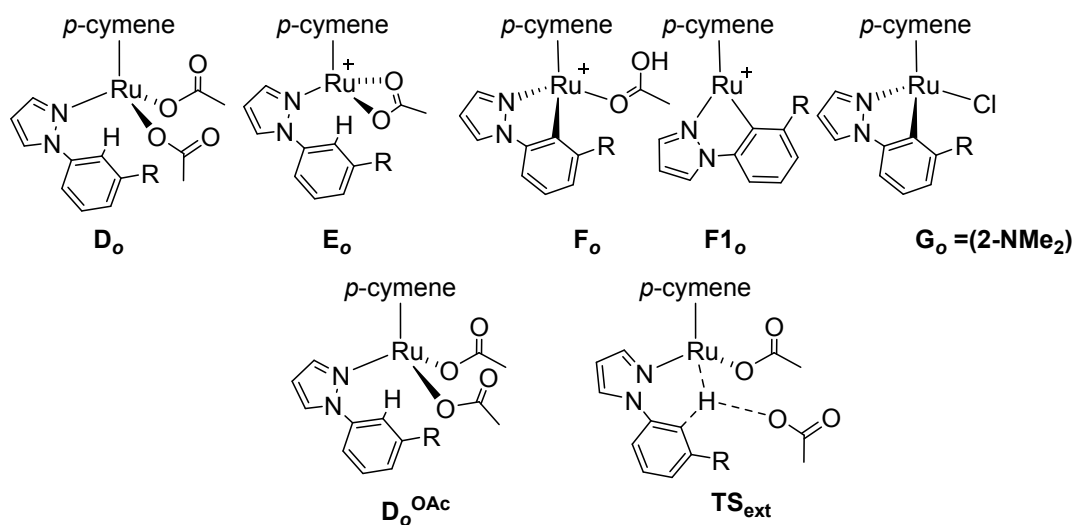
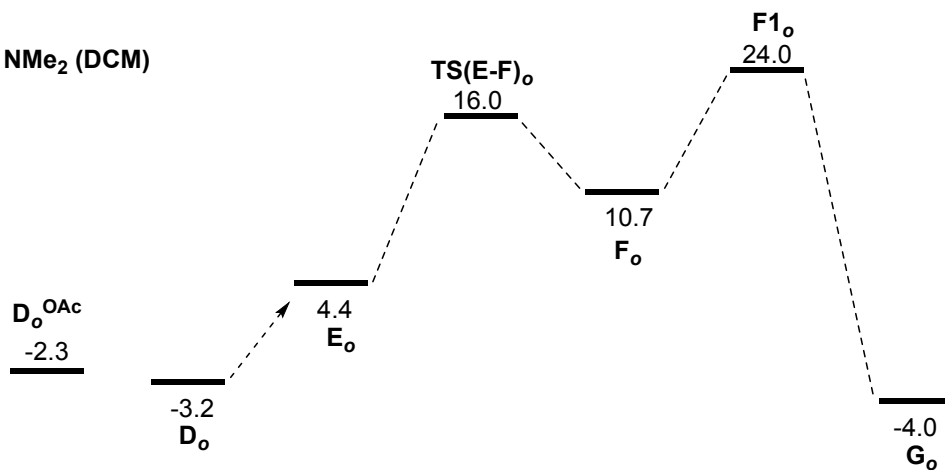
TS_{ext}
24.7

R = NMe₂ (MeOH)



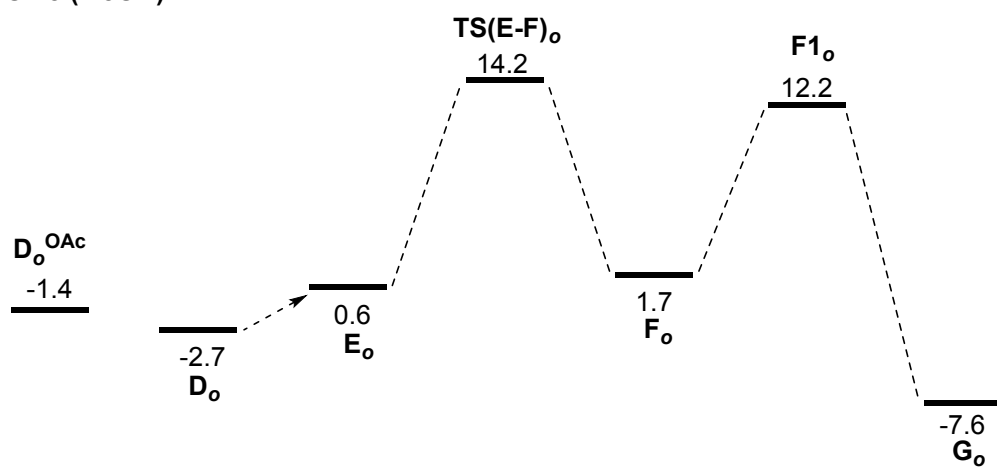
R = NMe₂ (DCM)

TS_{ext}
24.9



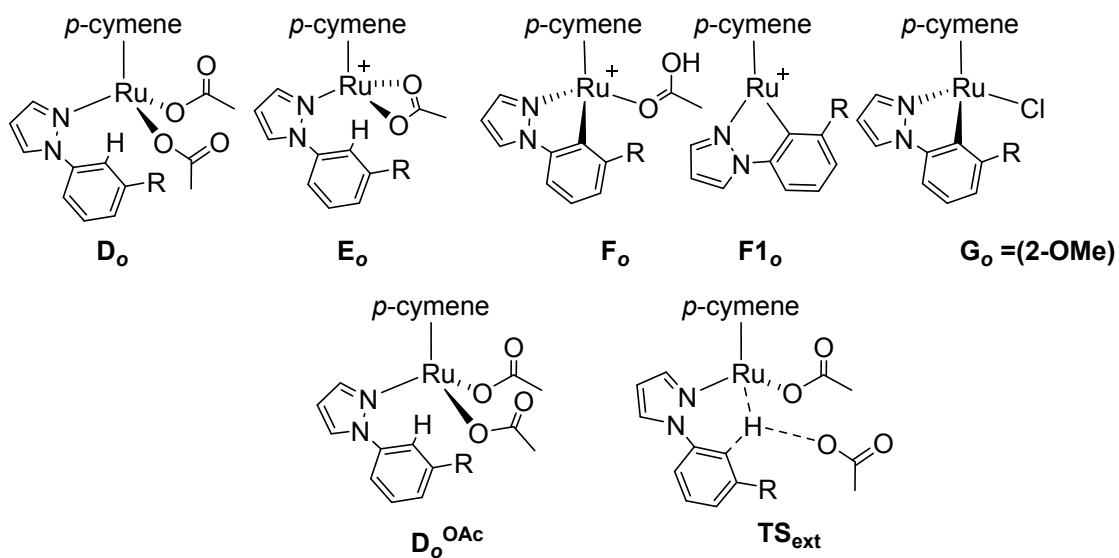
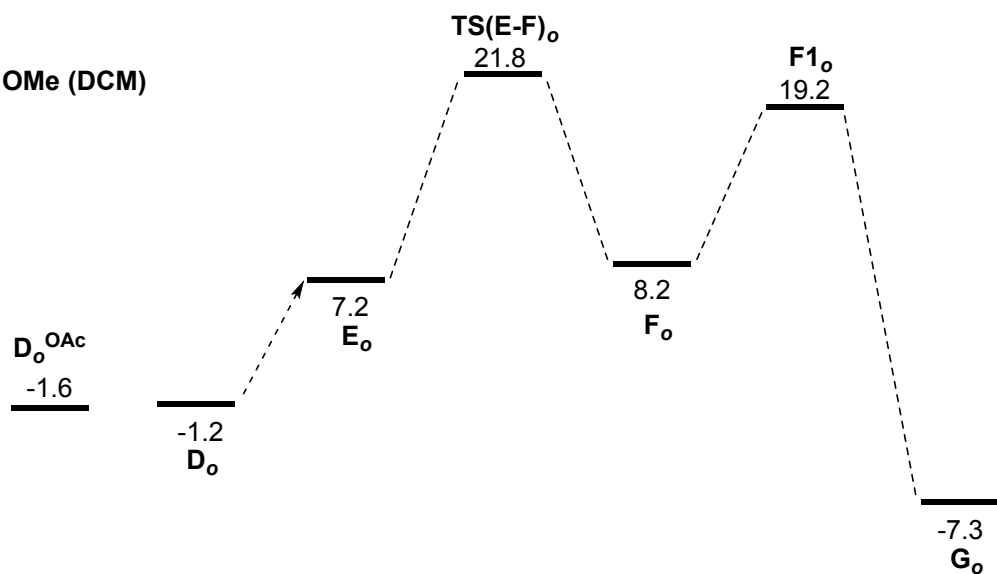
TS_{ext}
24.5

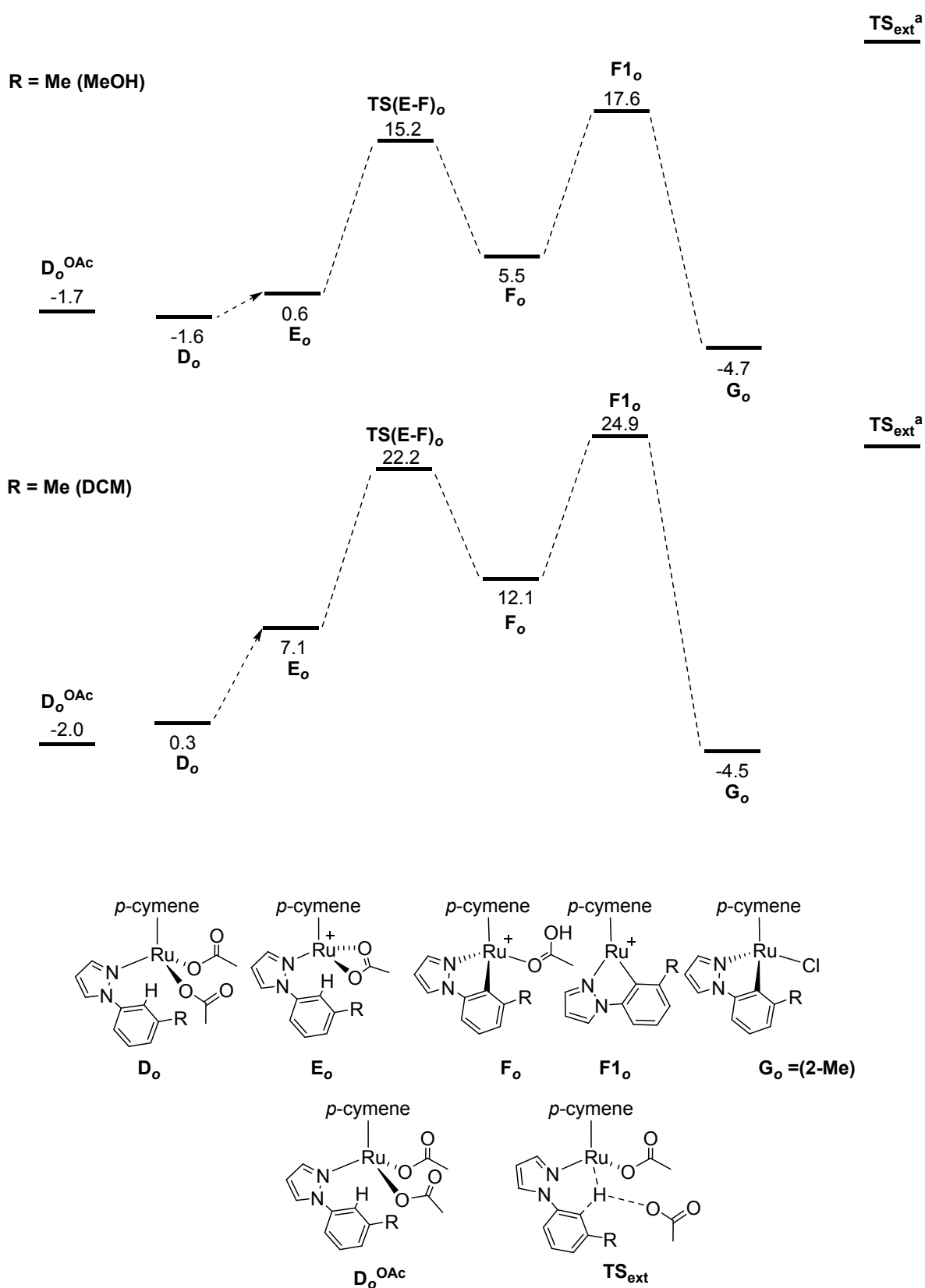
R = OMe (MeOH)



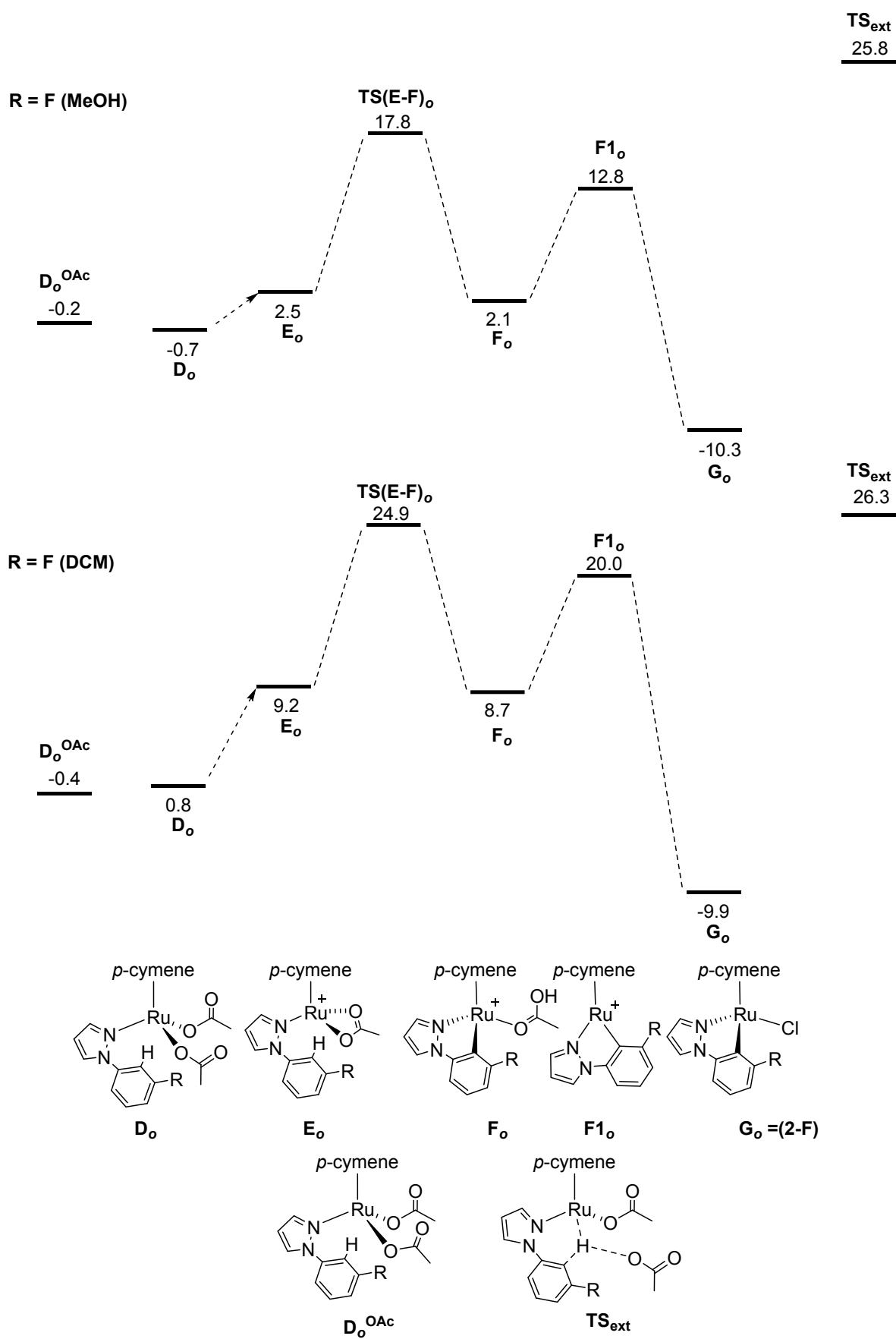
TS_{ext}
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R = OMe (DCM)



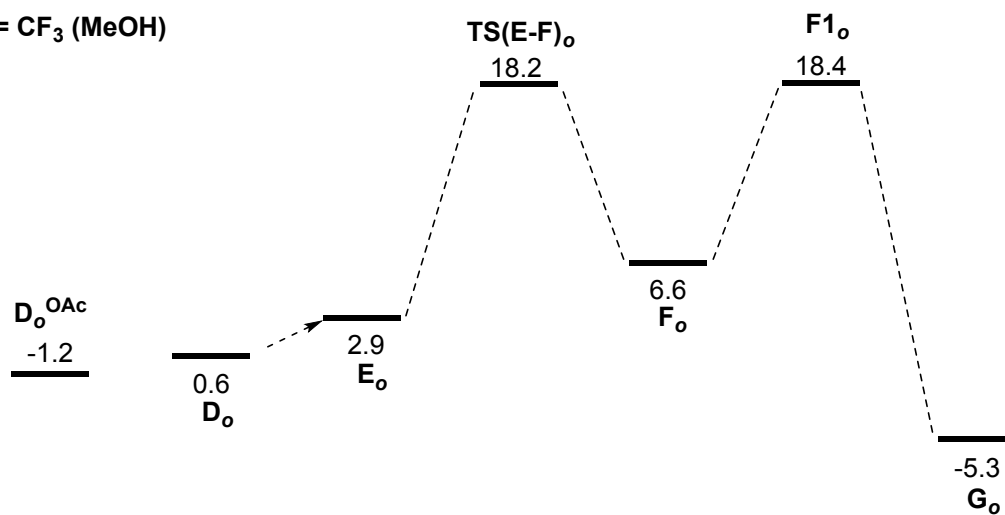


^aA transition state for external-CMD could not be located.

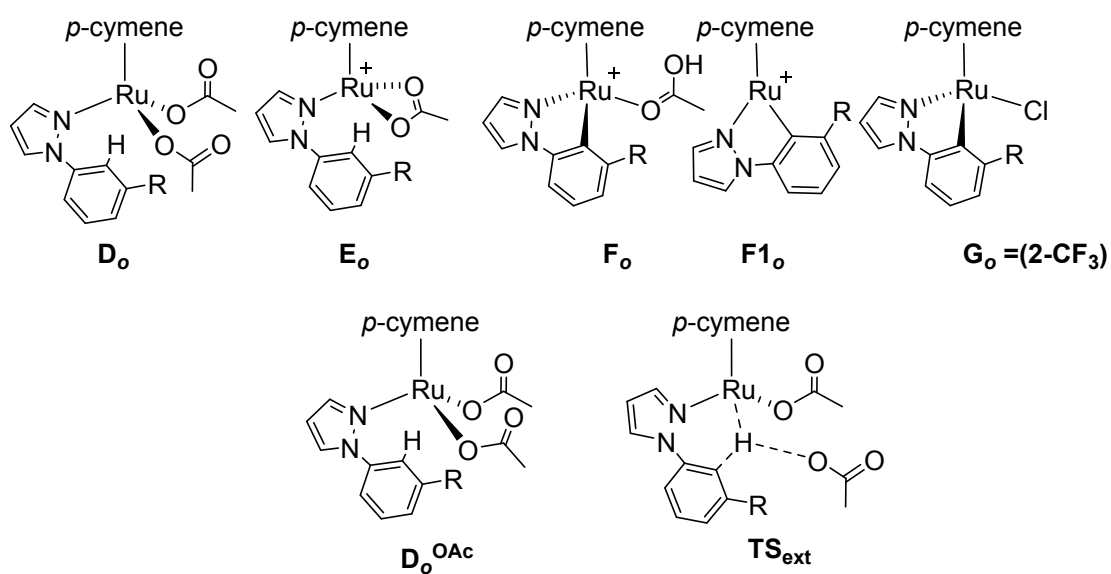
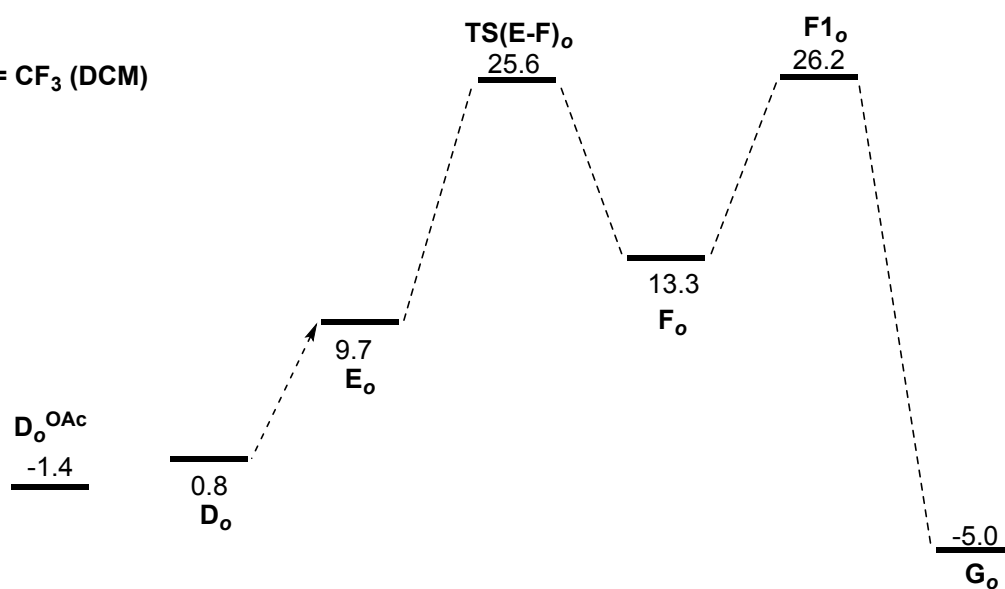


33.1
TS_{ext}

R = CF₃ (MeOH)

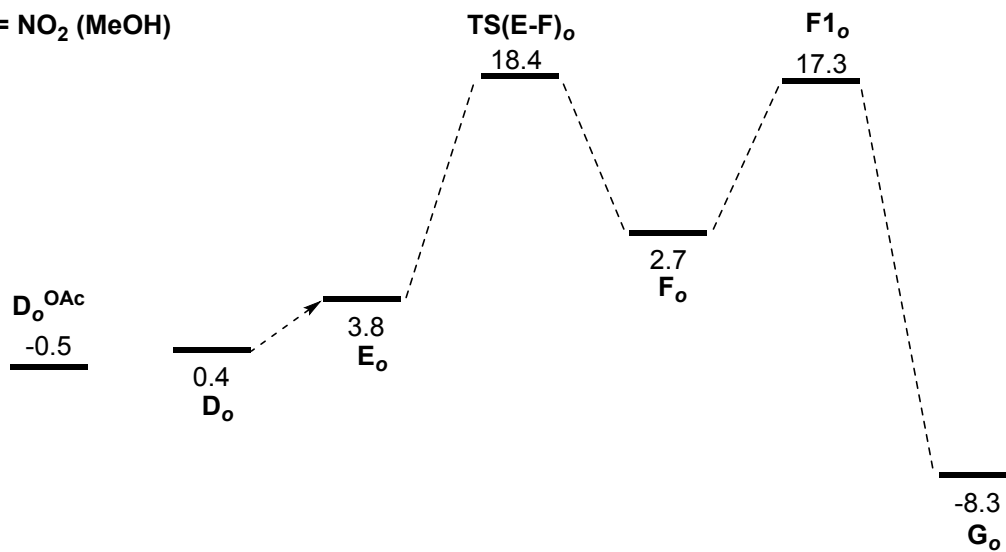


R = CF₃ (DCM)



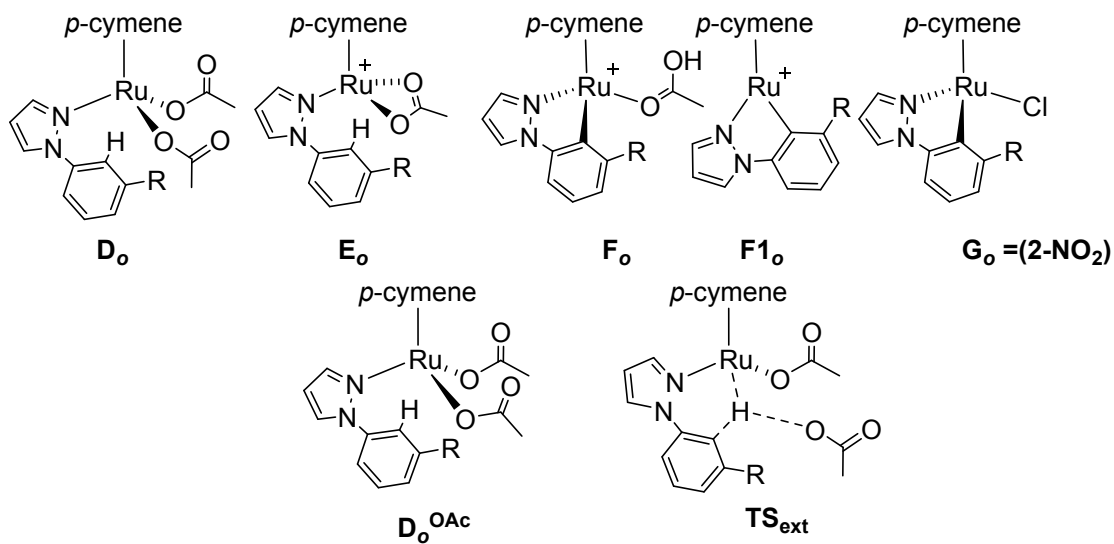
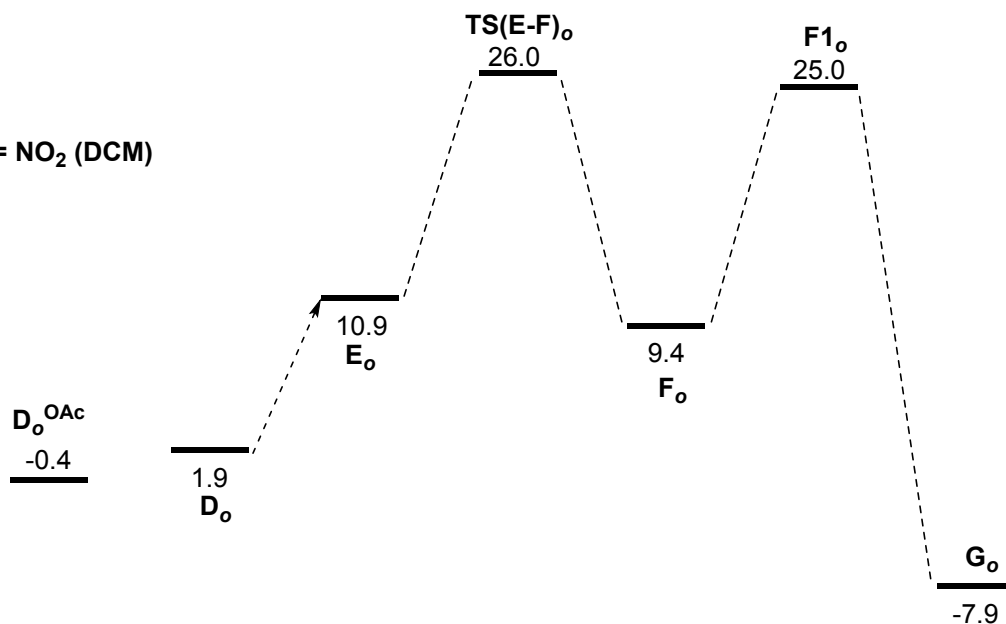
32.5
TS_{ext}

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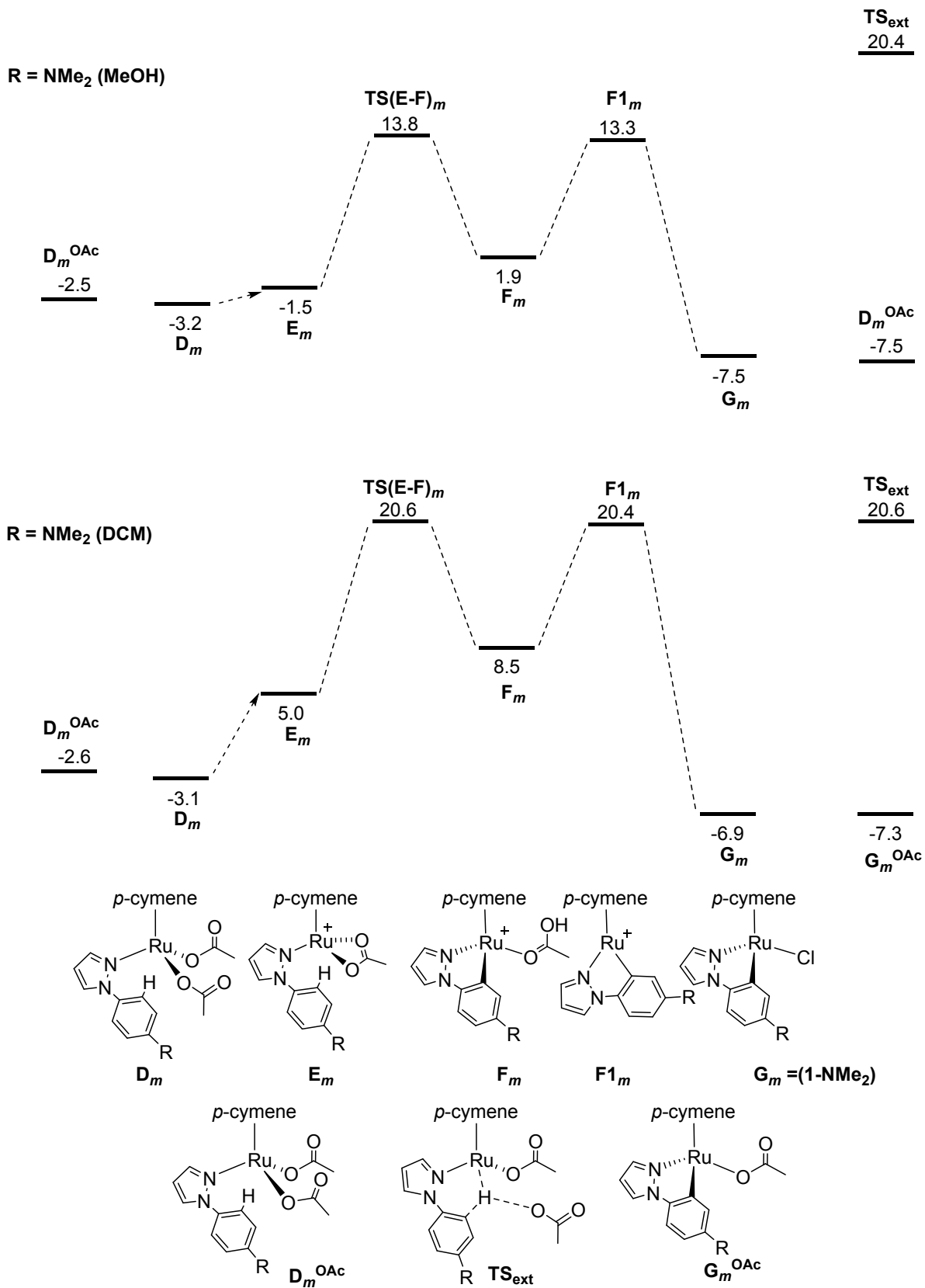


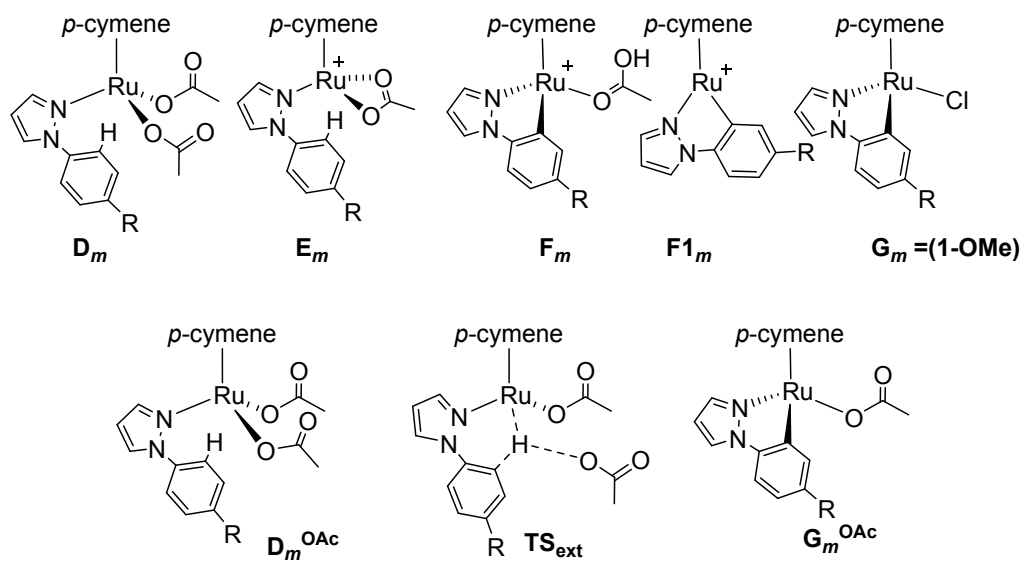
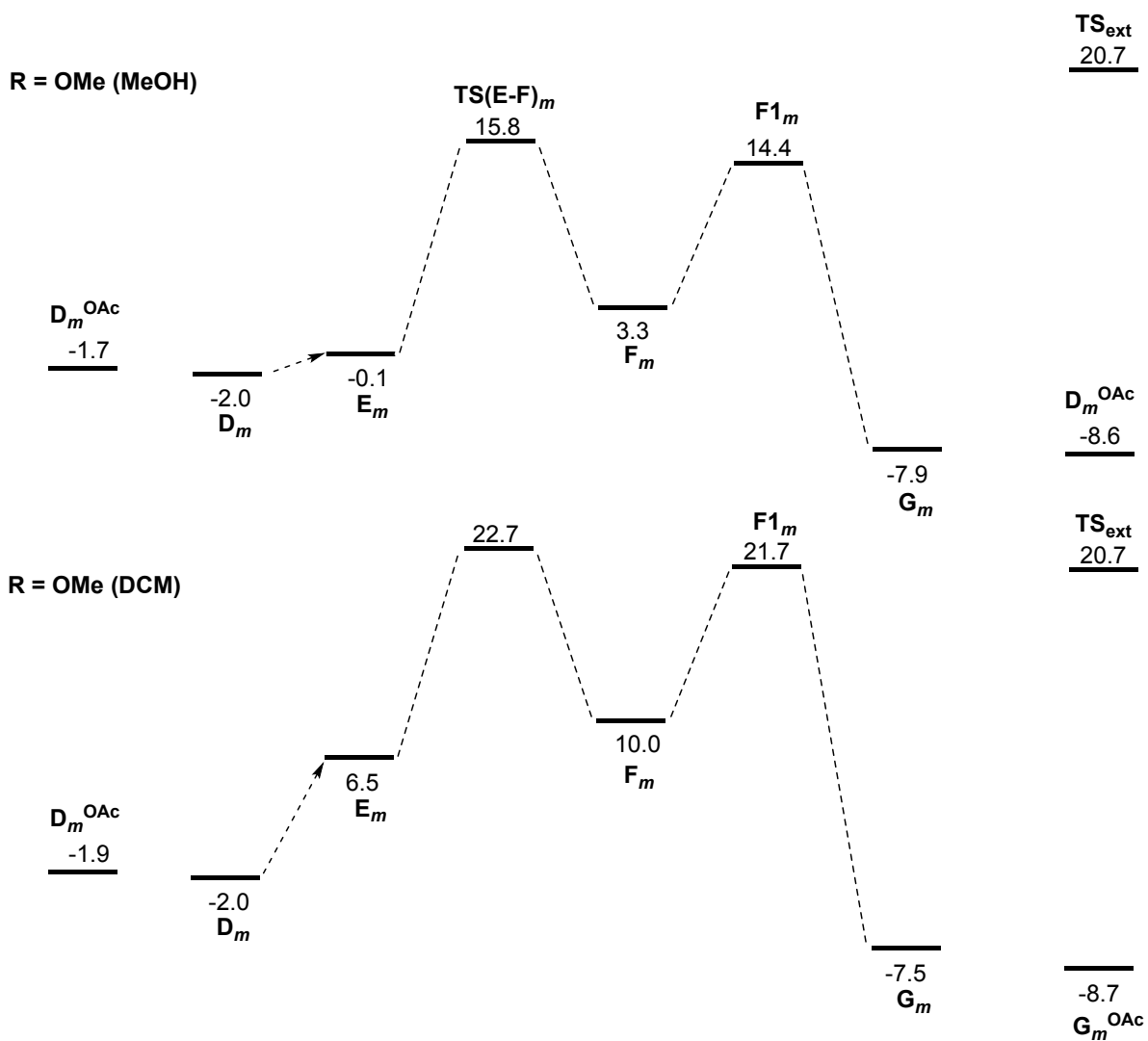
32.1
TS_{ext}

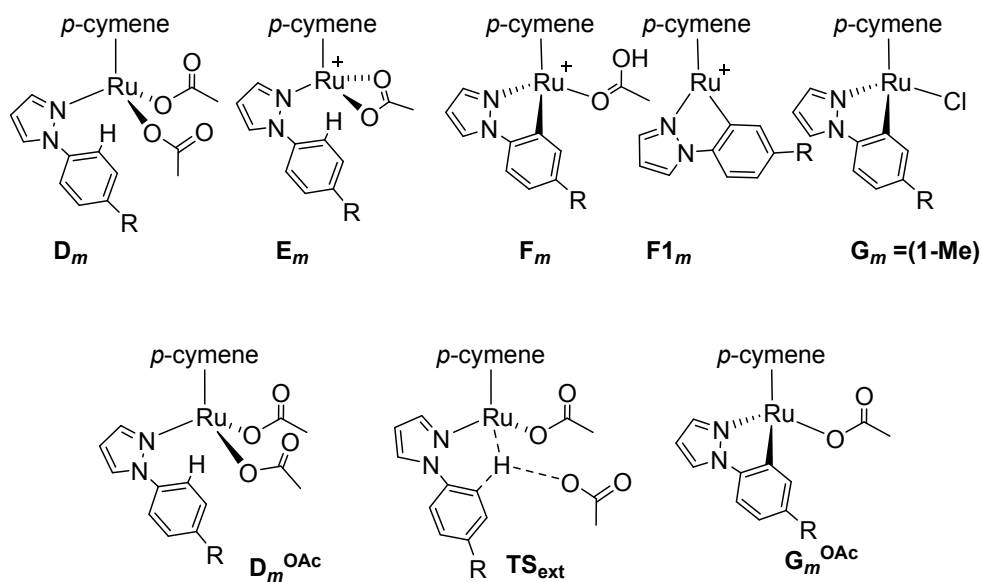
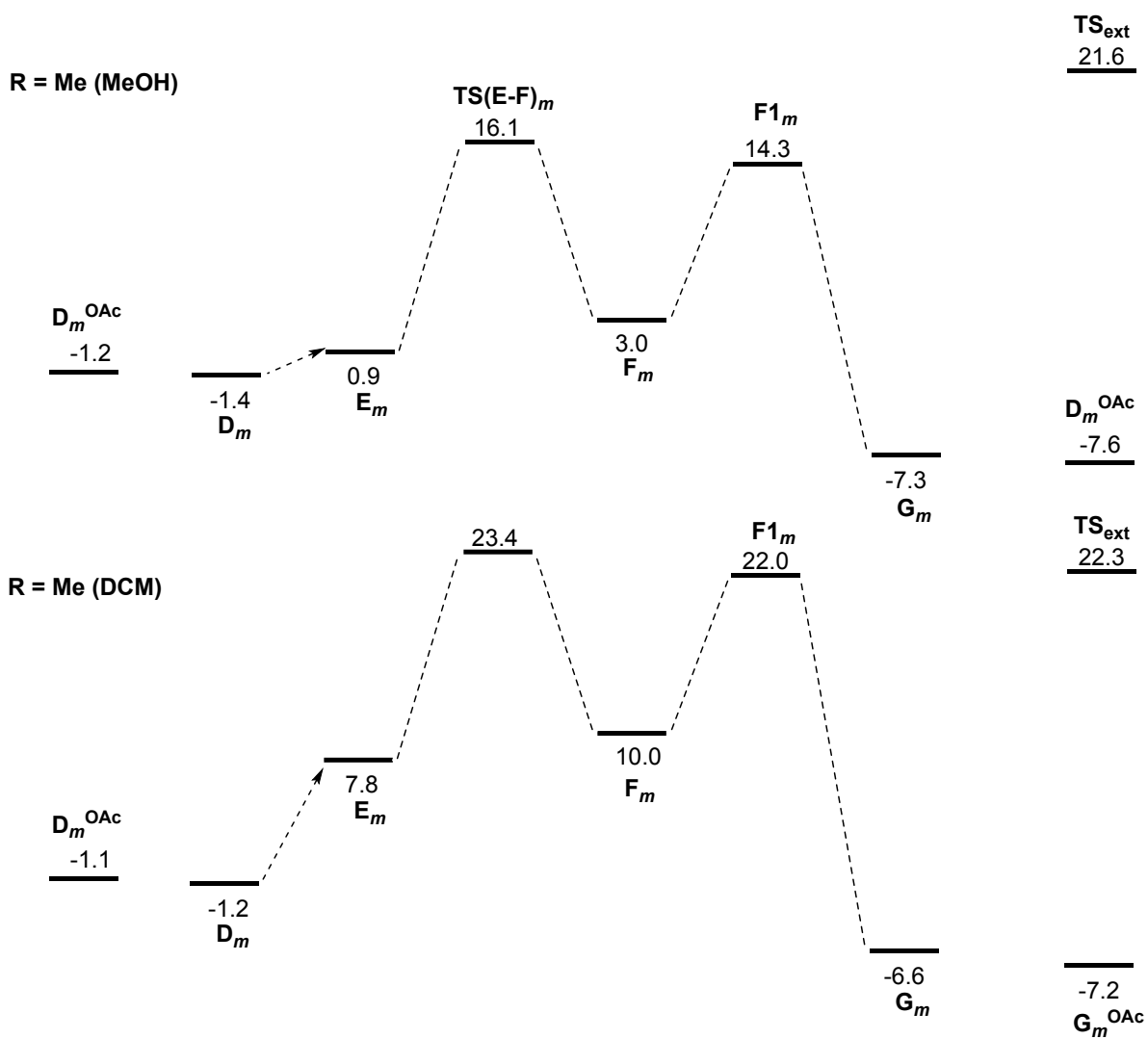
R = NO₂ (DCM)

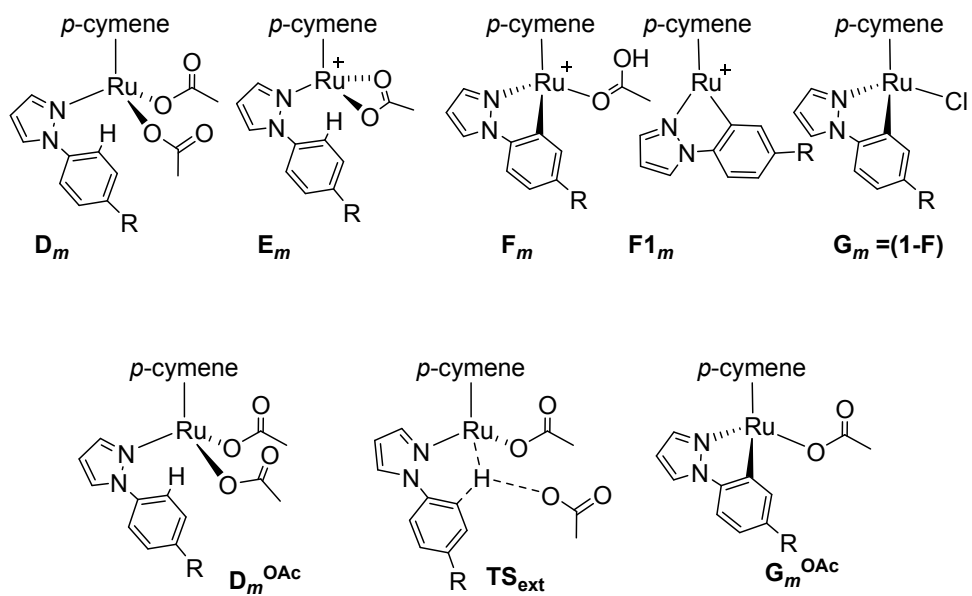
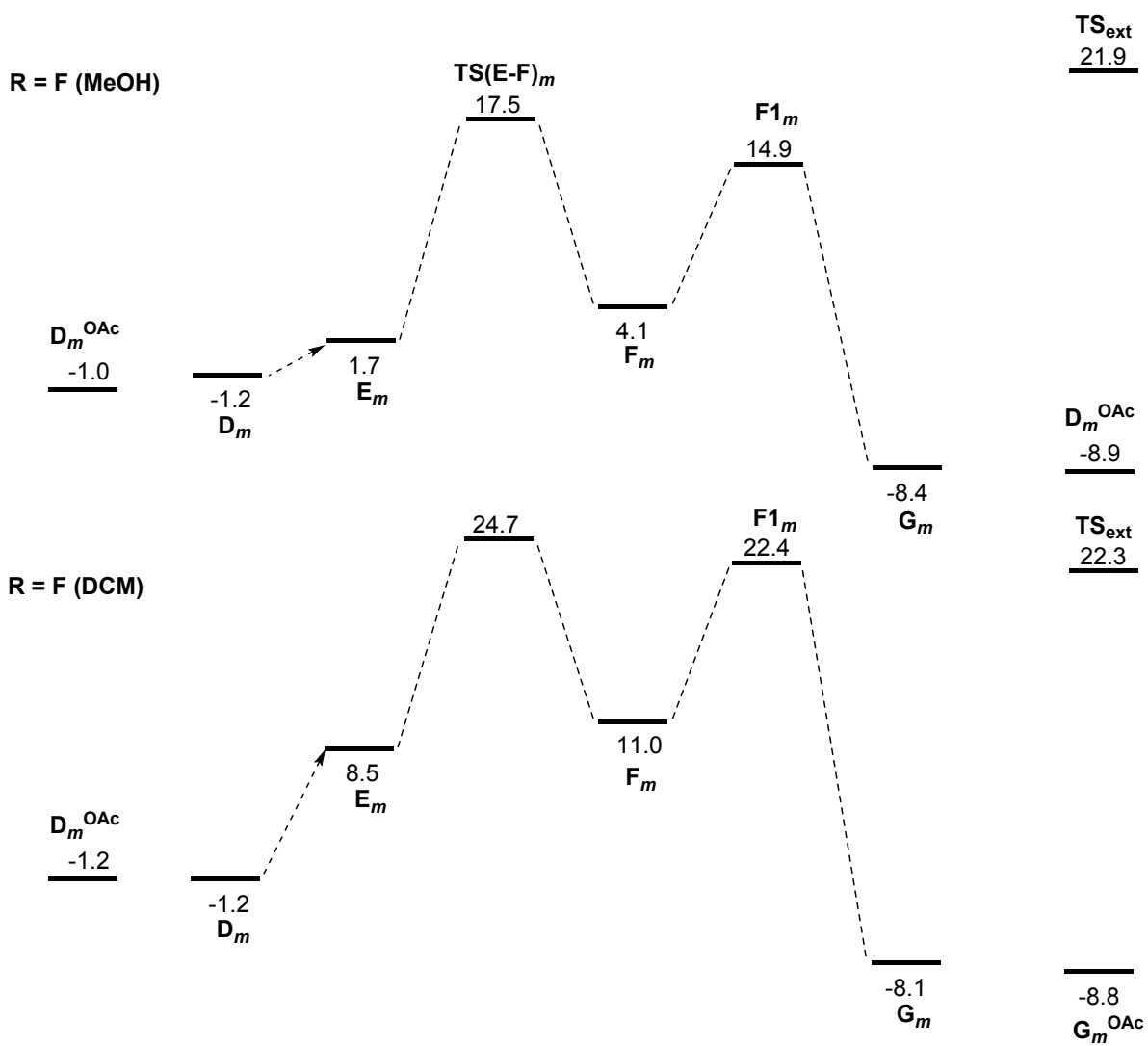


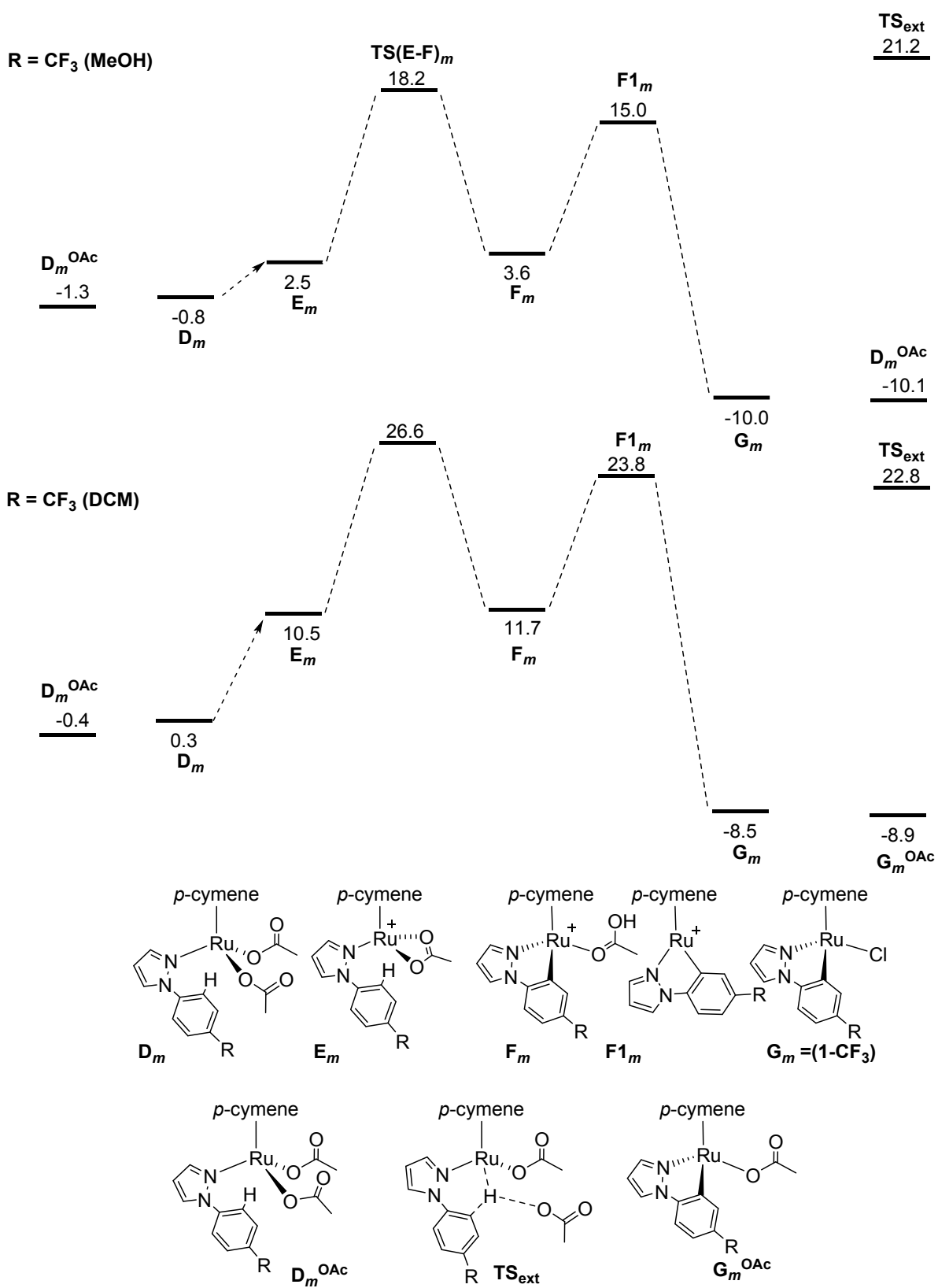
(iii) Computed profiles (G, kcal/mol) for cyclometallation of **L1-R** to give *meta*-substituted complexes **1-R**.

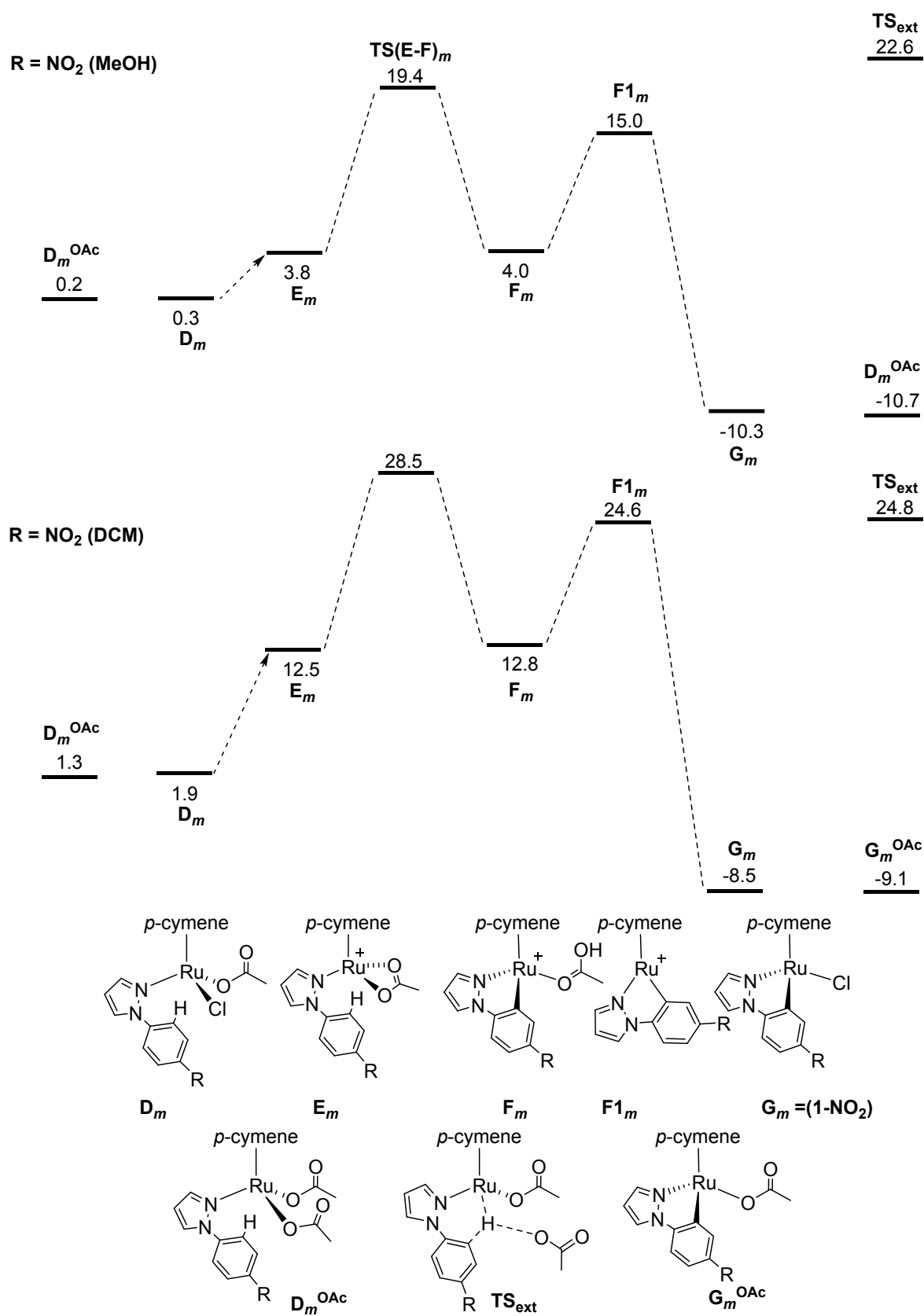




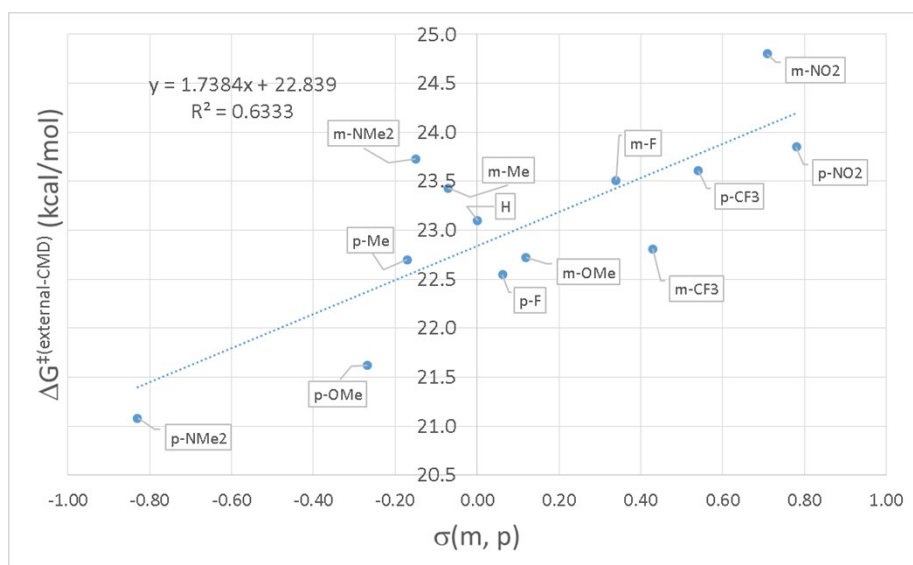
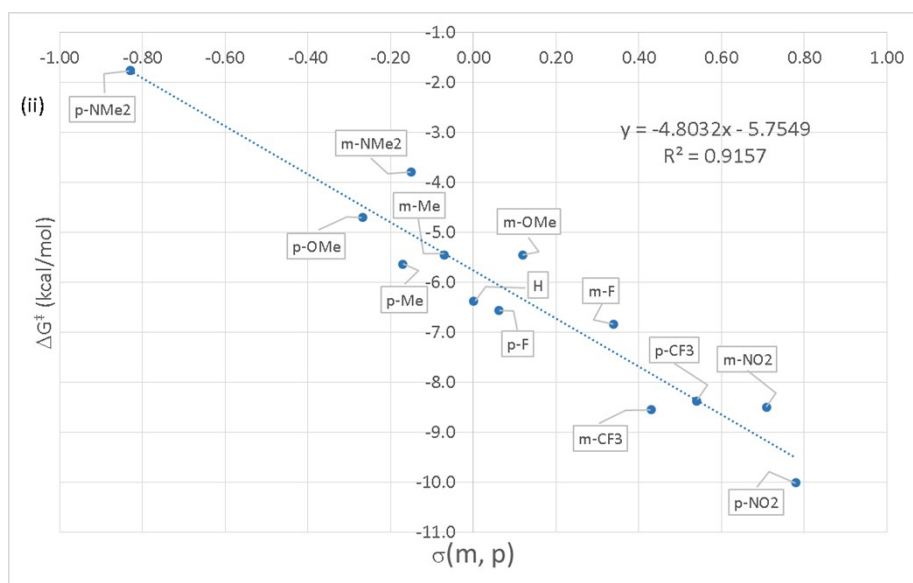
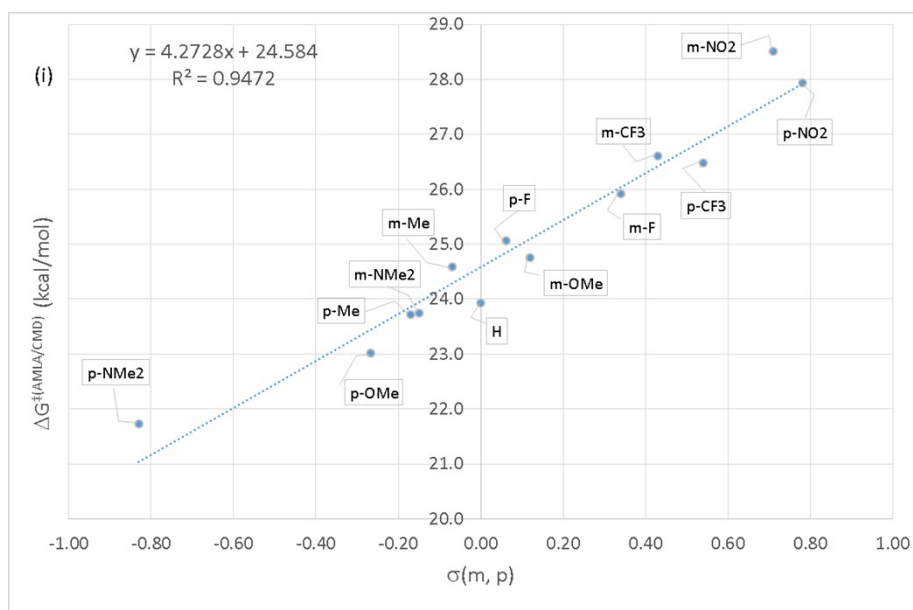








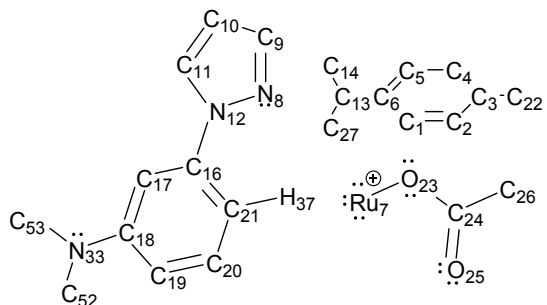
5. Plots of computed values of (i) $\Delta G^\ddagger(\text{AMLA/CMD})$, (ii) ΔG and (iii) $\Delta G^\ddagger(\text{external-CMD})$ (kcal/mol) against σ_m and σ_p Hammett constants for the reactions of **L1-R** and **L2-R**.



6. NBO Calculations.

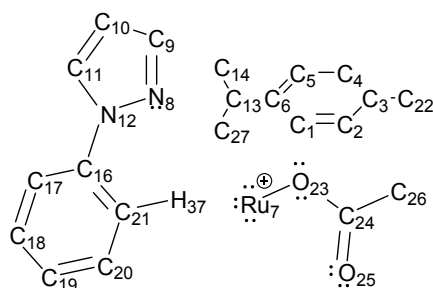
A common Lewis structure was imposed on **TS(E-F)_{1p}** (R = NMe₂), **TS(E-F)** (R = H) and **TS(E-F)_p** (R = NO₂) using the \$CHOOSE option. See below for atom labelling scheme employed (spectator H atoms omitted for clarity). All Lewis structure described in excess of 97% of the total electron density.

R = NMe₂, TS(E-F)_{1p}



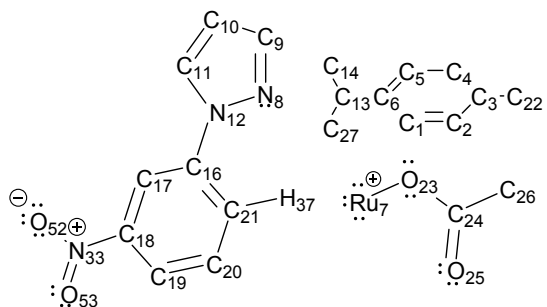
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$CHOOSE
LONE 7 3 8 1 12 1 23 2 25 2 33 1 END
BOND D 1 2 S 1 6 S 1 38 S 2 3 S 2 40 D 3 4 S 3 13 S 4 5 S 4 41 D 5 6 S 5 39
S 6 22 S 7 23 D 8 9 S 8 12 S 9 10 S 9 51 D 10 11 S 10 15 S 11 12 S 11 36
S 12 16 S 13 14 S 13 27 S 13 31 S 14 45 S 14 46 S 14 47 S 16 17 D 16 21
D 17 18 S 17 32 S 18 19 S 18 33 D 19 20 S 19 35 S 20 21 S 20 34 S 21 37
S 22 48 S 22 49 S 22 50 S 23 24 D 24 25 S 24 26 S 26 28 S 26 29 S 26 30
S 27 42 S 27 43 S 27 44 S 33 52 S 33 53 S 52 54 S 52 55 S 52 56 S 53 57
S 53 58 S 53 59 END
$END
```

R = H, TS(E-F)



```
$CHOOSE
LONE 7 3 8 1 12 1 23 2 25 2 END
BOND D 1 2 S 1 6 S 1 38 S 2 3 S 2 40 D 3 4 S 3 13 S 4 5 S 4 41 D 5 6 S 5 39
S 6 22 S 7 23 D 8 9 S 8 12 S 9 10 S 9 51 D 10 11 S 10 15 S 11 12 S 11 36
S 12 16 S 13 14 S 13 27 S 13 31 S 14 45 S 14 46 S 14 47 S 16 17 D 16 21
D 17 18 S 17 32 S 18 19 S 18 33 D 19 20 S 19 35 S 20 21 S 20 34 S 21 37
S 22 48 S 22 49 S 22 50 S 23 24 D 24 25 S 24 26 S 26 28 S 26 29 S 26 30
S 27 42 S 27 43 S 27 44 END
$END
```

R = NMe₂, TS(E-F)_{1p}



```
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LONE 7 3 8 1 12 1 23 2 25 2 52 3 53 2 END
BOND D 1 2 S 1 6 S 1 38 S 2 3 S 2 40 D 3 4 S 3 13 S 4 5 S 4 41 D 5 6 S 5 39
S 6 22 S 7 23 D 8 9 S 8 12 S 9 10 S 9 51 D 10 11 S 10 15 S 11 12 S 11 36
S 12 16 S 13 14 S 13 27 S 13 31 S 14 45 S 14 46 S 14 47 S 16 17 D 16 21
D 17 18 S 17 32 S 18 19 S 18 33 D 19 20 S 19 35 S 20 21 S 20 34 S 21 37
S 22 48 S 22 49 S 22 50 S 23 24 D 24 25 S 24 26 S 26 28 S 26 29 S 26 30
S 27 42 S 27 43 S 27 44 S 33 52 D 33 53 END
$END
```

Donor-acceptor interactions were quantified by a 2nd order perturbation analysis and the values quoted in the main paper (Figure 7) are a sum of all the interactions involved. The various components are summarised below:

R = NMe₂, TS(E-F)_{1p}	Donor	Acceptor	ΔE(kcal/mol)	Total
	78.BD(2)C16-C21	111.LV(1)Ru7	15.96	
	78.BD(2)C16-C21	112.LV(2)Ru7	3.13	19.09
	89.BD(1)C21-H37	111.LV(1)Ru7	7.36	
	89.BD(1)C21-H37	112.LV(2)Ru7	6.19	13.55
	Donor	Acceptor	ΔE(kcal/mol)	
	33.LP(1)Ru7	159.BD*(1)C21-H37	0.19	
	34.LP(2)Ru7	159.BD*(1)C21-H37	0.18	
	35.LP(3)Ru7	159.BD*(1)C21-H37	0.12	0.49
	40.LP(1)O25	159.BD*(1)C21-H37	1.17	
	41.LP(2)O25	159.BD*(1)C21-H37	1.82	2.99
R = H, TS(E-F)	Donor	Acceptor	ΔE(kcal/mol)	
	74.BD(2)C16-C21	99.LV(1)Ru7	13.54	
	74.BD(2)C16-C21	100.LV(2)Ru7	2.1	15.64
	85.BD(1)C21-H37	99.LV(1)Ru7	14.46	
	85.BD(1)C21-H37	100.LV(2)Ru7	10.08	24.54
	Donor	Acceptor	ΔE(kcal/mol)	
	30.LP(1)Ru7	147.BD*(1)C21-H37	0.31	
	31.LP(2)Ru7	147.BD*(1)C21-H37	0.76	
	32.LP(3)Ru7	147.BD*(1)C21-H37	0.13	
	30.LP(1)Ru7	147.BD*(1)C21-H37	0.31	1.51
	37.LP(1)O25	147.BD*(1)C21-H37	2.06	
	38.LP(2)O25	147.BD*(1)C21-H37	5.23	7.29
R = NO₂, TS(E-F)_p	Donor	Acceptor	ΔE(kcal/mol)	
	82.BD(2)C16-C21	110.LV(1)Ru7	7.47	
	82.BD(2)C16-C21	111.LV(2)Ru7	1.71	9.18
	93.BD(1)C21-H37	110.LV(1)Ru7	14.65	
	93.BD(1)C21-H37	111.LV(2)Ru7	10.72	25.37
	Donor	Acceptor	ΔE(kcal/mol)	
	33.LP(1)Ru7	158.BD*(1)C21-H37	0.22	
	34.LP(2)Ru7	158.BD*(1)C21-H37	0.08	
	35.LP(3)Ru7	158.BD*(1)C21-H37	1.07	1.37
	40.LP(1)O25	158.BD*(1)C21-H37	2.88	
	41.LP(2)O25	158.BD*(1)C21-H37	6.96	9.84

7. Computed Cartesian Coordinates (A)
and Energies (a.u.) for all species.

A [RuCl₂(p-cymene)]₂

SCF = -1029.38155006
H(0 K) = -1028.958494
H(298 K) = -1028.925916
G(298 K) = -1029.023879
BP86 (D3) = -1029.47775112
SCF (MeOH) = -1029.40716451
SCF (DCM) = -1029.40336604
SCF (BS2) = -2809.90308752
Lowest Frequencies = 12.8448cm⁻¹,
17.1216cm⁻¹

54

Ru	1.78347	-0.56569	0.37455
Cl	0.49307	1.55171	0.14492
Cl	1.70878	-0.21287	2.74116
C	3.57984	0.25121	-0.59738
C	2.64900	-0.21632	-1.60927
H	2.23779	0.49706	-2.33039
C	2.12349	-1.53574	-1.58711
H	1.32146	-1.79717	-2.28360
C	2.48556	-2.45051	-0.52576
C	3.41227	-2.00509	0.47268
H	3.62282	-2.64236	1.33628
C	3.95189	-0.66833	0.43391
H	4.54791	-0.32111	1.28126
C	4.07199	1.69203	-0.64434
H	3.22263	2.29383	-1.02091
C	5.22611	1.80179	-1.67098
H	6.10062	1.21192	-1.34399
H	5.54494	2.85309	-1.77355
H	4.92424	1.43869	-2.66806
C	4.48124	2.25866	0.72683
H	3.68246	2.12087	1.47435
H	4.68993	3.33789	0.63560
H	5.40248	1.78225	1.10749
C	1.85881	-3.81976	-0.44880
H	1.87637	-4.21038	0.58064
H	2.42096	-4.51993	-1.09412
H	0.81435	-3.79515	-0.79627
Ru	-1.75046	0.57242	-0.21095
Cl	-0.53574	-1.45040	0.53974
Cl	-1.06501	0.03451	-2.46110
C	-3.74141	-0.23862	0.27665
C	-3.12797	0.31829	1.46894
H	-2.93706	-0.33976	2.32278
C	-2.63261	1.65064	1.50532
H	-2.07498	1.99450	2.38125
C	-2.69953	2.48850	0.32644
C	-3.31134	1.95454	-0.85363
H	-3.28595	2.53154	-1.78228
C	-3.82167	0.60609	-0.87460
H	-4.15570	0.19048	-1.82827
C	-4.21176	-1.68730	0.28496
H	-3.49211	-2.24072	0.91883
C	-5.60264	-1.76945	0.96068
H	-6.36044	-1.22808	0.36729
H	-5.92388	-2.82176	1.04274
H	-5.59270	-1.33679	1.97555
C	-4.21950	-2.34836	-1.10482

H	-3.24641	-2.23219	-1.61020
H	-4.43285	-3.42561	-1.00242
H	-5.00501	-1.92343	-1.75512
C	-2.09423	3.86942	0.33416
H	-1.84120	4.19997	-0.68513
H	-2.81760	4.58810	0.76164
H	-1.17951	3.89788	0.94679

B Ru(OAc)(Cl)(p-cymene)

SCF = -728.133599061
H(0 K) = -727.873532
H(298 K) = -727.854774
G(298 K) = -727.921043
BP86 (D3) = -728.174755541
SCF (MeOH) = -728.151477240
SCF (DCM) = -728.148881511
SCF (BS2) = -1173.23217711
Lowest Frequencies = 19.0823cm⁻¹,
44.5539cm⁻¹

33

C	-0.10718	1.80082	-1.25786
C	-1.04525	0.74192	-1.44395
C	-1.81380	0.18939	-0.34459
C	-1.56960	0.73465	0.95314
C	-0.59878	1.77368	1.16896
C	0.16688	2.29468	0.07095
Ru	0.34995	0.11701	0.10007
Cl	0.73448	-1.31250	1.96474
C	-2.78790	-0.95260	-0.60654
C	-2.99701	-1.88069	0.60342
C	1.26520	3.30252	0.30126
O	1.19705	-1.48962	-1.06752
C	2.38744	-1.07031	-0.81324
O	2.49022	0.04392	-0.17553
C	3.60141	-1.86742	-1.20305
C	-4.13108	-0.37758	-1.11904
H	3.84986	-2.55335	-0.37488
H	3.39574	-2.46878	-2.10087
H	4.46151	-1.20249	-1.37108
H	-2.34323	-1.55561	-1.42239
H	0.50956	2.13597	-2.09714
H	-0.35319	2.07658	2.19016
H	-1.12758	0.27294	-2.43052
H	-2.01879	0.25674	1.82718
H	-4.82228	-1.19628	-1.38195
H	-4.61494	0.23861	-0.34089
H	-3.99368	0.25305	-2.01406
H	-3.59417	-2.75738	0.30184
H	-2.03449	-2.23367	1.00935
H	-3.55250	-1.37430	1.41304
H	2.10335	3.13958	-0.39437
H	0.87776	4.32538	0.14112
H	1.65309	3.23839	1.32956

C Ru(OAc)₂(p-cymene)

SCF = -941.572514204
H(0 K) = -941.263777
H(298 K) = -941.241282
G(298 K) = -941.316490
BP86 (D3) = -941.620367274
SCF (MeOH) = -941.585835902

SCF (DCM) = -941.583888511
 SCF (BS2) = -941.513267747
 Lowest Frequencies = 20.4399cm⁻¹,
 41.7952cm⁻¹

39

Ru	0.36306	-0.32771	-0.07682
O	0.93553	1.55376	-0.67281
C	0.14748	2.52163	-1.11325
C	0.93958	3.79751	-1.41690
C	-0.53105	-1.26398	-1.84983
O	-1.08470	2.47863	-1.25821
C	-2.84156	0.46884	0.75533
C	1.24632	-3.10085	-1.66681
O	1.27496	0.37248	1.75080
C	2.44852	0.13173	1.27765
C	3.68994	0.56862	2.00887
O	2.51604	-0.47077	0.14307
H	1.22787	4.28164	-0.46797
H	1.86736	3.56451	-1.96267
H	0.31792	4.49382	-1.99733
H	-2.74085	1.39959	0.16822
H	1.74356	-2.56580	-2.49092
H	3.95614	1.58767	1.67957
H	3.50952	0.59242	3.09379
H	4.53051	-0.10043	1.77219
C	0.14443	-2.26530	-1.06416
C	-0.22433	-2.42560	0.31704
C	-1.50687	-0.40766	-1.24552
C	-1.83802	-0.50155	0.14563
C	-1.15284	-1.51690	0.91337
H	-1.28735	-1.54653	1.99860
H	-1.88804	0.44843	-1.80676
H	-0.22023	-1.09052	-2.88389
H	0.32300	-3.13529	0.94421
C	-4.27541	-0.08388	0.57277
H	-5.01610	0.64134	0.95126
H	-4.50368	-0.27954	-0.48868
H	-4.41241	-1.02850	1.12961
C	-2.55735	0.80701	2.23065
H	-1.52023	1.15361	2.37060
H	-3.23627	1.60894	2.56601
H	-2.72914	-0.05868	2.89623
H	0.82835	-4.04143	-2.07003
H	2.00783	-3.35658	-0.91377

SCF = -728.133599061
 H(0 K)= -727.873532
 H(298 K)= -727.854774
 G(298 K)= -727.921043
 BP86 (D3) = -728.174755541
 SCF (MeOH) = -728.151477240
 SCF (DCM) = -728.148881511
 SCF (BS2) = -1173.23217711
 Lowest Frequencies = 19.0823cm⁻¹,
 44.5539cm⁻¹

33

C	-0.10718	1.80082	-1.25786
C	-1.04525	0.74192	-1.44395
C	-1.81380	0.18939	-0.34459
C	-1.56960	0.73465	0.95314
C	-0.59878	1.77368	1.16896

C	0.16688	2.29468	0.07095
Ru	0.34995	0.11701	0.10007
Cl	0.73448	-1.31250	1.96474
C	-2.78790	-0.95260	-0.60654
C	-2.99701	-1.88069	0.60342
C	1.26520	3.30252	0.30126
O	1.19705	-1.48962	-1.06752
C	2.38744	-1.07031	-0.81324
O	2.49022	0.04392	-0.17553
C	3.60141	-1.86742	-1.20305
C	-4.13108	-0.37758	-1.11904
H	3.84986	-2.55335	-0.37488
H	3.39574	-2.46878	-2.10087
H	4.46151	-1.20249	-1.37108
H	-2.34323	-1.55561	-1.42239
H	0.50956	2.13597	-2.09714
H	-0.35319	2.07658	2.19016
H	-1.12758	0.27294	-2.43052
H	-2.01879	0.25674	1.82718
H	-4.82228	-1.19628	-1.38195
H	-4.61494	0.23861	-0.34089
H	-3.99368	0.25305	-2.01406
H	-3.59417	-2.75738	0.30184
H	-2.03449	-2.23367	1.00935
H	-3.55250	-1.37430	1.41304
H	2.10335	3.13958	-0.39437
H	0.87776	4.32538	0.14112
H	1.65309	3.23839	1.32956

1-phenylpyrazole

SCF = -457.255768801
 H(0 K)= -457.108299
 H(298 K)= -457.099968
 G(298 K)= -457.142294
 BP86 (D3) = -457.269889531
 SCF (DCM) = -457.260735574
 SCF (MeOH) = -457.261572405
 Lowest Frequencies = 45.9004cm⁻¹,
 104.1130cm⁻¹

C	3.00299	-0.75368	-0.15015
C	3.15594	0.62888	0.13594
H	3.77689	-1.50657	-0.30315
H	4.07583	1.19530	0.26691
C	-0.40430	0.02630	-0.00631
C	-2.47891	-1.22294	0.13999
C	-2.53422	1.18641	-0.13183
C	-3.21479	-0.03266	0.01361
H	-2.99839	-2.18046	0.25034
H	-3.09461	2.12009	-0.24526
H	-4.30896	-0.05538	0.02269
N	1.01964	0.04176	-0.00289
N	1.71392	-1.11506	-0.23363
C	-1.07841	-1.20189	0.13504
H	-0.48783	-2.11508	0.23411
C	-1.13246	1.22277	-0.15105
H	-0.61413	2.17408	-0.30078
C	1.85774	1.11029	0.22626
H	1.47481	2.10033	0.46176

D (R = H)

SCF = -1185.38967343

H(0 K) = -1184.980752
 H(298 K) = -1184.952025
 G(298 K) = -1185.040575
 BP86 (D3) = -1185.47345356
 SCF (MeOH) = -1185.41042915
 SCF (DCM) = -1185.40707920
 SCF (BS2) = -1630.60248614
 Lowest Frequencies = 22.1021cm⁻¹,
 31.5743cm⁻¹

52

C	2.74672	0.28439	-1.14250
C	2.85781	-0.75592	-0.20348
C	3.90509	-0.78018	0.73708
C	4.85843	0.24988	0.73396
C	4.75779	1.29810	-0.19539
C	3.70287	1.31222	-1.12455
N	1.95737	-1.87068	-0.24258
N	0.58183	-1.78352	-0.27127
C	0.14112	-3.04880	-0.42562
C	1.21724	-3.95799	-0.49479
C	2.35766	-3.17623	-0.37954
Ru	-0.71377	-0.07624	0.12530
Cl	-0.54493	0.37611	-2.25156
H	3.62561	2.12418	-1.85463
C	-1.97355	0.39666	1.84217
C	-2.00455	1.50926	0.93160
C	-0.79308	2.14668	0.50893
C	0.45501	1.62497	0.99484
C	0.46323	0.49156	1.86987
C	-0.74715	-0.11995	2.36362
C	-0.88739	3.32368	-0.45565
C	-1.49578	4.53757	0.28994
C	-0.71296	-1.28784	3.31803
O	-2.12406	-1.47466	-0.51807
C	-3.42588	-1.24370	-0.59196
C	-4.15617	-2.36377	-1.34180
O	-4.03808	-0.25829	-0.15373
C	0.43991	3.70186	-1.13149
H	-2.96092	1.77881	0.48031
H	1.40231	2.02525	0.63064
H	1.42765	0.04997	2.14388
H	-2.91500	-0.11937	2.04732
H	-1.59230	3.01008	-1.24853
H	0.85861	2.84154	-1.67677
H	0.26687	4.51365	-1.85804
H	1.18235	4.06952	-0.39964
H	-1.63361	5.37942	-0.40975
H	-2.47692	4.29896	0.73270
H	-0.82914	4.87822	1.10221
H	0.18480	-1.90797	3.16147
H	-0.69736	-0.93234	4.36515
H	-1.60097	-1.92791	3.19325
H	-3.98678	-2.23282	-2.42432
H	-5.23536	-2.30807	-1.13959
H	-3.76815	-3.35688	-1.06389
H	-0.93470	-3.20033	-0.48439
H	1.16673	-5.03615	-0.62742
H	3.41719	-3.41794	-0.42785
H	1.91143	0.28396	-1.85369
H	5.50190	2.10100	-0.19734
H	5.67508	0.23323	1.46258
H	3.96515	-1.59898	1.46149

D^{OAc} (R = H)

SCF = -1398.82452353
 H(0 K) = -1398.366676
 H(298 K) = -1398.334301
 G(298 K) = -1398.431658
 BP86 (D3) = -1398.91691244
 SCF (MeOH) = -1398.84217244
 SCF (DCM) = -1398.83952494
 SCF (BS2) = -1398.87836777
 Lowest Frequencies = 19.9574cm⁻¹,
 25.7153cm⁻¹

58

Ru	-0.48890	-0.09014	-0.17705
C	-1.71229	0.21517	-1.99135
C	-2.36923	-0.78590	-1.17796
C	-1.61127	-1.91018	-0.74011
C	-0.22718	-2.05913	-1.12179
C	0.41393	-1.12154	-1.98060
C	-0.35080	0.04559	-2.36580
H	-2.23320	1.14830	-2.21568
C	-3.83351	-0.59309	-0.80659
H	-2.01752	-2.61441	-0.01446
H	0.34281	-2.88375	-0.68674
C	1.82284	-1.33096	-2.47457
H	0.15559	0.85313	-2.90600
H	-3.99089	0.49703	-0.72049
C	-4.24269	-1.25338	0.52153
C	-4.70388	-1.10920	-1.98015
H	-3.58868	-0.92774	1.34577
H	-5.28118	-0.97590	0.76957
H	-4.20562	-2.35541	0.46109
H	-5.77071	-0.92037	-1.77119
H	-4.44943	-0.60865	-2.92978
H	-4.57147	-2.19660	-2.12090
H	2.42001	-1.91967	-1.76117
H	1.79905	-1.87935	-3.43508
H	2.34019	-0.37495	-2.64959
O	-1.64860	1.02729	1.17812
C	-2.46418	2.01398	0.88910
O	-2.64037	2.54067	-0.23181
C	-3.19112	2.54691	2.12943
H	-3.51464	1.72319	2.78428
H	-4.05239	3.15932	1.82567
H	-2.49657	3.17616	2.71261
O	0.20681	-0.66246	1.71320
C	-0.03609	-1.83045	2.28404
O	-0.52019	-2.84166	1.74964
C	0.34059	-1.82477	3.77116
H	-0.43743	-1.28066	4.33361
H	0.39896	-2.85560	4.14928
H	1.29263	-1.29805	3.94550
N	0.92603	1.55729	0.00127
C	0.48592	2.83427	-0.03884
H	-0.58304	3.01796	-0.16521
C	1.55689	3.74762	0.05433
H	1.50116	4.83343	0.06664
C	2.69339	2.96028	0.14616
H	3.74482	3.21160	0.26495
N	2.30380	1.64434	0.10867
C	3.22860	0.55047	0.04492

C 3.06896 -0.58842 0.84962
H 2.18512 -0.66138 1.49148
C 4.03439 -1.60578 0.78597
H 3.91094 -2.49658 1.41036
C 5.15694 -1.48211 -0.04988
H 5.90895 -2.27692 -0.08358
C 5.31103 -0.33305 -0.84291
H 6.17780 -0.22896 -1.50332
C 4.34443 0.68231 -0.80674
H 4.44218 1.56685 -1.44398

E (R = H)

SCF = -1170.15092882
H(0 K) = -1169.741883
H(298 K) = -1169.715219
G(298 K) = -1169.799693
BP86 (D3) = -1170.22383350
SCF (MeOH) = -1170.20562902
SCF (DCM) = -1170.20082891
SCF (BS2) = -1170.12434678
Lowest Frequencies = 15.6952cm⁻¹,
37.2386cm⁻¹

51

C 1.64346 0.76048 -2.23358
C 2.54087 0.13127 -1.32182
C 2.20866 -1.08935 -0.62186
C 0.89560 -1.60763 -0.84341
C -0.03435 -0.98174 -1.74158
C 0.32350 0.21688 -2.44074
Ru 0.67830 0.51705 -0.26717
N -0.38750 0.04813 1.51465
C 0.14308 0.08628 2.76082
C -0.74654 -0.46908 3.69974
C -1.86246 -0.84660 2.96089
N -1.62710 -0.53297 1.64972
C 3.23993 -1.74297 0.28910
C 2.63880 -2.65930 1.36871
H -0.60213 -0.56809 4.77286
C -2.56053 -0.68524 0.56874
C -3.10360 -1.95954 0.32595
C -4.06380 -2.11169 -0.68712
C -4.46772 -1.00192 -1.44823
C -3.91615 0.26621 -1.19279
C -2.96100 0.43672 -0.17829
C -0.65979 0.92370 -3.33459
O 1.54005 2.02582 0.97785
C 0.57951 2.84871 0.71109
O -0.30528 2.42420 -0.12767
C 0.48804 4.19820 1.35611
C 4.26233 -2.51122 -0.58752
H -0.05003 4.10884 2.31610
H 1.49462 4.58972 1.56475
H -0.06969 4.89324 0.71190
H 3.78148 -0.92002 0.79533
H -2.77609 -2.81650 0.92305
H -4.49457 -3.09877 -0.87935
H -4.24725 1.13501 -1.77014
H -5.22027 -1.12304 -2.23314
H -2.81908 -1.27181 3.25737
H -2.53298 1.41954 0.03831
H 1.91612 1.71294 -2.69671

H -1.04977 -1.37527 -1.83193
H 3.48595 0.63098 -1.08245
H 0.55406 -2.45878 -0.24793
H 5.05817 -2.93486 0.04667
H 3.77423 -3.34345 -1.12338
H 4.73863 -1.85615 -1.33588
H 3.43609 -3.00983 2.04345
H 1.88343 -2.13735 1.98009
H 2.17341 -3.55877 0.92841
H -0.55024 2.01724 -3.26473
H -0.47089 0.63132 -4.38377
H -1.69624 0.65241 -3.08455
H 1.13465 0.51201 2.90169

TS(E-F) (R = H)

SCF = -1170.11902155
H(0 K) = -1169.711776
H(298 K) = -1169.685514
G(298 K) = -1169.769597
BP86 (D3) = -1170.19305893
SCF (MeOH) = -1170.17849054
SCF (DCM) = -1170.17302249
SCF (BS2) = -1170.09316150
Lowest Frequencies = -97.6200cm⁻¹,
8.3243cm⁻¹

51

C 2.08268 1.82282 -0.63424
C 2.58059 0.56326 -0.14496
C 2.16202 -0.68917 -0.73006
C 1.18677 -0.64130 -1.78756
C 0.64278 0.60733 -2.19444
C 1.10259 1.87538 -1.66246
Ru 0.43785 0.49808 0.00303
N -0.27301 -1.04567 1.25439
C 0.18988 -1.59796 2.39246
C -0.73216 -2.54809 2.88425
C -1.79545 -2.53291 1.98859
N -1.49630 -1.61669 1.01393
C 2.78019 -1.98738 -0.23293
C 1.94991 -3.24858 -0.52652
H -0.64128 -3.15308 3.78322
C -2.26466 -1.14149 -0.08238
C -3.13916 -1.99191 -0.77564
C -3.86167 -1.47899 -1.86488
C -3.70049 -0.14033 -2.26697
C -2.81582 0.69688 -1.57139
C -2.08928 0.20605 -0.46823
C 0.52147 3.18082 -2.13900
O 0.44989 1.48231 1.85082
C -0.38507 2.50245 1.85797
O -1.12317 2.77529 0.88417
C -0.40447 3.31158 3.14231
C 4.20352 -2.10664 -0.84201
H -1.35041 3.11047 3.67297
H 0.43709 3.06067 3.80250
H -0.39044 4.38474 2.89718
H 2.89367 -1.88878 0.86438
H -3.23992 -3.04199 -0.48592
H -4.54768 -2.13558 -2.40802
H -2.71814 1.75286 -1.84088
H -4.27760 0.25015 -3.11017

H -2.74310 -3.06664 1.98219
H -1.63420 0.98181 0.20952
H 2.36838 2.74460 -0.11841
H -0.18934 0.61253 -2.90517
H 3.25784 0.55340 0.71453
H 0.78398 -1.56577 -2.20643
H 4.69791 -3.01158 -0.45298
H 4.15587 -2.19117 -1.94100
H 4.83554 -1.23900 -0.59142
H 2.42196 -4.12093 -0.04707
H 0.92083 -3.16702 -0.14071
H 1.90445 -3.46307 -1.60841
H 0.46403 3.91567 -1.32257
H 1.15738 3.59659 -2.94173
H -0.49018 3.04433 -2.54995
H 1.14445 -1.27372 2.80108

F (R = H)

SCF = -1170.14594827
H(0 K) = -1169.737445
H(298 K) = -1169.710814
G(298 K) = -1169.794566
BP86 (D3) = -1170.22006822
SCF (MeOH) = -1170.20164714
SCF (DCM) = -1170.19668557
SCF (BS2) = -1170.11842680
Lowest Frequencies = 19.1348cm⁻¹,
32.2901cm⁻¹

51

C 1.21916 1.61344 -1.71478
C 1.12619 2.58811 -0.67839
C 1.76152 2.31564 0.59522
C 2.37757 1.07094 0.83092
C 2.42669 0.03834 -0.18976
C 1.84847 0.34338 -1.46304
Ru 0.29254 0.60631 0.04280
N -0.16389 -0.81462 1.48438
C 0.05967 -0.97700 2.80619
C -0.58840 -2.14313 3.26694
C -1.22585 -2.68215 2.15196
N -0.95706 -1.86257 1.09080
C 3.13751 -1.27500 0.11198
C 2.69760 -2.45096 -0.77722
C 0.41123 3.89725 -0.89901
H -0.59140 -2.54183 4.27859
C -1.35442 -1.85717 -0.27132
C -2.10516 -2.90009 -0.83222
C -2.46150 -2.81778 -2.18710
C -2.06633 -1.70793 -2.95000
C -1.30700 -0.67589 -2.36450
C -0.92231 -0.71129 -1.00096
O -1.36481 1.69442 0.93214
C -2.57752 1.78100 0.60988
O -3.12121 1.11946 -0.39808
C -3.52683 2.66632 1.36661
C 4.66833 -1.04918 0.02204
H -4.30936 2.04604 1.83491
H -2.99037 3.23269 2.13778
H -4.03421 3.35192 0.66865
H 2.89457 -1.52906 1.16263
H -2.40874 -3.76545 -0.23480

H -3.04881 -3.62087 -2.64088
H -1.01845 0.17994 -2.98495
H -2.34691 -1.64118 -4.00579
H -1.84435 -3.56935 2.04037
H -2.42007 0.52024 -0.80236
H 0.65935 -0.25030 3.35010
H 0.75507 1.81155 -2.68483
H 1.83264 -0.42084 -2.24373
H 2.78555 0.85016 1.82326
H 1.67318 3.04559 1.40499
H 5.20268 -1.96998 0.30789
H 4.96660 -0.78871 -1.00804
H 5.00814 -0.23978 0.68971
H 1.60348 -2.58809 -0.76648
H 3.02101 -2.31535 -1.82407
H 3.16255 -3.38280 -0.41721
H -0.15463 4.20038 -0.00403
H 1.15176 4.69036 -1.10823
H -0.27796 3.84505 -1.75585

F1 (R = H)

SCF = -941.016843875
H(0 K) = -940.670419
H(298 K) = -940.649224
G(298 K) = -940.721381
BP86 (D3) = -941.069997225
SCF (MeOH) = -941.075736007
SCF (DCM) = -941.070435004
SCF (BS2) = -940.920436213
Lowest Frequencies = 13.7645cm⁻¹,
24.0182cm⁻¹

43

C 1.29896 -0.95468 0.30198
C 2.46394 -0.29479 -0.19191
C 3.71308 -0.91327 -0.30909
C 3.82754 -2.25963 0.07865
C 2.71052 -2.95642 0.57104
C 1.46825 -2.31028 0.67470
N 2.26335 1.06809 -0.56213
N 0.99332 1.55836 -0.38348
C 1.03262 2.85955 -0.77016
C 2.32579 3.20370 -1.19609
C 3.08378 2.03734 -1.05149
Ru -0.35650 0.21719 0.44095
C -1.71116 -1.00966 1.66873
C -1.75847 0.35751 2.12938
C -2.19089 1.38459 1.21055
C -2.38596 1.08156 -0.15239
C -2.16970 -0.25697 -0.66246
C -1.90582 -1.31092 0.29382
C -1.43485 0.69579 3.56173
C -2.35475 -0.53209 -2.14800
C -3.86448 -0.76929 -2.41756
C -1.50112 -1.69259 -2.69043
H 2.67144 4.16648 -1.56437
H -2.05715 0.39270 -2.67922
H 4.58795 -0.37668 -0.68880
H 4.79586 -2.76116 -0.00653
H 0.61235 -2.87389 1.06122
H 2.81047 -4.00386 0.87148
H 4.13346 1.84235 -1.26011

H 0.13060 3.46624 -0.71907
H -1.40302 -1.79579 2.36402
H -1.74528 -2.33122 -0.06340
H -2.58896 1.88726 -0.86530
H -2.23942 2.42150 1.55595
H -4.03199 -0.90321 -3.49882
H -4.21864 -1.67934 -1.90367
H -4.48351 0.07815 -2.07938
H -0.43416 -1.56457 -2.44323
H -1.83638 -2.66835 -2.29786
H -1.59650 -1.74036 -3.78706
H -1.03026 1.71562 3.65605
H -2.35931 0.64372 4.16721
H -0.71173 -0.01381 3.99257

G (R = H)

SCF = -956.295830707
H(0 K) = -955.948786
H(298 K) = -955.925991
G(298 K) = -956.000670
BP86 (D3) = -956.361335057
SCF (MeOH) = -956.316329438
SCF (DCM) = -956.313089443
SCF (BS2) = -1401.43491923
Lowest Frequencies = 16.6691cm⁻¹,
44.5593cm⁻¹

44

C 1.35765 -0.64386 -0.71031
C 2.36811 0.26596 -0.30415
C 3.65742 0.30608 -0.85693
C 3.98013 -0.61203 -1.86581
C 3.01881 -1.54625 -2.28843
C 1.73468 -1.56069 -1.71446
N 1.97044 1.14409 0.73687
N 0.67266 1.01964 1.15163
C 0.51168 1.88153 2.17739
C 1.71556 2.57882 2.41704
C 2.62471 2.08243 1.48398
Ru -0.44895 -0.46339 0.24609
Cl 0.50720 -1.89534 1.95421
C -1.66662 -1.48551 -1.30871
C -2.14425 -1.92944 -0.04386
C -2.61444 -0.93313 0.90440
C -2.52900 0.43943 0.60526
C -1.95478 0.90546 -0.64564
C -1.55299 -0.07935 -1.60509
C -2.17002 -3.39052 0.32593
C -1.86943 2.40465 -0.90924
C -3.25891 2.94172 -1.33011
C -0.78970 2.80041 -1.93184
H 1.90162 3.33884 3.17216
H -1.60356 2.87616 0.05799
H 4.40109 1.03079 -0.50841
H 4.97946 -0.60110 -2.31157
H 1.01860 -2.31996 -2.04691
H 3.27243 -2.27483 -3.06652
H 3.67190 2.31340 1.30703
H -0.44395 1.93317 2.69364
H -1.30526 -2.22208 -2.03212
H -1.10279 0.23084 -2.55114
H -2.82300 1.17688 1.36050

H -2.93741 -1.25733 1.89772
H -3.23023 4.03839 -1.44968
H -3.57093 2.50223 -2.29383
H -4.03422 2.70064 -0.58315
H 0.19096 2.37225 -1.66713
H -1.05042 2.46333 -2.95076
H -0.69082 3.89818 -1.96983
H -1.60995 -3.54836 1.26372
H -3.21036 -3.73337 0.47051
H -1.70505 -4.00853 -0.45773

G^{OAc} (R = H)

SCF = -1169.73348298
H(0 K) = -1169.337687
H(298 K) = -1169.311255
G(298 K) = -1169.394812
BP86 (D3) = -1169.80557072
SCF (MeOH) = -1169.74895750
SCF (BS2) = -1169.71485240
Lowest Frequencies = 16.3812cm⁻¹,
32.3996cm⁻¹

50

0.0000000000
C 2.20970 -0.64491 1.03288
C 2.44100 0.75446 1.31518
C 2.34061 1.70831 0.27678
C 2.07526 1.23853 -1.07060
C 1.97072 -0.15380 -1.34409
C 2.05502 -1.14710 -0.30087
Ru 0.45603 0.34280 0.16517
O -0.86774 1.96622 0.27617
C -0.93026 2.92631 -0.62695
O -0.16955 3.10074 -1.59543
C 2.45330 3.18895 0.53826
C 1.97106 -2.62869 -0.64581
C 1.38567 -3.50068 0.47903
C -1.05610 -0.49533 -0.93861
C -1.19925 -0.54164 -2.34180
C -2.31461 -1.14323 -2.95408
C -3.33696 -1.71109 -2.17528
C -3.25152 -1.66386 -0.77632
C -2.12836 -1.05524 -0.19553
N -1.98439 -0.93857 1.21251
N -0.83183 -0.34038 1.64344
C -0.91443 -0.27352 2.98810
C -2.12801 -0.84462 3.42992
C -2.78634 -1.25692 2.27239
C -2.11749 3.86648 -0.38065
C 3.36409 -3.14382 -1.08117
H -0.43902 -0.07261 -2.97511
H -2.38888 -1.16017 -4.04714
H -0.10858 0.18736 3.55488
H -2.33399 3.97179 0.69354
H -1.91692 4.84955 -0.83167
H -3.01398 3.44018 -0.86368
H -4.20406 -2.17989 -2.65081
H -4.05050 -2.08777 -0.15831
H -2.48060 -0.94314 4.45393
H -3.75098 -1.73600 2.12615
H 1.74739 -0.47973 -2.36551
H 2.58859 1.08417 2.34811

H	2.16950	-1.34615	1.87226
H	1.87533	1.96898	-1.85553
H	1.29162	-2.70597	-1.51698
H	3.77310	-2.55088	-1.91667
H	4.08210	-3.08634	-0.24378
H	3.30519	-4.19685	-1.40667
H	1.72317	3.73411	-0.08002
H	2.28107	3.42746	1.59973
H	3.46421	3.54392	0.26469
H	2.05873	-3.54691	1.35402
H	0.40731	-3.11744	0.81215
H	1.24822	-4.53533	0.12248

1. para-substituted species

1-C6H4R-pyrazole (R = p-NMe2)

SCF = -591.225615108
H(0 K) = -591.007435
H(298 K) = -590.994515
G(298 K) = -591.047568
BP86 (D3) = -591.249486698
SCF (DCM) = -591.232090603
SCF (MeOH) = -591.233178322
SCF (BS2) = -591.373943916
Lowest Frequencies = 39.7831cm⁻¹,
57.8987cm⁻¹

C -0.40691 -0.34719 -0.05798
C -1.74375 0.12898 -0.05855
C -1.95405 1.53408 0.03340
C -0.86330 2.40604 0.11534
C 0.45847 1.93877 0.11722
C 0.66709 0.55010 0.02255
H -0.17012 -1.40955 -0.11106
N -2.81197 -0.75745 -0.16232
H -2.96536 1.94518 0.04965
H -1.04964 3.48208 0.19779
H 1.29425 2.63334 0.22781
N 1.99378 0.02237 0.01093
N 2.21222 -1.29774 0.29443
C 3.16258 0.68697 -0.28121
C 4.19071 -0.24017 -0.17740
C 3.54096 -1.45013 0.18047
H 5.25154 -0.06457 -0.34495
H 3.98115 -2.43059 0.36571
H 3.16801 1.73671 -0.56412
C -4.17079 -0.26560 0.02112
C -2.56559 -2.19104 -0.06057
H -3.51780 -2.72811 -0.18172
H -1.88462 -2.53446 -0.86046
H -2.12093 -2.48428 0.91301
H -4.87630 -1.09667 -0.12491
H -4.34486 0.16329 1.03059
H -4.41611 0.51255 -0.72498

D (R = p-NMe2)

SCF = -1319.35972754
H(0 K) = -1318.880192
H(298 K) = -1318.846821
G(298 K) = -1318.946111
BP86 (D3) = -1319.45403747
SCF (MeOH) = -1319.38294824
SCF (DCM) = -1319.37924456
SCF (BS2) = -1764.60507290
Lowest Frequencies = 17.4808cm⁻¹,
23.9289cm⁻¹

60

C 3.31341 -0.94222 -0.04335
C 2.14784 -0.84985 -0.82269
C 1.92955 0.19994 -1.72694
C 2.92934 1.18175 -1.82103
C 4.10539 1.11810 -1.06368
C 4.33633 0.03865 -0.16412
N 1.20747 -1.93120 -0.72527

N -0.14503 -1.79444 -0.50032
C -0.65905 -3.03742 -0.60404
C 0.34818 -3.98154 -0.89141
C 1.52181 -3.24417 -0.96607
Ru -1.27717 -0.04993 0.14981
Cl -1.54949 0.42124 -2.21198
H 4.85031 1.90861 -1.17650
C -0.90761 -0.11822 2.35550
C -2.18036 0.46536 2.06488
C -2.31827 1.58888 1.17854
C -1.17086 2.16888 0.54464
C 0.11580 1.58089 0.79602
C 0.22295 0.43740 1.65239
C -0.76352 -1.30002 3.28227
C -1.37716 3.35785 -0.38720
C -1.77963 4.59408 0.45479
O -2.83922 -1.39080 -0.20926
C -4.12084 -1.09879 -0.05271
C -5.02458 -2.18549 -0.64717
O -4.59975 -0.08421 0.47609
C -0.17514 3.67393 -1.29063
H 2.79005 2.02010 -2.51139
H -3.32524 1.91067 0.90733
H 1.00074 1.93298 0.26416
H 1.19656 -0.05717 1.74095
H -3.09481 -0.00661 2.43337
H -2.22763 3.08635 -1.04057
H 0.09721 2.79619 -1.89723
H -0.43483 4.49666 -1.97813
H 0.70331 4.00052 -0.70435
H -1.99766 5.44813 -0.20890
H -2.67631 4.40100 1.06667
H -0.96175 4.89373 1.13430
H 0.06769 -1.95385 2.97121
H -0.55763 -0.96206 4.31510
H -1.68627 -1.90177 3.30275
H -5.05316 -2.05953 -1.74313
H -6.04460 -2.08364 -0.24966
H -4.63456 -3.19490 -0.43970
H -1.73291 -3.14749 -0.46837
H 0.23021 -5.05231 -1.04037
H 2.54505 -3.51951 -1.21176
H 0.99968 0.24752 -2.30306
N 5.51506 -0.05930 0.56770
H 3.41090 -1.77842 0.65211
C 5.62751 -1.06815 1.61316
C 6.44537 1.06416 0.57895
H 6.80589 1.29045 -0.44070
H 5.99960 1.98994 0.99890
H 7.32168 0.79750 1.18731
H 6.63186 -1.01560 2.05762
H 4.88181 -0.93574 2.42585
H 5.50212 -2.08496 1.19819

D^{OAc} (R = p-NMe2)

SCF = -1532.79427033
H(0 K) = -1532.265571
H(298 K) = -1532.228649
G(298 K) = -1532.336106
BP86 (D3) = -1532.89708729
SCF (MeOH) = -1532.81289468
SCF (DCM) = -1532.81095434

SCF (BS2) = -1532.88000548
 Lowest Frequencies = 19.6561cm⁻¹,
 24.7297cm⁻¹

66

C	3.78862	0.76641	-0.04473
C	2.57329	0.57055	0.63722
C	2.31371	-0.59433	1.37045
C	3.31183	-1.58183	1.39025
C	4.53634	-1.41301	0.73401
C	4.81323	-0.21666	0.01360
N	1.62922	1.65268	0.59927
N	0.28590	1.55678	0.28093
C	-0.16361	2.83007	0.21945
C	0.86595	3.74961	0.50740
C	1.98706	2.96949	0.74382
Ru	-1.06886	-0.09512	-0.15268
O	-0.65906	-0.71307	1.80367
C	-0.97727	-1.89438	2.30330
C	-0.81162	-1.92770	3.82836
C	-1.99343	0.25146	-2.13065
C	-2.76500	-0.76735	-1.45152
C	-2.08123	-1.90168	-0.92526
C	-0.65402	-2.04115	-1.08798
C	0.11085	-1.08378	-1.81352
C	-0.58886	0.09118	-2.28831
C	-4.26983	-0.58340	-1.30636
C	-4.94843	-1.07211	-2.61067
C	1.58169	-1.27979	-2.07948
O	-2.43723	0.97150	1.04180
C	-3.20961	1.96221	0.66369
C	-4.12072	2.45099	1.79627
C	-4.87368	-1.27502	-0.07161
O	-3.22116	2.52412	-0.45408
O	-1.38067	-2.89119	1.68109
H	-2.47701	1.18828	-2.41539
H	-2.59344	-2.62003	-0.28573
H	-0.15599	-2.87386	-0.58519
H	-0.00651	0.91121	-2.72285
H	-4.44221	0.50434	-1.21924
H	-4.34870	-0.97244	0.84823
H	-5.93751	-0.99965	0.02588
H	-4.82789	-2.37537	-0.15377
H	-6.03562	-0.88955	-2.56302
H	-4.55424	-0.54881	-3.49834
H	-4.79096	-2.15573	-2.75512
H	2.06043	-1.87607	-1.28737
H	1.71564	-1.81178	-3.04039
H	2.11432	-0.31873	-2.15028
H	-4.53559	1.60441	2.36490
H	-4.92933	3.07321	1.38615
H	-3.52681	3.05918	2.50041
H	-1.65612	-1.38882	4.29112
H	-0.81302	-2.96783	4.18501
H	0.11116	-1.41542	4.14494
H	-1.20358	3.00701	-0.06195
H	0.79214	4.83360	0.55042
H	3.00465	3.22402	1.03052
H	1.35211	-0.71062	1.87629
H	3.13265	-2.50889	1.94498
H	5.27957	-2.21159	0.78298
N	6.03839	-0.01428	-0.61471
H	3.91899	1.67592	-0.63397

C	6.21390	1.13543	-1.49195
C	6.98119	-1.12209	-0.71796
H	7.25044	1.15358	-1.85872
H	5.53563	1.11937	-2.37156
H	6.03947	2.08033	-0.94529
H	7.27377	-1.48863	0.28265
H	6.57773	-1.98141	-1.29328
H	7.89383	-0.77007	-1.22045

E (R = p-NMe₂)

SCF = -1304.12679308
 H(0 K) = -1303.647018
 H(298 K) = -1303.615710
 G(298 K) = -1303.711336
 BP86 (D3) = -1304.21038456
 SCF (MeOH) = -1304.17922232
 SCF (DCM) = -1304.17456735
 SCF (BS2) = -1304.13283602
 Lowest Frequencies = 9.6180cm⁻¹,
 25.1994cm⁻¹

59

C	-2.11191	0.23013	-2.40217
C	-2.71293	1.11033	-1.45507
C	-1.93428	1.93017	-0.55357
C	-0.51596	1.76703	-0.61588
C	0.11331	0.87123	-1.54605
C	-0.67742	0.08252	-2.44393
Ru	-1.40260	-0.24177	-0.37024
N	-0.46831	-0.54785	1.51678
C	-1.10383	-0.49073	2.71283
C	-0.17740	-0.53220	3.77118
C	1.06766	-0.62548	3.15721
N	0.87355	-0.62782	1.80383
C	-2.64106	2.89366	0.39143
C	-1.81874	3.27754	1.63367
H	-0.38723	-0.51322	4.83788
C	1.89661	-0.79181	0.80516
C	2.96136	0.12140	0.81602
C	4.04225	-0.03280	-0.10267
C	3.96197	-1.11586	-1.03066
C	2.88246	-2.00442	-1.01062
C	1.82820	-1.87071	-0.08964
C	-0.04036	-0.91383	-3.37506
O	-3.02226	-1.27103	0.57719
C	-2.54032	-2.42059	0.23371
O	-1.46785	-2.38862	-0.48229
C	-3.17533	-3.70784	0.66586
C	-3.06630	4.15333	-0.40580
H	-2.77368	-3.99989	1.65196
H	-4.26372	-3.58229	0.76397
H	-2.94286	-4.50852	-0.05111
H	-3.56316	2.38293	0.73157
H	2.94768	0.94085	1.53747
N	5.11439	0.83279	-0.09500
H	2.87341	-2.84056	-1.71736
H	4.76213	-1.27337	-1.75641
H	2.07146	-0.73343	3.56237
H	0.99428	-2.57508	-0.05654
H	-2.74111	-0.41382	-3.02305
H	1.19543	0.72292	-1.50750
H	-3.80354	1.10906	-1.35127
H	0.10964	2.26999	0.12656

H -3.64168 4.83377 0.24313
H -2.18267 4.70130 -0.77602
H -3.69751 3.89852 -1.27338
H -2.43379 3.89239 2.31019
H -1.48067 2.39073 2.19574
H -0.93390 3.88209 1.36660
H -0.66167 -1.81704 -3.47991
H 0.06639 -0.45817 -4.37656
H 0.95899 -1.20763 -3.02121
H -2.18967 -0.42258 2.73301
C 6.19959 0.66332 -1.06018
C 5.16932 1.92184 0.87497
H 6.95273 1.44523 -0.89418
H 6.69779 -0.31794 -0.94793
H 5.83987 0.75385 -2.10282
H 5.13976 1.54501 1.91526
H 6.10949 2.47437 0.74528
H 4.33447 2.63824 0.74180

TS (E-F) 1 (R = p-NMe2)

SCF = -1304.10128918
H(0 K) = -1303.622662
H(298 K) = -1303.591810
G(298 K) = -1303.685261
BP86 (D3) = -1304.18615594
SCF (MeOH) = -1304.15782165
SCF (DCM) = -1304.15254940
SCF (BS2) = -1304.10809525
Lowest Frequencies = -100.9087cm-1,
16.2590cm-1

59
C -2.60722 -0.96714 -1.67326
C -2.88617 0.37267 -1.22517
C -1.89222 1.41402 -1.30673
C -0.59096 1.05856 -1.82242
C -0.30799 -0.28051 -2.19703
C -1.31767 -1.32248 -2.15560
Ru -1.15192 -0.31368 -0.15189
N -0.45592 0.83221 1.49229
C -1.07213 1.57055 2.43601
C -0.12151 2.11443 3.32831
C 1.11312 1.65238 2.88329
N 0.88357 0.88170 1.77483
C -2.26265 2.83348 -0.89688
C -1.06393 3.74292 -0.57578
H -0.31243 2.74559 4.19299
C 1.75890 0.07185 0.99569
C 3.02600 0.53733 0.65145
C 3.88558 -0.28263 -0.14633
C 3.37064 -1.53826 -0.60945
C 2.09456 -1.96260 -0.25302
C 1.25000 -1.17621 0.56614
C -0.99402 -2.74152 -2.54529
O -2.37538 -1.07340 1.38584
C -2.12776 -2.35448 1.53345
O -1.25287 -2.94337 0.85281
C -2.94541 -3.06774 2.59467
C -3.13564 3.45275 -2.02062
H -2.30959 -3.23614 3.48059
H -3.82512 -2.48254 2.89699
H -3.25343 -4.05560 2.21973

H -2.89405 2.75049 0.00943
H 3.33722 1.53395 0.96946
N 5.15252 0.13049 -0.46921
H 1.74599 -2.95078 -0.56858
H 3.99748 -2.19235 -1.21819
H 2.11854 1.77235 3.28017
H 0.38089 -1.65981 1.04482
H -3.35661 -1.74974 -1.52225
H 0.71693 -0.55306 -2.46571
H -3.85160 0.59066 -0.75806
H 0.21371 1.79726 -1.82748
H -3.46252 4.46332 -1.72564
H -2.56324 3.54151 -2.95988
H -4.03548 2.84954 -2.22415
H -1.42649 4.71349 -0.20070
H -0.40625 3.30814 0.19407
H -0.46165 3.95234 -1.47718
H -1.47476 -3.45718 -1.86127
H -1.35601 -2.93605 -3.57119
H 0.09115 -2.92269 -2.53086
H -2.15618 1.66011 2.42786
C 5.99988 -0.69197 -1.33740
C 5.66747 1.40310 0.03826
H 6.95620 -0.17688 -1.49618
H 6.21266 -1.67626 -0.88192
H 5.53114 -0.85421 -2.32518
H 5.62330 1.44148 1.14186
H 6.71822 1.51142 -0.26055
H 5.10582 2.26601 -0.36799

INT (E-F) (R = p-NMe2)

SCF = -1304.10414380
H(0 K) = -1303.625344
H(298 K) = -1303.593779
G(298 K) = -1303.689670
BP86 (D3) = -1304.18975553
SCF (MeOH) = -1304.16264069
SCF (DCM) = -1304.15711349
SCF (BS2) = -1304.11128253
Lowest Frequencies = 13.1154cm-1,
20.8564cm-1

59
C -2.58726 -1.13132 -1.40938
C -2.95817 0.20344 -1.02998
C -2.07293 1.31096 -1.27893
C -0.80460 1.04381 -1.90329
C -0.44019 -0.29539 -2.22588
C -1.33898 -1.41235 -2.04074
Ru -1.02837 -0.28292 -0.10820
N -0.48272 0.99798 1.48497
C -1.10355 1.75213 2.40932
C -0.15580 2.33155 3.28638
C 1.08373 1.87706 2.85076
N 0.85714 1.07222 1.76462
C -2.52437 2.71839 -0.90682
C -1.38403 3.73807 -0.74274
H -0.35352 2.98253 4.13471
C 1.71037 0.25357 0.97704
C 2.97076 0.69051 0.59879
C 3.78638 -0.14792 -0.23334
C 3.23230 -1.39332 -0.69121

C	1.96678	-1.79424	-0.29553
C	1.14692	-0.98643	0.54577
C	-0.96152	-2.81843	-2.43168
O	-1.81319	-1.35160	1.50690
C	-1.66647	-2.67102	1.54520
O	-0.96799	-3.32996	0.75425
C	-2.45036	-3.33273	2.67371
C	-3.54367	3.20095	-1.97249
H	-1.81550	-4.08686	3.16338
H	-2.81523	-2.60367	3.41038
H	-3.31449	-3.86457	2.24006
H	-3.06383	2.63726	0.05721
H	3.31220	1.68259	0.89926
N	5.04591	0.23874	-0.58999
H	1.58546	-2.77869	-0.58226
H	3.83236	-2.05744	-1.31562
H	2.08890	2.02999	3.23686
H	0.42723	-1.52306	1.18506
H	-3.23916	-1.96564	-1.13282
H	0.56824	-0.49347	-2.60316
H	-3.89680	0.37239	-0.49415
H	-0.08387	1.85048	-2.05189
H	-3.92957	4.19634	-1.69776
H	-3.06606	3.28317	-2.96383
H	-4.40187	2.51524	-2.06247
H	-1.79160	4.69403	-0.37624
H	-0.62236	3.39638	-0.02324
H	-0.88769	3.94943	-1.70599
H	-1.14389	-3.50907	-1.59273
H	-1.56196	-3.14033	-3.30094
H	0.10026	-2.88229	-2.71562
H	-2.18842	1.83302	2.40385
C	5.84834	-0.58630	-1.50233
C	5.62249	1.48056	-0.06343
H	6.78883	-0.06478	-1.72146
H	6.09277	-1.56556	-1.05300
H	5.32015	-0.75441	-2.45709
H	5.59409	1.49487	1.04017
H	6.67252	1.54939	-0.37525
H	5.09123	2.37177	-0.44638

TS (E-F) 2 (R = p-NMe2)

SCF	=	-1304.10413370
H(0 K)	=	-1303.625536
H(298 K)	=	-1303.594834
G(298 K)	=	-1303.687504
BP86 (D3)	=	-1304.18955268
SCF (MeOH)	=	-1304.16256422
SCF (DCM)	=	-1304.15704818
SCF (BS2)	=	-1304.11119575

Lowest Frequencies = -28.0120cm⁻¹,
17.3237cm⁻¹

59

C	-2.63589	-1.08515	-1.39498
C	-2.97296	0.25535	-1.00541
C	-2.06694	1.34475	-1.26084
C	-0.81459	1.05359	-1.90574
C	-0.48452	-0.29195	-2.24016
C	-1.40262	-1.39081	-2.04512
Ru	-1.04085	-0.27748	-0.11334
N	-0.46970	0.97583	1.49063

C	-1.08142	1.71774	2.43098
C	-0.12670	2.26820	3.31883
C	1.10718	1.80858	2.87285
N	0.87111	1.02859	1.77070
C	-2.48147	2.75925	-0.87350
C	-1.31578	3.75032	-0.71254
H	-0.31642	2.90378	4.18055
C	1.71772	0.22346	0.96285
C	2.98536	0.65790	0.60499
C	3.79667	-0.16165	-0.24926
C	3.23172	-1.38544	-0.74917
C	1.95911	-1.78368	-0.37384
C	1.14309	-0.99523	0.48905
C	-1.05885	-2.80379	-2.44334
O	-1.82859	-1.35340	1.49727
C	-1.66754	-2.67018	1.53931
O	-0.95200	-3.32167	0.75662
C	-2.45325	-3.34105	2.66091
C	-3.49987	3.27404	-1.92480
H	-1.79894	-4.05487	3.18470
H	-2.86920	-2.61358	3.37147
H	-3.27917	-3.92206	2.21642
H	-3.01286	2.68289	0.09536
H	3.33586	1.63606	0.93879
N	5.06246	0.22248	-0.58692
H	1.57050	-2.75514	-0.69335
H	3.82793	-2.03675	-1.39055
H	2.11424	1.94231	3.26109
H	0.41670	-1.55428	1.10462
H	-3.30169	-1.90602	-1.11112
H	0.51366	-0.50932	-2.63362
H	-3.90027	0.44159	-0.45579
H	-0.07898	1.84511	-2.06253
H	-3.85995	4.27565	-1.63791
H	-3.03033	3.35374	-2.92018
H	-4.37455	2.60905	-2.01176
H	-1.69677	4.71203	-0.33273
H	-0.55494	3.38360	-0.00457
H	-0.82474	3.95917	-1.67904
H	-1.21921	-3.48926	-1.59548
H	-1.69404	-3.12174	-3.28889
H	-0.00884	-2.88300	-2.76468
H	-2.16537	1.81008	2.42875
C	5.85990	-0.58086	-1.52249
C	5.64897	1.44085	-0.01871
H	6.80791	-0.06387	-1.71881
H	6.09003	-1.57772	-1.10540
H	5.33526	-0.71016	-2.48528
H	5.61365	1.42128	1.08464
H	6.70172	1.50769	-0.32174
H	5.12998	2.34948	-0.37690

F (R = p-NMe2)

SCF	=	-1304.12140900
H(0 K)	=	-1303.642545
H(298 K)	=	-1303.611182
G(298 K)	=	-1303.706312
BP86 (D3)	=	-1304.20564022
SCF (MeOH)	=	-1304.17399518
SCF (DCM)	=	-1304.16929729
SCF (BS2)	=	-1304.12649420

Lowest Frequencies = 10.9996cm⁻¹,
25.1168cm⁻¹

59
C 1.88186 -0.01935 -2.24531
C 2.87825 0.76564 -1.59335
C 3.53466 0.22730 -0.41988
C 3.12723 -1.01164 0.11663
C 2.07475 -1.80112 -0.49863
C 1.47379 -1.28434 -1.69010
Ru 1.23749 0.21891 -0.13359
N 0.45973 -0.18844 1.75032
C 0.94945 -0.31892 3.00186
C -0.10694 -0.50892 3.91834
C -1.27188 -0.48069 3.15500
N -0.90520 -0.28492 1.85267
C 1.70038 -3.14694 0.10963
C 0.28654 -3.63218 -0.25473
C 3.26718 2.12470 -2.11847
H -0.03233 -0.64826 4.99418
C -1.62919 -0.12423 0.63987
C -3.01179 -0.32031 0.59194
C -3.69917 -0.15302 -0.64568
C -2.91620 0.19529 -1.78746
C -1.53112 0.36882 -1.69218
C -0.81613 0.23547 -0.47299
O 1.30595 2.27387 0.59051
C 0.45429 3.19819 0.51813
O -0.74314 3.05129 -0.01654
C 0.75012 4.57399 1.04841
C 2.77064 -4.19488 -0.28753
H 0.03247 4.82077 1.84830
H 1.77452 4.62284 1.43788
H 0.60943 5.31857 0.24792
H 1.74585 -3.01751 1.20904
H -3.55812 -0.60863 1.49192
N -5.06427 -0.31917 -0.73133
H -0.99040 0.64512 -2.60477
H -3.39628 0.33459 -2.75817
H -2.31650 -0.57479 3.44079
H -0.84121 2.07674 -0.29901
H 2.02199 -0.26063 3.17452
H 1.38105 0.37469 -3.13389
H 0.64913 -1.82788 -2.15695
H 3.57451 -1.36768 1.05111
H 4.27768 0.83460 0.10486
H 2.55623 -5.15889 0.20247
H 2.77113 -4.36053 -1.37865
H 3.78594 -3.88270 0.00930
H -0.47801 -2.86892 -0.03368
H 0.21028 -3.90151 -1.32276
H 0.04427 -4.53917 0.32243
H 3.45148 2.83307 -1.29556
H 4.20115 2.04166 -2.70322
H 2.49091 2.54130 -2.77868
C -5.73712 -0.19428 -2.02326
C -5.83204 -0.70231 0.44982
H -6.81496 -0.35174 -1.88298
H -5.59628 0.81275 -2.45836
H -5.37419 -0.94327 -2.75291
H -5.72201 0.04004 1.26317
H -6.89715 -0.75350 0.18703
H -5.52970 -1.69448 0.83917

F1 (R = p-NMe₂)

SCF = -1075.00233361
H(0 K) = -1074.584850
H(298 K) = -1074.559004
G(298 K) = -1074.641673
BP86 (D3) = -1075.06481951
SCF (MeOH) = -1075.05654816
SCF (DCM) = -1075.05170664
SCF (BS2) = -1074.93740059
Lowest Frequencies = 13.9735cm⁻¹,
25.1547cm⁻¹

51
C -2.12862 -1.69480 0.51742
C -1.96701 -1.12611 1.81135
C -2.42345 0.21833 2.09027
C -3.16929 0.90690 1.06888
C -3.32339 0.34278 -0.21923
C -2.74694 -0.93748 -0.54824
Ru -1.09575 0.22431 0.33381
N -0.23295 1.94121 -0.48730
N 1.12981 1.88047 -0.63605
C 1.60440 3.03905 -1.17844
C 0.51523 3.88321 -1.39030
C -0.60756 3.15678 -0.94490
C 1.74334 0.66519 -0.20989
C 0.82920 -0.31210 0.30792
C 1.45011 -1.52236 0.73251
C 2.81936 -1.74683 0.65702
C 3.69683 -0.74324 0.13333
C 3.11749 0.49013 -0.30642
C -2.19921 0.84234 3.44443
C -2.90774 -1.49697 -1.95569
C -1.73523 -2.37919 -2.42237
C -4.25413 -2.26158 -2.03863
H 0.53535 4.88603 -1.80971
H -2.97029 -0.62472 -2.63481
H 3.75352 1.27975 -0.71044
N 5.04908 -0.95044 0.05337
H 0.82341 -2.32239 1.14155
H 3.22433 -2.69983 1.00260
H 2.66407 3.18512 -1.37455
H -1.65815 3.44008 -0.92834
H -1.40916 -1.66854 2.58072
H -1.69003 -2.67189 0.29963
H -3.78710 0.93081 -1.01748
H -3.51192 1.92803 1.26179
H -4.42133 -2.61744 -3.06869
H -4.24933 -3.14143 -1.37225
H -5.10730 -1.62339 -1.75507
H -0.76852 -1.86067 -2.30897
H -1.68854 -3.33025 -1.86354
H -1.86577 -2.63912 -3.48540
H -2.15831 1.94098 3.38157
H -3.03326 0.57406 4.11961
H -1.26578 0.48209 3.90421
C 5.63118 -2.21763 0.50782
C 5.93259 0.08741 -0.48377
H 6.71840 -2.18547 0.36096
H 5.43361 -2.38879 1.58126
H 5.23125 -3.07247 -0.06653

H 5.88202 1.01256 0.11928
H 6.96828 -0.27511 -0.46156
H 5.67888 0.33091 -1.53182

G (R = p-NMe2)

SCF = -1090.26230063
H(0 K)= -1089.844542
H(298 K)= -1089.817197
G(298 K)= -1089.902105
BP86 (D3) = -1090.33765767
SCF (MeOH) = -1090.28485585
SCF (DCM) = -1090.28125279
SCF (BS2) = -1535.43397228
Lowest Frequencies = 14.2247cm⁻¹,
34.4390cm⁻¹

52

C 0.89374 -0.50953 -0.16548
C 1.67179 0.55711 0.34198
C 3.05429 0.70304 0.15795
C 3.75969 -0.27238 -0.59005
C 3.01400 -1.37614 -1.08806
C 1.63061 -1.47783 -0.87675
N 0.92924 1.49895 1.10209
N -0.41609 1.26240 1.18467
C -0.92647 2.21652 1.99115
C 0.09856 3.08612 2.42160
C 1.26780 2.59830 1.83895
Ru -1.11281 -0.45899 0.27066
Cl -0.51018 -1.52124 2.37091
C -1.75857 -1.81741 -1.36167
C -2.50614 -2.16914 -0.20271
C -3.31165 -1.14228 0.43754
C -3.29441 0.18325 -0.03648
C -2.46014 0.57101 -1.16109
C -1.71824 -0.45493 -1.83145
C -2.47663 -3.56471 0.36663
C -2.46300 2.02578 -1.61802
C -3.74204 2.31301 -2.44123
C -1.20092 2.44270 -2.39365
H 0.00309 3.95163 3.07300
H -2.50859 2.64117 -0.69725
H 3.57734 1.55588 0.59562
N 5.13441 -0.14378 -0.83708
H 1.12097 -2.36759 -1.26293
H 3.51720 -2.17489 -1.63821
H 2.29788 2.93876 1.90260
H -1.98714 2.20924 2.23068
H -1.14093 -2.57663 -1.85029
H -1.06711 -0.19968 -2.67080
H -3.85195 0.95772 0.50209
H -3.84979 -1.38749 1.35752
H -3.79623 3.38119 -2.71333
H -3.74490 1.72332 -3.37485
H -4.65628 2.05771 -1.87894
H -0.28411 2.18993 -1.83639
H -1.15044 1.95310 -3.38240
H -1.21060 3.53114 -2.57184
H -2.17945 -3.52872 1.42889
H -3.47458 -4.03317 0.29147
H -1.75311 -4.19857 -0.16925
C 5.86329 -1.30415 -1.33622

C 5.89079 0.83035 -0.06162
H 6.91613 -1.02408 -1.49260
H 5.83172 -2.17543 -0.64666
H 5.46141 -1.62829 -2.31227
H 5.51447 1.85342 -0.24378
H 5.85818 0.64380 1.03440
H 6.94261 0.80819 -0.38453

G^{OAc} (R = p-NMe2)

SCF = -1303.69999544
H(0 K)= -1303.233534
H(298 K)= -1303.202530
G(298 K)= -1303.296297
BP86 (D3) = -1303.78207692
SCF (MeOH) = -1303.71773311
SCF (DCM) = -1303.71496369
SCF (BS2) = -1303.71415240
Lowest Frequencies = 14.8482cm⁻¹,
28.7497cm⁻¹

58

C 1.44564 -0.06872 3.28532
N 1.01260 -0.00328 1.99097
N -0.35316 -0.07411 1.93689
C -0.78135 -0.19581 3.21033
C 0.31799 -0.19165 4.09625
C 1.67570 0.07145 0.73585
C 0.80564 0.02602 -0.37904
C 1.45987 0.02590 -1.62787
C 2.85520 0.10997 -1.75391
C 3.69693 0.20120 -0.61176
C 3.07333 0.15799 0.66095
Ru -1.19711 -0.14052 0.03908
O -0.71964 -2.16902 0.29770
C -0.67783 -3.04095 -0.69039
C -0.11107 -4.39346 -0.23712
C -2.64051 1.45348 0.45597
C -3.46174 0.26459 0.41014
C -3.35270 -0.62325 -0.68520
C -2.46739 -0.26814 -1.77934
C -1.75985 0.96675 -1.76617
C -1.83822 1.88174 -0.65331
C -4.09034 -1.93782 -0.72453
C -1.08550 3.20549 -0.69690
C -1.91455 4.25510 -1.47543
O -1.01933 -2.85855 -1.87268
C -0.67872 3.73902 0.68806
H 0.86986 -0.08078 -2.54446
H 3.28988 0.09125 -2.75619
H -1.84587 -0.28897 3.41348
H -0.37470 -4.61215 0.80916
H -0.47208 -5.19325 -0.90064
H 0.99025 -4.35745 -0.30523
N 5.08726 0.33759 -0.73383
H 3.67061 0.18333 1.57492
H 0.29651 -0.26807 5.18087
H 2.50421 -0.03194 3.52889
H -1.07560 1.19599 -2.59014
H -4.08254 -0.00233 1.27089
H -2.64623 2.05570 1.36996
H -2.28029 -0.99949 -2.56674
H -0.15560 3.01342 -1.26706

H -2.17412 3.89808 -2.48645
H -2.85720 4.48080 -0.94564
H -1.34988 5.19776 -1.58076
H -3.44489 -2.71547 -1.16191
H -4.40871 -2.25406 0.28146
H -4.99162 -1.84659 -1.35878
H -1.55810 4.04060 1.28527
H -0.11488 2.98131 1.25632
H -0.04177 4.63270 0.57699
C 5.91401 0.13559 0.44804
C 5.70275 0.07759 -2.03007
H 5.54315 -0.96023 -2.39450
H 5.31027 0.77014 -2.79532
H 6.78628 0.25461 -1.95273
H 6.96955 0.29329 0.17961
H 5.66247 0.87208 1.23289
H 5.81505 -0.88085 0.88886

D_{para} - D_{ortho} TS (R = p-NMe₂)

SCF = -1319.34465201
H(0 K) = -1318.865097
H(298 K) = -1318.832643
G(298 K) = -1318.928575
BP86 (D3) = -1319.43574477
SCF (MeOH) = -1319.37025492
SCF (DCM) = -1319.36602646
SCF (BS2) = -1764.59039088
Lowest Frequencies = -30.3920cm⁻¹,
24.5056cm⁻¹

60

C 3.92809 -0.61137 0.06071
C 2.53913 -0.37778 0.10457
C 2.02565 0.91382 -0.07011
C 2.93103 1.96839 -0.25949
C 4.31344 1.77068 -0.26166
C 4.84382 0.46159 -0.09647
N 1.67063 -1.50725 0.32323
N 0.32105 -1.55365 0.01783
C -0.04402 -2.84105 0.19245
C 1.03697 -3.63325 0.62621
C 2.10530 -2.75523 0.70388
Ru -1.44750 -0.12046 0.06947
Cl -0.76286 0.77511 -2.05711
C -3.26477 0.95427 0.59615
C -2.19868 1.91298 0.65409
C -1.04912 1.59919 1.45610
C -0.97778 0.34885 2.14931
C -2.07855 -0.58424 2.17990
C -3.20346 -0.26423 1.36039
C -2.32548 3.19939 -0.15404
C -3.39478 4.10269 0.50950
C -2.00921 -1.85946 2.98283
O -2.17827 -1.64077 -1.14662
C -3.42644 -1.71832 -1.58159
C -3.57884 -2.79054 -2.66548
C -1.00545 3.96087 -0.35456
O -4.39071 -1.02571 -1.22087
H -4.09108 1.08127 -0.10569
H -0.18383 2.26447 1.46471
H -0.04221 0.07996 2.65305
H -3.99914 -0.99863 1.21128

H -2.69245 2.89579 -1.15241
H -0.26063 3.32300 -0.85702
H -1.18152 4.84224 -0.99417
H -0.59351 4.32995 0.60260
H -3.54952 5.01111 -0.09708
H -4.36502 3.58781 0.60606
H -3.07518 4.41967 1.51825
H -0.98662 -2.27041 2.99985
H -2.31393 -1.67079 4.02903
H -2.68422 -2.62664 2.57083
H -3.23503 -2.36736 -3.62492
H -4.63550 -3.07922 -2.76205
H -2.95567 -3.67346 -2.45351
H -1.07677 -3.10546 -0.02397
H 1.03844 -4.69619 0.85599
H 3.13374 -2.92091 1.00824
H 0.95166 1.07526 -0.14220
H 2.53750 2.97653 -0.42531
H 4.97605 2.62389 -0.41902
N 6.21916 0.23218 -0.09573
H 4.31030 -1.62987 0.09633
C 6.71746 -1.13623 -0.13719
C 7.11655 1.30196 -0.51937
H 6.93715 1.63020 -1.56446
H 7.01804 2.18416 0.13812
H 8.15524 0.94858 -0.44222
H 7.81593 -1.12046 -0.08327
H 6.35383 -1.71404 0.73246
H 6.42352 -1.68202 -1.05921

1-C6H4R-pyrazole (R = p-OMe)

SCF = -571.781603533
H(0 K) = -571.602555
H(298 K) = -571.591601
G(298 K) = -571.640035
BP86 (D3) = -571.800753353
SCF (DCM) = -571.787461439
SCF (MeOH) = -571.788401986
SCF (BS2) = -571.930217690
Lowest Frequencies = 37.1157cm⁻¹,
95.0353cm⁻¹

23

C -0.00687 1.90177 -0.09693
C -0.27390 0.52391 -0.02862
C 0.77133 -0.41872 0.02475
C 2.10172 0.03371 0.01425
C 2.38604 1.41661 -0.03736
C 1.33135 2.33097 -0.09288
N -1.61644 0.04457 -0.01063
N -1.87513 -1.27346 -0.27297
C -3.20785 -1.38210 -0.16375
C -3.82109 -0.14593 0.17014
C -2.76598 0.75054 0.26376
O 3.19363 -0.79368 0.05963
C 2.95073 -2.20236 0.10317
H 0.50616 -1.47536 0.06623
H 3.43008 1.74101 -0.03954
H 1.54945 3.40238 -0.14620
H -0.81724 2.62996 -0.17816
H -4.87670 0.06521 0.32898
H -3.67779 -2.35135 -0.33372
H -2.74253 1.80518 0.52658
H 3.94292 -2.67585 0.12344
H 2.38812 -2.49150 1.01104
H 2.39658 -2.54835 -0.78965

D (R = p-OMe)

SCF = -1299.91426364
H(0 K) = -1299.473903
H(298 K) = -1299.442463
G(298 K) = -1299.537313
BP86 (D3) = -1300.00327901
SCF (MeOH) = -1299.93702998
SCF (DCM) = -1299.93341293
SCF (BS2) = -1745.16027549
Lowest Frequencies = 18.1952cm⁻¹,
26.3694cm⁻¹

56

C 3.60994 -0.64184 0.08414
C 2.44155 -0.61816 -0.70695
C 2.16116 0.43488 -1.58745
C 3.08491 1.49422 -1.66262
C 4.25573 1.49688 -0.89768
C 4.52595 0.42317 -0.02072
N 1.58588 -1.76806 -0.64793
N 0.21932 -1.73861 -0.47046
C -0.19041 -3.01787 -0.59286
C 0.89734 -3.87917 -0.84562
C 2.01101 -3.05229 -0.87884

Ru -1.07793 -0.09606 0.13955
Cl -1.27083 0.39043 -2.22749
H 4.98120 2.31280 -0.96188
C -0.78778 -0.16940 2.35788
C -2.09696 0.29916 2.02697
C -2.30512 1.42070 1.15107
C -1.19455 2.11642 0.57210
C 0.13088 1.64490 0.86575
C 0.31239 0.50180 1.70850
C -0.56815 -1.34859 3.27299
C -1.47387 3.29996 -0.34748
C -2.01967 4.47694 0.49891
O -2.50728 -1.54968 -0.31736
C -3.81455 -1.37715 -0.19724
C -4.59788 -2.52224 -0.84963
O -4.39891 -0.42466 0.34074
C -0.27232 3.74370 -1.19657
H 2.88776 2.32626 -2.34584
H -3.32692 1.65317 0.84636
H 0.99857 2.08953 0.37620
H 1.32407 0.09954 1.83157
H -2.97681 -0.26065 2.35431
H -2.27053 2.96561 -1.03847
H 0.10231 2.90831 -1.80852
H -0.58032 4.55406 -1.87866
H 0.54914 4.13679 -0.56996
H -2.28992 5.32078 -0.15850
H -2.91725 4.19062 1.07162
H -1.25880 4.83592 1.21480
H 0.32272 -1.92598 2.97593
H -0.41726 -1.00922 4.31474
H -1.43720 -2.02569 3.26213
H -4.59899 -2.37136 -1.94276
H -5.63604 -2.51942 -0.48776
H -4.12858 -3.49909 -0.65070
H -1.25652 -3.21244 -0.49644
H 0.86893 -4.95526 -0.99997
H 3.05989 -3.24695 -1.09147
H 1.23724 0.42358 -2.17659
O 5.69595 0.51088 0.68607
H 3.77938 -1.48063 0.76308
C 6.01120 -0.55766 1.58141
H 6.97993 -0.29633 2.03029
H 5.25335 -0.65702 2.38220
H 6.10459 -1.52305 1.04822

D^{OAc} (R = p-OMe)

SCF = -1513.34958855
H(0 K) = -1512.860161
H(298 K) = -1512.825118
G(298 K) = -1512.928517
BP86 (D3) = -1513.44712280
SCF (MeOH) = -1513.36828023
SCF (DCM) = -1513.36547487
SCF (BS2) = -1513.43684537
Lowest Frequencies = 17.5083cm⁻¹,
23.3889cm⁻¹

62

C 3.93998 0.88570 -0.37011
C 2.76132 0.73823 0.37840
C 2.57508 -0.35675 1.23947

C	3.59743	-1.31079	1.32612
C	4.79448	-1.18439	0.59895
C	4.96724	-0.07333	-0.25071
N	1.78607	1.78556	0.28124
N	0.42947	1.62105	0.06021
C	-0.06344	2.86874	-0.10214
C	0.95155	3.84008	0.02439
C	2.10996	3.11948	0.26679
Ru	-0.88882	-0.10256	-0.15445
O	-0.35770	-0.54052	1.82207
C	-0.60338	-1.68718	2.43229
C	-0.36797	-1.58675	3.94508
C	-1.93130	0.04752	-2.09789
C	-2.62777	-0.93439	-1.29437
C	-1.87579	-1.99876	-0.71757
C	-0.45523	-2.10612	-0.94921
C	0.23385	-1.18908	-1.79315
C	-0.53278	-0.08139	-2.32283
C	-4.12797	-0.78565	-1.07839
C	-4.85904	-1.40202	-2.29751
C	1.69390	-1.36178	-2.12710
O	-2.22302	1.02573	1.02037
C	-3.04822	1.95669	0.60314
C	-3.91095	2.51802	1.73971
C	-4.63837	-1.39018	0.24129
O	-3.13989	2.41658	-0.55669
O	-0.99311	-2.74667	1.91401
H	-2.46312	0.94151	-2.43037
H	-2.32674	-2.67860	0.00487
H	0.09877	-2.87821	-0.40970
H	-0.00532	0.71668	-2.85688
H	-4.33375	0.29976	-1.07082
H	-4.07479	-0.99636	1.10183
H	-5.70418	-1.14008	0.37724
H	-4.55884	-2.49165	0.24637
H	-5.94768	-1.24909	-2.20273
H	-4.53238	-0.94286	-3.24597
H	-4.67195	-2.48862	-2.36176
H	2.23831	-1.86497	-1.31296
H	1.79321	-1.97944	-3.03957
H	2.18480	-0.39595	-2.32292
H	-4.25770	1.71532	2.40864
H	-4.76615	3.07057	1.32438
H	-3.30229	3.21074	2.34646
H	-1.21958	-1.05541	4.40360
H	-0.29798	-2.59279	4.38336
H	0.53832	-1.00402	4.17572
H	-1.12363	2.98813	-0.33494
H	0.84531	4.92029	-0.03966
H	3.13417	3.43031	0.45905
H	1.63958	-0.44318	1.79913
H	3.46800	-2.17130	1.99054
H	5.57455	-1.94234	0.70071
O	6.07969	0.16697	-1.01495
H	4.07688	1.72270	-1.05997
C	7.14490	-0.78468	-0.94284
H	7.92522	-0.41106	-1.62111
H	7.55638	-0.85976	0.08151
H	6.81925	-1.78788	-1.27755

E (R = p-OMe)

SCF = -1284.67863600

H(0 K) = -1284.237994
H(298 K) = -1284.208700
G(298 K) = -1284.299177
BP86 (D3) = -1284.75678027
SCF (MeOH) = -1284.73257631
SCF (DCM) = -1284.72782405
SCF (BS2) = -1284.68531971
Lowest Frequencies = 11.7245cm⁻¹,
29.6268cm⁻¹

55

C	-1.89449	0.42267	-2.39596
C	-2.63157	1.07256	-1.36300
C	-1.99298	1.84283	-0.31928
C	-0.56439	1.86973	-0.33720
C	0.20213	1.20605	-1.35455
C	-0.45258	0.46383	-2.39096
Ru	-1.18668	-0.25127	-0.42074
N	-0.27786	-0.71294	1.44680
C	-0.95138	-0.89190	2.60911
C	-0.05968	-0.97104	3.69520
C	1.20586	-0.83727	3.13420
N	1.05463	-0.67797	1.78386
C	-2.84545	2.56439	0.71667
C	-2.11715	2.85973	2.03915
H	-0.30330	-1.12035	4.74429
C	2.12039	-0.59337	0.82314
C	3.08242	0.40792	1.00020
C	4.18721	0.47149	0.11839
C	4.29109	-0.46316	-0.93550
C	3.30501	-1.45385	-1.08614
C	2.21093	-1.54163	-0.21358
C	0.33527	-0.29564	-3.42435
O	-2.68410	-1.60295	0.28837
C	-2.04470	-2.62065	-0.18773
O	-0.96233	-2.34979	-0.83615
C	-2.51943	-4.02618	0.02524
C	-3.40187	3.86607	0.08440
H	-2.11959	-4.40576	0.98185
H	-3.61774	-4.05334	0.07993
H	-2.15769	-4.67878	-0.78248
H	-3.70551	1.90164	0.93546
H	3.00355	1.13981	1.80884
O	5.07517	1.46835	0.37454
H	3.40893	-2.18840	-1.89098
H	5.13737	-0.43500	-1.62524
H	2.20189	-0.88181	3.56961
H	1.45385	-2.32213	-0.31954
H	-2.41654	-0.19614	-3.13119
H	1.29297	1.19562	-1.29035
H	-3.71516	0.91961	-1.31186
H	-0.03140	2.33597	0.49600
H	-4.07831	4.36992	0.79408
H	-2.58380	4.56491	-0.16138
H	-3.96898	3.66597	-0.83995
H	-2.82618	3.28867	2.76522
H	-1.68563	1.94809	2.48570
H	-1.30925	3.60043	1.90432
H	-0.16065	-1.24254	-3.68924
H	0.41257	0.31457	-4.34284
H	1.35337	-0.51396	-3.06928
H	-2.03778	-0.95132	2.58858
C	6.23400	1.57338	-0.47053

H 6.80727 2.42368 -0.07774
H 6.85081 0.65820 -0.42011
H 5.94969 1.77432 -1.51949

TS(E-F) (R = p-OMe)

SCF = -1284.64950691
H(0 K)= -1284.210565
H(298 K)= -1284.181582
G(298 K)= -1284.271187
BP86 (D3) = -1284.72896979
SCF (MeOH) = -1284.70722085
SCF (DCM) = -1284.70184560
SCF (BS2) = -1284.65680729
Lowest Frequencies = -97.5981cm⁻¹,
12.1602cm⁻¹

55

C -2.48419 -1.04873 -1.56884
C -2.78715 0.26916 -1.07339
C -1.85355 1.36001 -1.22004
C -0.58460 1.07721 -1.84349
C -0.27228 -0.24556 -2.25424
C -1.22371 -1.33694 -2.15948
Ru -0.94761 -0.35000 -0.15117
N -0.31409 0.81265 1.50039
C -0.96959 1.45596 2.48586
C -0.04927 2.05006 3.37787
C 1.20981 1.71916 2.88883
N 1.02301 0.97149 1.75602
C -2.25419 2.75256 -0.75379
C -1.07658 3.70851 -0.49675
H -0.27407 2.62932 4.27027
C 1.95251 0.28750 0.92519
C 3.19413 0.84901 0.63580
C 4.08812 0.14018 -0.20589
C 3.69965 -1.10063 -0.76947
C 2.43915 -1.62951 -0.46866
C 1.54166 -0.95594 0.38495
C -0.86537 -2.72967 -2.60882
O -1.98391 -1.30875 1.40279
C -1.59072 -2.55975 1.51116
O -0.68059 -3.03894 0.79457
C -2.29629 -3.37511 2.57951
C -3.23116 3.35015 -1.80187
H -1.60751 -3.51799 3.42944
H -3.20865 -2.88041 2.94042
H -2.53462 -4.37302 2.18078
H -2.81642 2.62444 0.19183
H 3.49524 1.82622 1.02207
O 5.27686 0.75015 -0.41590
H 2.15626 -2.61246 -0.85762
H 4.38407 -1.65935 -1.41116
H 2.20991 1.92026 3.26617
H 0.69630 -1.54600 0.80499
H -3.18315 -1.86713 -1.37156
H 0.74011 -0.46516 -2.60624
H -3.72245 0.43446 -0.52980
H 0.18099 1.85370 -1.90461
H -3.58106 4.33864 -1.46229
H -2.73038 3.48327 -2.77601
H -4.11537 2.71018 -1.95555
H -1.45390 4.65351 -0.07428

H -0.34740 3.28847 0.21474
H -0.54910 3.96394 -1.43231
H -1.27705 -3.48575 -1.92364
H -1.27397 -2.90948 -3.61979
H 0.22533 -2.86675 -2.65819
H -2.05712 1.44573 2.50719
C 6.24281 0.10117 -1.26636
H 7.11154 0.77209 -1.28375
H 6.54003 -0.87877 -0.85368
H 5.85058 -0.02359 -2.29118

F (R = p-OMe)

SCF = -1284.67309145
H(0 K)= -1284.233221
H(298 K)= -1284.203884
G(298 K)= -1284.293748
BP86 (D3) = -1284.75226692
SCF (MeOH) = -1284.72803497
SCF (DCM) = -1284.72314602
SCF (BS2) = -1284.67867504
Lowest Frequencies = 19.2811cm⁻¹,
22.7987cm⁻¹

55

C 1.60985 0.12067 -2.27527
C 2.53676 1.00309 -1.64738
C 3.27749 0.53077 -0.49467
C 3.01923 -0.74544 0.04419
C 2.03401 -1.63617 -0.54429
C 1.34961 -1.18079 -1.71548
Ru 1.00291 0.28792 -0.14299
N 0.31986 -0.22199 1.75082
C 0.85323 -0.33645 2.98587
C -0.15531 -0.65099 3.92231
C -1.33785 -0.71735 3.18971
N -1.02607 -0.45329 1.88489
C 1.82094 -3.01641 0.06460
C 0.46273 -3.65483 -0.27369
C 2.77376 2.39501 -2.17692
H -0.03835 -0.80925 4.99174
C -1.79408 -0.33580 0.69722
C -3.15516 -0.64040 0.67438
C -3.86126 -0.50301 -0.54273
C -3.17811 -0.06624 -1.69775
C -1.80124 0.22083 -1.63121
C -1.04916 0.10809 -0.43760
O 0.89455 2.32149 0.62081
C -0.02585 3.17795 0.56184
O -1.20534 2.95054 0.01253
C 0.15486 4.55901 1.12678
C 2.99197 -3.93842 -0.36081
H -0.57344 4.71960 1.93914
H 1.17465 4.68608 1.51048
H -0.05903 5.31023 0.34916
H 1.87530 -2.88647 1.16353
H -3.70053 -0.98651 1.55671
O -5.18332 -0.81390 -0.48121
H -1.30809 0.56367 -2.54786
H -3.70473 0.05412 -2.64714
H -2.36052 -0.92246 3.49663
H -1.23037 1.98309 -0.28922
H 1.91932 -0.17904 3.13495

H 1.04805 0.46169 -3.14926
H 0.57332 -1.80558 -2.16325
H 3.53125 -1.05763 0.96084
H 3.96779 1.21038 0.01330
H 2.89516 -4.92143 0.12859
H 2.98721 -4.09992 -1.45251
H 3.97297 -3.51758 -0.08350
H -0.37922 -2.98669 -0.02738
H 0.39280 -3.92347 -1.34229
H 0.33785 -4.58759 0.29953
H 2.89443 3.11989 -1.35647
H 3.70408 2.40950 -2.77309
H 1.95063 2.72805 -2.82769
C -5.95692 -0.70956 -1.68773
H -6.97600 -1.01039 -1.41012
H -5.97023 0.32820 -2.06755
H -5.57283 -1.38825 -2.47077

F1 (R = p-OMe)

SCF = -1055.54897283
H(0 K) = -1055.170911
H(298 K) = -1055.146993
G(298 K) = -1055.225225
BP86 (D3) = -1055.60672173
SCF (MeOH) = -1055.60498666
SCF (DCM) = -1055.60001230
SCF (BS2) = -1055.48497805
Lowest Frequencies = 14.4284cm⁻¹,
21.2006cm⁻¹

47

C -1.87483 -1.69075 0.59128
C -1.68015 -1.08429 1.86181
C -2.12918 0.26892 2.10990
C -2.91500 0.92387 1.09300
C -3.10014 0.32322 -0.17170
C -2.51786 -0.96241 -0.47936
Ru -0.86128 0.23336 0.32355
N -0.01905 1.93139 -0.54183
N 1.34077 1.87060 -0.72028
C 1.80082 3.01830 -1.29300
C 0.70422 3.85804 -1.49628
C -0.40610 3.14043 -1.01408
C 1.97006 0.66677 -0.28847
C 1.07753 -0.30763 0.26994
C 1.69901 -1.50751 0.70416
C 3.07561 -1.73594 0.60112
C 3.90540 -0.73522 0.04022
C 3.34129 0.48649 -0.41201
C -1.85761 0.93998 3.43182
C -2.69952 -1.55458 -1.87037
C -1.54346 -2.46266 -2.32809
C -4.05651 -2.30476 -1.91582
H 0.71444 4.85311 -1.93415
H -2.76127 -0.69888 -2.57028
H 4.01215 1.23700 -0.83877
O 5.24415 -0.83067 -0.11481
H 1.08062 -2.29854 1.14215
H 3.49986 -2.67916 0.95220
H 2.85630 3.16054 -1.51432
H -1.45647 3.42309 -0.97959
H -1.09588 -1.59945 2.63016

H -1.43510 -2.67014 0.38725
H -3.58855 0.88450 -0.97445
H -3.25808 1.94817 1.26743
H -4.23937 -2.68377 -2.93477
H -4.05320 -3.16770 -1.22790
H -4.89919 -1.64988 -1.63910
H -0.56811 -1.95582 -2.23815
H -1.50414 -3.40196 -1.74928
H -1.68886 -2.74388 -3.38355
H -1.80628 2.03489 3.32670
H -2.67623 0.70717 4.13848
H -0.91645 0.58460 3.87914
C 5.90611 -2.03617 0.31883
H 6.96929 -1.87983 0.09483
H 5.77359 -2.19157 1.40369
H 5.53393 -2.91376 -0.23793

G (R = p-OMe)

SCF = -1070.81906185
H(0 K) = -1070.440512
H(298 K) = -1070.415014
G(298 K) = -1070.495792
BP86 (D3) = -1070.88949453
SCF (MeOH) = -1070.84087950
SCF (DCM) = -1070.83743085
SCF (BS2) = -1515.99139317
Lowest Frequencies = 13.8251cm⁻¹,
39.8926cm⁻¹

48

C 1.13840 -0.43891 -0.14938
C 1.85942 0.66538 0.37560
C 3.23029 0.87611 0.19236
C 3.95942 -0.07172 -0.55032
C 3.29937 -1.19833 -1.07939
C 1.91561 -1.36497 -0.86961
N 1.06740 1.56343 1.13588
N -0.26557 1.26203 1.20698
C -0.82496 2.18373 2.01792
C 0.15576 3.09688 2.46315
C 1.35023 2.67038 1.88500
Ru -0.87402 -0.47834 0.26607
Cl -0.24688 -1.53902 2.35748
C -1.44408 -1.84163 -1.39083
C -2.18547 -2.24226 -0.24392
C -3.04097 -1.26030 0.40186
C -3.07878 0.07075 -0.05475
C -2.25327 0.51036 -1.16679
C -1.46043 -0.47263 -1.84269
C -2.09922 -3.64249 0.30760
C -2.31752 1.96927 -1.60550
C -3.60225 2.20944 -2.43495
C -1.06982 2.45155 -2.36631
H 0.01540 3.95030 3.12228
H -2.39703 2.57025 -0.67756
H 3.75840 1.73889 0.60864
O 5.30210 0.19839 -0.69290
H 1.44412 -2.26828 -1.27166
H 3.84934 -1.95472 -1.64533
H 2.36361 3.05635 1.95825
H -1.88545 2.12446 2.25095
H -0.78980 -2.56635 -1.88413

H -0.81421 -0.17762 -2.67281
H -3.67550 0.81207 0.48836
H -3.57587 -1.54132 1.31347
H -3.70197 3.27748 -2.69417
H -3.57206 1.63212 -3.37576
H -4.50824 1.90673 -1.88296
H -0.14659 2.23418 -1.80473
H -0.99003 1.97653 -3.36021
H -1.12709 3.54043 -2.53200
H -1.81370 -3.60738 1.37311
H -3.07464 -4.15359 0.21685
H -1.34344 -4.23657 -0.22929
C 6.08322 -0.75341 -1.41325
H 7.11225 -0.36483 -1.40693
H 6.06671 -1.74897 -0.92898
H 5.74064 -0.85856 -2.46120

G^{OAc} (R = p-OMe)

SCF = -1284.25697734
H(0 K) = -1283.829616
H(298 K) = -1283.800507
G(298 K) = -1283.889738
BP86 (D3) = -1284.33415833
SCF (MeOH) = -1284.27398251
SCF (DCM) = -1284.27140732
SCF (BS2) = -1284.27166057
Lowest Frequencies = 17.1124cm⁻¹,
32.0295cm⁻¹

54

C 1.55596 -0.07339 3.34844
N 1.15968 -0.01094 2.04206
N -0.20384 -0.08256 1.94742
C -0.66837 -0.20058 3.20801
C 0.40529 -0.19392 4.12572
C 1.85986 0.05790 0.80881
C 1.02395 0.01232 -0.33804
C 1.70472 0.01535 -1.57000
C 3.10909 0.09901 -1.66298
C 3.88711 0.17220 -0.49119
C 3.25551 0.14586 0.76729
Ru -0.99134 -0.14361 0.02545
O -0.52856 -2.17353 0.28927
C -0.44708 -3.03505 -0.70635
C 0.09409 -4.39454 -0.24417
C -2.44698 1.44900 0.41031
C -3.26388 0.25879 0.33360
C -3.12277 -0.62121 -0.76484
C -2.20800 -0.25748 -1.83097
C -1.50142 0.97733 -1.78764
C -1.61343 1.88531 -0.67207
C -3.85650 -1.93668 -0.83347
C -0.86313 3.21110 -0.68630
C -1.67478 4.26403 -1.47869
O -0.73657 -2.83639 -1.89959
C -0.49388 3.73572 0.71251
H 1.13498 -0.08255 -2.49994
H 3.58088 0.09409 -2.64903
H -1.73822 -0.29386 3.38084
H -0.21593 -4.62376 0.78698
H -0.24067 -5.18515 -0.93193
H 1.19745 -4.36271 -0.26345

O 5.26092 0.26166 -0.45739
H 3.87526 0.18483 1.66797
H 0.35208 -0.26821 5.20937
H 2.60760 -0.03633 3.62068
H -0.79423 1.21315 -2.59011
H -3.90788 -0.01520 1.17477
H -2.48005 2.04524 1.32765
H -1.99916 -0.98195 -2.61924
H 0.08157 3.02581 -1.23399
H -1.90708 3.91363 -2.49860
H -2.63134 4.48353 -0.97183
H -1.11009 5.20878 -1.56258
H -3.19919 -2.70990 -1.26085
H -4.19951 -2.26187 0.16144
H -4.74160 -1.84134 -1.48943
H -1.38922 4.03095 1.28871
H 0.05707 2.97574 1.29035
H 0.14328 4.63173 0.62437
C 5.94212 0.26460 -1.71105
H 7.01327 0.33664 -1.47144
H 5.75793 -0.66658 -2.28098
H 5.64980 1.13080 -2.33604

1-C6H4R-pyrazole (R = p-Me)
 SCF = -496.573116995
 H(0 K) = -496.399094
 H(298 K) = -496.388804
 G(298 K) = -496.436747
 BP86 (D3) = -496.590469175
 SCF (DCM) = -496.578118196
 SCF (MeOH) = -496.578958781
 SCF (BS2) = -496.696488978
 Lowest Frequencies = 20.2631cm⁻¹,
 41.3532cm⁻¹

22

C -3.16549 -1.10436 -0.16540
 N -1.83294 -1.21074 -0.27736
 N -1.36629 0.04737 -0.00715
 C -2.38731 0.92712 0.27445
 C -3.57255 0.21193 0.17805
 C 0.03494 0.30560 -0.02559
 C 0.93062 -0.77399 0.06113
 C 2.32028 -0.55258 0.05161
 C 2.79628 0.77076 -0.03622
 C 1.89893 1.84614 -0.12655
 C 0.51579 1.62542 -0.13039
 H 0.51904 -1.78437 0.13138
 C 3.27546 -1.72493 0.13851
 H 3.87581 0.95740 -0.03920
 H 2.27894 2.86977 -0.20778
 H -0.17456 2.46642 -0.23763
 H -4.58052 0.58803 0.34143
 H -3.78523 -1.98432 -0.34098
 H -2.19415 1.96232 0.54525
 H 4.32427 -1.38823 0.16939
 H 3.08708 -2.33166 1.04180
 H 3.16219 -2.39852 -0.72971

D (R = p-Me)

SCF = -1224.70714658
 H(0 K) = -1224.271639
 H(298 K) = -1224.240944
 G(298 K) = -1224.334548
 BP86 (D3) = -1224.79427603
 SCF (MeOH) = -1224.72808957
 SCF (DCM) = -1224.72471657
 SCF (BS2) = -1669.92794743
 Lowest Frequencies = 21.6297cm⁻¹,
 29.6196cm⁻¹

55

C 3.74059 -0.83228 0.39136
 C 2.62542 -0.79234 -0.46687
 C 2.45491 0.24804 -1.39445
 C 3.42874 1.25825 -1.44091
 C 4.54789 1.22281 -0.59413
 C 4.72410 0.17385 0.33239
 N 1.70987 -1.89546 -0.43097
 N 0.33749 -1.79188 -0.35202
 C -0.12895 -3.05268 -0.46249
 C 0.92749 -3.97530 -0.60979
 C 2.08242 -3.20653 -0.58999
 Ru -0.90608 -0.06950 0.13208
 Cl -0.91455 0.37650 -2.25097

H 5.29879 2.01906 -0.65174
 C -0.77130 -0.10881 2.36675
 C -2.02772 0.42054 1.93770
 C -2.11521 1.53188 1.02914
 C -0.93207 2.15496 0.51495
 C 0.34318 1.62062 0.90751
 C 0.40510 0.48838 1.78179
 C -0.67748 -1.27575 3.31834
 C -1.08508 3.33124 -0.44301
 C -1.62558 4.55244 0.34192
 O -2.37694 -1.45462 -0.39698
 C -3.67789 -1.20958 -0.37135
 C -4.47618 -2.32422 -1.05736
 O -4.24426 -0.21589 0.10812
 C 0.19312 3.69560 -1.21439
 H 3.31309 2.07842 -2.15676
 H -3.09991 1.81113 0.65054
 H 1.26468 2.00893 0.47117
 H 1.38263 0.03608 1.98227
 H -2.95671 -0.08457 2.21432
 H -1.84868 3.02310 -1.18186
 H 0.56429 2.83037 -1.78555
 H -0.02492 4.50692 -1.92927
 H 0.98976 4.05858 -0.53938
 H -1.80568 5.39454 -0.34781
 H -2.57408 4.32452 0.85571
 H -0.89804 4.88767 1.10258
 H 0.19282 -1.91198 3.08822
 H -0.56746 -0.91931 4.35949
 H -1.58388 -1.90022 3.27064
 H -4.39219 -2.19717 -2.15029
 H -5.53533 -2.25729 -0.77026
 H -4.07694 -3.32051 -0.80829
 H -1.20777 -3.19097 -0.43554
 H 0.85400 -5.05349 -0.73094
 H 3.13200 -3.46115 -0.71954
 H 1.56846 0.26377 -2.03977
 C 5.94524 0.11791 1.22576
 H 3.83680 -1.65419 1.10993
 H 5.77199 -0.51258 2.11301
 H 6.81296 -0.30403 0.68609
 H 6.23761 1.12306 1.57236

D^{OAc} (R = p-Me)

SCF = -1438.14201052
 H(0 K) = -1437.657445
 H(298 K) = -1437.623186
 G(298 K) = -1437.725039
 BP86 (D3) = -1438.23788910
 SCF (MeOH) = -1438.15964509
 SCF (DCM) = -1438.15696619
 SCF (BS2) = -1438.20394340
 Lowest Frequencies = 20.5091cm⁻¹,
 25.0611cm⁻¹

61

C 4.16634 0.70334 -0.48780
 C 3.00645 0.57690 0.30357
 C 2.80775 -0.54692 1.11771
 C 3.78588 -1.55421 1.11492
 C 4.94741 -1.43125 0.33777
 C 5.15805 -0.29438 -0.47084

N	2.07315	1.66595	0.29310
N	0.70553	1.56838	0.10187
C	0.26041	2.84184	0.02126
C	1.31776	3.76339	0.17056
C	2.45138	2.98460	0.34074
Ru	-0.68346	-0.09048	-0.16454
O	-0.11527	-0.65791	1.76805
C	-0.37190	-1.83279	2.31723
C	-0.09883	-1.82538	3.82703
C	-1.78960	0.20276	-2.05489
C	-2.48880	-0.80174	-1.28181
C	-1.75174	-1.91993	-0.79520
C	-0.34506	-2.05865	-1.08754
C	0.34223	-1.11606	-1.90394
C	-0.40561	0.04385	-2.34066
C	-3.97418	-0.61855	-0.99996
C	-4.77012	-1.14723	-2.21964
C	1.78147	-1.31495	-2.30575
O	-1.93636	1.02300	1.10937
C	-2.73693	2.00497	0.76773
C	-3.53980	2.53952	1.95972
C	-4.45510	-1.27502	0.30594
O	-2.84737	2.52779	-0.36345
O	-0.79710	-2.85210	1.74867
H	-2.30246	1.13121	-2.31433
H	-2.19794	-2.62573	-0.09504
H	0.20222	-2.87775	-0.61470
H	0.12785	0.85450	-2.84919
H	-4.14389	0.47082	-0.92898
H	-3.84973	-0.94180	1.16367
H	-5.50729	-1.00181	0.49368
H	-4.40909	-2.37712	0.25305
H	-5.84880	-0.96553	-2.07497
H	-4.46385	-0.64964	-3.15544
H	-4.62168	-2.23430	-2.34632
H	2.33519	-1.89891	-1.55457
H	1.82355	-1.86422	-3.26520
H	2.30194	-0.35520	-2.44770
H	-3.88320	1.71890	2.60816
H	-4.39403	3.13216	1.60150
H	-2.88922	3.19016	2.56964
H	-0.92660	-1.30260	4.33622
H	-0.04226	-2.85637	4.20504
H	0.82603	-1.27722	4.06857
H	-0.79975	3.01656	-0.17340
H	1.25464	4.84888	0.16775
H	3.49203	3.24372	0.52138
H	1.89174	-0.61896	1.71177
H	3.64011	-2.44130	1.73992
H	5.70227	-2.22568	0.35541
C	6.42034	-0.14658	-1.29411
H	4.28626	1.58038	-1.13337
H	6.30024	0.60442	-2.09176
H	7.27063	0.17344	-0.66435
H	6.70884	-1.10146	-1.76476

E (R = p-Me)

SCF	=	-1209.46977198
H(0 K)	=	-1209.034025
H(298 K)	=	-1209.005501
G(298 K)	=	-1209.094411
BP86 (D3)	=	-1209.54615878

SCF (MeOH)	=	-1209.52349759
SCF (DCM)	=	-1209.51877428
SCF (BS2)	=	-1209.45130551
Lowest Frequencies	=	15.2307cm ⁻¹ , 34.0375cm ⁻¹

54

C	1.82503	0.01920	-2.35633
C	2.61051	-0.62827	-1.35851
C	2.05276	-1.58914	-0.43299
C	0.64501	-1.81452	-0.52731
C	-0.17214	-1.15958	-1.51074
C	0.40529	-0.22582	-2.43155
Ru	0.95439	0.36913	-0.36190
N	-0.08820	0.49433	1.48939
C	0.50670	0.62240	2.70018
C	-0.43325	0.47004	3.73663
C	-1.64641	0.24758	3.09408
N	-1.41931	0.26028	1.74482
C	2.96287	-2.28967	0.56776
C	2.23547	-2.83706	1.80781
H	-0.25557	0.52953	4.80768
C	-2.42389	0.15211	0.72310
C	-3.26868	-0.97212	0.73621
C	-4.31084	-1.08894	-0.20554
C	-4.46283	-0.05865	-1.15949
C	-3.61364	1.05915	-1.16452
C	-2.58438	1.18250	-0.21740
C	-0.44528	0.52092	-3.42353
O	2.21424	1.82494	0.56750
C	1.45848	2.79276	0.16362
O	0.45301	2.45041	-0.56991
C	1.72102	4.21760	0.54672
C	3.73697	-3.41514	-0.16558
H	1.22615	4.43421	1.50965
H	2.80078	4.38560	0.67256
H	1.31091	4.89962	-0.21214
H	3.70150	-1.53587	0.90388
H	-3.11230	-1.75756	1.48387
C	-5.25286	-2.27201	-0.18019
H	-3.76578	1.85541	-1.90002
H	-5.26587	-0.13082	-1.90095
H	-2.65768	0.12381	3.47579
H	-1.92266	2.05265	-0.20216
H	2.27803	0.78109	-2.99690
H	-1.25455	-1.31018	-1.50379
H	3.65776	-0.33086	-1.23613
H	0.15601	-2.43842	0.22585
H	4.45359	-3.89006	0.52429
H	3.04604	-4.19505	-0.52938
H	4.30334	-3.03076	-1.03015
H	2.97179	-3.23590	2.52379
H	1.65162	-2.05582	2.32305
H	1.55678	-3.66899	1.54926
H	-0.08172	1.55037	-3.56762
H	-0.39969	0.00613	-4.40071
H	-1.49686	0.55583	-3.10225
H	1.57650	0.81616	2.74743
H	-5.48252	-2.62651	-1.19835
H	-4.83615	-3.11538	0.39271
H	-6.21377	-1.99506	0.28963

TS (E-F) (R = p-Me)

SCF = -1209.43884841
H(0 K) = -1209.004921
H(298 K) = -1208.976758
G(298 K) = -1209.064986
BP86 (D3) = -1209.51634434
SCF (MeOH) = -1209.49702480
SCF (DCM) = -1209.49166413
SCF (BS2) = -1209.42114264
Lowest Frequencies = -93.3547cm⁻¹,
12.8662cm⁻¹

54

C -2.51633 -1.04438 -1.23363
C -2.72805 0.27519 -0.69646
C -1.83291 1.36512 -1.00414
C -0.68778 1.07854 -1.83039
C -0.45138 -0.24724 -2.28173
C -1.37519 -1.33679 -2.02865
Ru -0.76155 -0.34549 -0.09413
N 0.10661 0.81613 1.44193
C -0.39726 1.44964 2.51889
C 0.64563 2.01783 3.28319
C 1.81987 1.68005 2.61933
N 1.46895 0.95343 1.51169
C -2.14780 2.75902 -0.48087
C -0.94244 3.71327 -0.42656
H 0.55470 2.58515 4.20638
C 2.26902 0.28068 0.54850
C 3.49095 0.82119 0.12427
C 4.26081 0.14703 -0.84637
C 3.75776 -1.05834 -1.39166
C 2.53174 -1.58540 -0.97052
C 1.76713 -0.92495 0.01306
C -1.10119 -2.72874 -2.53516
O -1.51879 -1.33010 1.59357
C -1.10073 -2.57868 1.64140
O -0.30296 -3.05315 0.80057
C -1.63638 -3.39652 2.80288
C -3.28584 3.35499 -1.35286
H -0.82054 -3.55964 3.52724
H -2.47145 -2.89534 3.31143
H -1.95061 -4.38640 2.43776
H -2.54459 2.63424 0.54563
H 3.83941 1.77687 0.52933
C 5.59789 0.69417 -1.28645
H 2.17594 -2.54334 -1.36187
H 4.34941 -1.59290 -2.14228
H 2.86475 1.86445 2.85828
H 0.95755 -1.52333 0.50782
H -3.17453 -1.86010 -0.91959
H 0.48772 -0.46962 -2.79742
H -3.55832 0.44373 -0.00379
H 0.05722 1.85314 -2.02404
H -3.57336 4.34435 -0.96137
H -2.95457 3.48590 -2.39709
H -4.18374 2.71563 -1.35524
H -1.24204 4.65913 0.05237
H -0.10490 3.29217 0.15268
H -0.57920 3.96712 -1.43765
H -1.42443 -3.48833 -1.80801
H -1.64800 -2.89165 -3.48170
H -0.02994 -2.87883 -2.73694

H -1.47116 1.45034 2.69223
H 5.73981 0.58460 -2.37397
H 5.71275 1.75792 -1.02641
H 6.42029 0.14150 -0.79671

F (R = p-Me)

SCF = -1209.46469213
H(0 K) = -1209.029664
H(298 K) = -1209.001082
G(298 K) = -1209.089792
BP86 (D3) = -1209.54218144
SCF (MeOH) = -1209.51913775
SCF (DCM) = -1209.51428725
SCF (BS2) = -1209.44522913
Lowest Frequencies = 18.4255cm⁻¹,
30.5171cm⁻¹

54

C 1.73089 0.46566 -2.06219
C 2.41421 1.40491 -1.23553
C 3.02968 0.93765 -0.00944
C 2.87378 -0.40136 0.39970
C 2.12580 -1.35950 -0.39586
C 1.57429 -0.90009 -1.63412
Ru 0.78110 0.37262 -0.05152
N -0.09928 -0.36543 1.67762
C 0.25227 -0.50341 2.97416
C -0.83391 -1.01089 3.71888
C -1.87230 -1.17023 2.80412
N -1.40616 -0.77243 1.58184
C 2.01883 -2.80243 0.08119
C 0.81876 -3.57199 -0.49735
C 2.53099 2.85515 -1.63193
H -0.85934 -1.23344 4.78294
C -1.99385 -0.66075 0.29458
C -3.29250 -1.11603 0.02998
C -3.82871 -0.98146 -1.26613
C -3.01898 -0.39150 -2.25913
C -1.71480 0.05209 -1.97547
C -1.14775 -0.06175 -0.68180
O 0.24782 2.30594 0.78760
C -0.74539 3.05333 0.59438
O -1.76219 2.73871 -0.18986
C -0.85270 4.39778 1.25722
C 3.35119 -3.53254 -0.22544
H -1.74364 4.41571 1.90675
H 0.04620 4.60516 1.85072
H -0.99587 5.17888 0.49275
H 1.90181 -2.76110 1.18207
H -3.89615 -1.58041 0.81747
C -5.23883 -1.43287 -1.57214
H -1.13067 0.50657 -2.78374
H -3.41366 -0.27877 -3.27502
H -2.89186 -1.52497 2.93326
H -1.61528 1.80448 -0.54184
H 1.25250 -0.22550 3.29948
H 1.27059 0.80292 -2.99494
H 0.97360 -1.58126 -2.24147
H 3.27868 -0.72099 1.36605
H 3.53253 1.65560 0.64485
H 3.32077 -4.55813 0.17757
H 3.52014 -3.59969 -1.31394

H 4.21815 -3.01855 0.22242
H -0.13022 -3.03375 -0.33697
H 0.93516 -3.75722 -1.57948
H 0.74005 -4.55756 -0.01089
H 2.42307 3.51867 -0.75944
H 3.52997 3.03866 -2.06728
H 1.77846 3.13268 -2.38597
H -5.32108 -1.82533 -2.59853
H -5.57547 -2.21811 -0.87649
H -5.94950 -0.59064 -1.48769

F1 (R = p-Me)

SCF = -980.336858121
H(0 K) = -979.963905
H(298 K) = -979.940721
G(298 K) = -980.018398
BP86 (D3) = -980.393071891
SCF (MeOH) = -980.393587898
SCF (DCM) = -980.388518268
SCF (BS2) = -980.248346072
Lowest Frequencies = 10.4188cm⁻¹,
20.0284cm⁻¹

46

C -1.88383 -1.51897 0.51945
C -1.69003 -0.98894 1.82302
C -1.96502 0.40377 2.09638
C -2.60728 1.19316 1.07221
C -2.79441 0.66554 -0.22232
C -2.36145 -0.67499 -0.55403
Ru -0.62096 0.26014 0.37114
N 0.47079 1.77131 -0.54863
N 1.80951 1.50563 -0.69622
C 2.44347 2.56016 -1.27835
C 1.48729 3.55120 -1.51951
C 0.27558 3.01704 -1.05008
C 2.25045 0.23533 -0.21772
C 1.22183 -0.58101 0.34143
C 1.64573 -1.84861 0.81409
C 2.98191 -2.26040 0.73948
C 3.97537 -1.42268 0.18187
C 3.58923 -0.15411 -0.30517
C -1.66329 0.99465 3.44937
C -2.53785 -1.18824 -1.97629
C -1.50439 -2.24724 -2.40104
C -3.98683 -1.72107 -2.13130
H 1.65429 4.52405 -1.97523
H -2.42591 -0.31112 -2.64278
H 4.34726 0.50373 -0.74364
C 5.41829 -1.86075 0.12826
H 0.91078 -2.53235 1.25275
H 3.26795 -3.24859 1.11587
H 3.51231 2.54094 -1.47953
H -0.72200 3.45198 -1.04327
H -1.22015 -1.60081 2.59860
H -1.55961 -2.53864 0.29718
H -3.16069 1.31225 -1.02604
H -2.82638 2.24618 1.27277
H -4.15772 -2.03587 -3.17384
H -4.15710 -2.59552 -1.48008
H -4.73839 -0.95475 -1.87915
H -0.47167 -1.90076 -2.22915

H -1.64757 -3.20054 -1.86307
H -1.61919 -2.46644 -3.47473
H -1.45141 2.07313 3.38184
H -2.54062 0.86440 4.11060
H -0.80621 0.49511 3.92684
H 5.50320 -2.93364 -0.10939
H 5.99329 -1.29226 -0.61945
H 5.90703 -1.70823 1.10831

G (R = p-Me)

SCF = -995.612639167
H(0 K) = -995.238978
H(298 K) = -995.214230
G(298 K) = -995.293960
BP86 (D3) = -995.681404147
SCF (MeOH) = -995.633134185
SCF (DCM) = -995.629857156
SCF (BS2) = -1440.75953171
Lowest Frequencies = 17.2239cm⁻¹,
27.1851cm⁻¹

47

C 1.27717 -0.56302 -0.38842
C 2.14656 0.42674 0.13313
C 3.50530 0.53713 -0.20119
C 4.07375 -0.38515 -1.09636
C 3.23879 -1.39435 -1.62270
C 1.88120 -1.48198 -1.27252
N 1.52670 1.31606 1.04857
N 0.18775 1.11835 1.24946
C -0.19625 2.00792 2.18889
C 0.90464 2.79652 2.58751
C 1.98664 2.32710 1.84396
Ru -0.67233 -0.47378 0.24648
Cl 0.07109 -1.76900 2.15843
C -1.53879 -1.62673 -1.44384
C -2.18928 -2.06929 -0.25794
C -2.87841 -1.08389 0.55907
C -2.84092 0.28197 0.22240
C -2.09819 0.75318 -0.93436
C -1.47579 -0.22520 -1.77534
C -2.17655 -3.51712 0.16145
C -2.07493 2.24647 -1.24126
C -3.41170 2.66493 -1.90024
C -0.87425 2.69338 -2.09380
H 0.91369 3.59765 3.32276
H -2.00312 2.76433 -0.26392
H 4.12888 1.32847 0.23122
C 5.54248 -0.31687 -1.45885
H 1.28517 -2.30094 -1.68977
H 3.66319 -2.13046 -2.31657
H 3.03242 2.62270 1.83049
H -1.22642 2.01463 2.53693
H -1.01059 -2.35422 -2.06696
H -0.89668 0.09108 -2.64620
H -3.30772 1.01636 0.88819
H -3.33844 -1.40296 1.49861
H -3.44066 3.75674 -2.05813
H -3.53158 2.17551 -2.88280
H -4.27926 2.38754 -1.27772
H 0.07871 2.35125 -1.65808
H -0.94128 2.30648 -3.12608

H	-0.84956	3.79389	-2.16196
H	-1.77764	-3.60594	1.18658
H	-3.19976	-3.93364	0.14059
H	-1.54148	-4.12020	-0.50586
H	6.12412	-1.09686	-0.93368
H	5.69999	-0.47114	-2.54033
H	5.98193	0.65788	-1.18944

G^{OAc} (R = p-Me)

SCF = -1209.05035924
H(0 K) = -1208.627931
H(298 K) = -1208.599561
G(298 K) = -1208.687783
BP86 (D3) = -1209.12574799
SCF (MeOH) = -1209.06589308
SCF (DCM) = -1209.06341410
SCF (BS2) = -1209.03963196
Lowest Frequencies = 18.4774cm⁻¹,
33.1024cm⁻¹

H	-2.13840	3.90645	-2.24169
H	-2.57473	4.47844	-0.60979
H	-1.18569	5.20290	-1.46712
H	-3.19151	-2.71286	-0.77774
H	-3.93760	-2.25247	0.79010
H	-4.74724	-1.83787	-0.74884
H	-0.94407	4.02841	1.38967
H	0.47884	2.97296	1.13045
H	0.44281	4.62863	0.45861
H	6.06765	0.05140	-0.73459
H	5.69057	-0.22654	-2.45501
H	5.68668	1.42386	-1.79959

53

C	2.27808	-0.06978	2.94709
N	1.67091	-0.00462	1.72455
N	0.31160	-0.08713	1.85718
C	0.06234	-0.21513	3.17673
C	1.27282	-0.20402	3.90373
C	2.15490	0.08217	0.39206
C	1.14148	0.03551	-0.59840
C	1.60599	0.05630	-1.93060
C	2.97384	0.15664	-2.23903
C	3.95487	0.23246	-1.22795
C	3.52570	0.18472	0.11051
Ru	-0.78153	-0.14355	0.09227
O	-0.25882	-2.16900	0.26548
C	-0.38382	-3.04584	-0.71203
C	0.25458	-4.39485	-0.35539
C	-2.14947	1.45022	0.71701
C	-2.96873	0.26058	0.78819
C	-3.02461	-0.62265	-0.31414
C	-2.30612	-0.26550	-1.52367
C	-1.60404	0.96885	-1.61119
C	-1.51896	1.88107	-0.49639
C	-3.76493	-1.93466	-0.25033
C	-0.78351	3.20676	-0.64718
C	-1.72564	4.25833	-1.28109
O	-0.92167	-2.86846	-1.81947
C	-0.16765	3.73263	0.66137
H	0.88903	-0.04211	-2.75254
H	3.28848	0.16570	-3.28987
H	-0.96346	-0.31755	3.52371
H	0.17319	-4.60867	0.72143
H	-0.21247	-5.19811	-0.94423
H	1.32813	-4.35788	-0.61013
C	5.42335	0.37450	-1.56932
H	4.26612	0.21984	0.91853
H	1.40044	-0.28403	4.98074
H	3.35986	-0.02496	3.04262
H	-1.05047	1.20195	-2.52699
H	-3.45783	-0.00807	1.72950
H	-2.02249	2.05049	1.62339
H	-2.24168	-0.99246	-2.33426
H	0.04661	3.02116	-1.35644

1-C6H4R-pyrazole (R = p-F)
 SCF = -556.489303649
 H(0 K) = -556.349894
 H(298 K) = -556.340701
 G(298 K) = -556.385328
 BP86 (D3) = -556.504108729
 SCF (DCM) = -556.494124306
 SCF (MeOH) = -556.494917359
 SCF (BS2) = -556.642014142
 Lowest Frequencies = 34.5861cm-1,
 101.7399cm-1

19

C	-3.17081	-1.04631	-0.12831
N	-1.84137	-1.19509	-0.21382
N	-1.34260	0.06305	-0.00662
C	-2.34277	0.98569	0.21014
C	-3.54500	0.29861	0.13552
C	0.06362	0.27579	-0.01993
C	0.91566	-0.84161	0.05377
C	2.29430	-0.62251	0.04485
C	2.85778	0.65757	-0.02629
C	1.98674	1.75449	-0.10253
C	0.59549	1.57792	-0.10668
H	0.49932	-1.84812	0.11148
F	3.11806	-1.69752	0.11608
H	3.94381	0.77707	-0.02697
H	2.39801	2.76632	-0.17093
H	-0.06197	2.44555	-0.19915
H	-4.54413	0.71077	0.26156
H	-3.81265	-1.91740	-0.26334
H	-2.12721	2.02986	0.42246

D (R = p-F)

SCF = -1284.62214740
 H(0 K) = -1284.221301
 H(298 K) = -1284.191689
 G(298 K) = -1284.282355
 BP86 (D3) = -1284.70647927
 SCF (MeOH) = -1284.64261658
 SCF (DCM) = -1284.63931927
 SCF (BS2) = -1729.87249512
 Lowest Frequencies = 21.7855cm-1,
 29.7560cm-1

52

C	3.75574	-0.84533	0.44367
C	2.64279	-0.79709	-0.41747
C	2.47651	0.24640	-1.34460
C	3.45037	1.25686	-1.39819
C	4.57701	1.23303	-0.55927
C	4.70807	0.17572	0.34815
N	1.72883	-1.89902	-0.38457
N	0.35487	-1.79236	-0.33784
C	-0.10983	-3.05282	-0.45337
C	0.94856	-3.97795	-0.57348
C	2.10391	-3.21207	-0.53043
Ru	-0.89852	-0.06975	0.12936
Cl	-0.86364	0.38282	-2.25266
H	5.34595	2.00877	-0.60085
C	-0.80593	-0.11430	2.36695
C	-2.05442	0.41477	1.91540

C	-2.12554	1.52757	1.00735
C	-0.93358	2.15398	0.51789
C	0.33432	1.61969	0.93307
C	0.38068	0.48527	1.80547
C	-0.72900	-1.28186	3.31921
C	-1.07000	3.33368	-0.43817
C	-1.62281	4.55198	0.34286
O	-2.35684	-1.45464	-0.43064
C	-3.65870	-1.21033	-0.42982
C	-4.44298	-2.32456	-1.13192
O	-4.23379	-0.21718	0.03967
C	0.22085	3.70050	-1.18702
H	3.33423	2.07181	-2.11912
H	-3.10306	1.80687	0.61064
H	1.26317	2.01190	0.51624
H	1.35442	0.03415	2.02638
H	-2.98795	-0.09161	2.17373
H	-1.82165	3.02901	-1.19056
H	0.60023	2.83749	-1.75625
H	0.01498	4.51510	-1.90170
H	1.00658	4.06023	-0.49764
H	-1.79125	5.39677	-0.34646
H	-2.57974	4.32239	0.83995
H	-0.90778	4.88384	1.11667
H	0.14900	-1.91437	3.10908
H	-0.64396	-0.92541	4.36261
H	-1.63164	-1.90979	3.25079
H	-4.34020	-2.19497	-2.22295
H	-5.50705	-2.25951	-0.86331
H	-4.04699	-3.32089	-0.87801
H	-1.18926	-3.18966	-0.44814
H	0.87601	-5.05647	-0.69199
H	3.15546	-3.46948	-0.63689
H	1.59038	0.26226	-1.99053
F	5.78425	0.13526	1.17063
H	3.88167	-1.64961	1.17302

D^{OAc} (R = p-F)

SCF = -1498.05726951
 H(0 K) = -1497.607407
 H(298 K) = -1497.574195
 G(298 K) = -1497.673432
 BP86 (D3) = -1498.15036208
 SCF (MeOH) = -1498.07452169
 SCF (DCM) = -1498.07192720
 SCF (BS2) = -1498.14864738
 Lowest Frequencies = 20.5166cm-1,
 24.5886cm-1

58

C	4.17989	0.72785	-0.51825
C	3.01948	0.58450	0.26938
C	2.81949	-0.55341	1.06634
C	3.79418	-1.56439	1.05871
C	4.96542	-1.44612	0.29315
C	5.13584	-0.29193	-0.47987
N	2.08807	1.67215	0.27280
N	0.71663	1.57103	0.10905
C	0.26771	2.84364	0.04562
C	1.32578	3.76760	0.17958
C	2.46472	2.99222	0.32122
Ru	-0.67541	-0.08729	-0.16690

O -0.08587 -0.68728 1.75001
 C -0.33250 -1.87322 2.28111
 C -0.04741 -1.89094 3.78834
 C -1.80733 0.23719 -2.03692
 C -2.49355 -0.78268 -1.27241
 C -1.74681 -1.90733 -0.81610
 C -0.34405 -2.03761 -1.13054
 C 0.32949 -1.07817 -1.93856
 C -0.42718 0.08720 -2.34453
 C -3.97512 -0.60851 -0.96656
 C -4.78690 -1.11964 -2.18333
 C 1.76412 -1.26492 -2.36274
 O -1.91254 1.00453 1.14050
 C -2.71792 1.99128 0.82391
 C -3.51050 2.50297 2.03239
 C -4.43532 -1.28749 0.33528
 O -2.83896 2.53331 -0.29707
 O -0.75731 -2.88385 1.69754
 H -2.32585 1.16880 -2.27272
 H -2.18181 -2.62705 -0.12304
 H 0.21130 -2.86427 -0.68087
 H 0.09697 0.90809 -2.84625
 H -4.14690 0.47905 -0.87564
 H -3.81771 -0.96743 1.18932
 H -5.48498 -1.01941 0.54320
 H -4.38846 -2.38845 0.26337
 H -5.86380 -0.94351 -2.02004
 H -4.49568 -0.60585 -3.11516
 H -4.63737 -2.20402 -2.32987
 H 2.32897 -1.86160 -1.62994
 H 1.79583 -1.79666 -3.33223
 H 2.27942 -0.30095 -2.49580
 H -3.85691 1.66916 2.66219
 H -4.36212 3.11016 1.69300
 H -2.85209 3.13317 2.65516
 H -0.87664 -1.38635 4.31325
 H 0.02210 -2.92809 4.14680
 H 0.87347 -1.33772 4.03339
 H -0.79643 3.01720 -0.12873
 H 1.25948 4.85286 0.18521
 H 3.50755 3.25413 0.48479
 H 1.90169 -0.63157 1.65729
 H 3.64314 -2.45574 1.67541
 H 5.73626 -2.22102 0.28807
 F 6.25440 -0.15703 -1.23400
 H 4.33455 1.59663 -1.16265

E (R = p- F)

SCF = -1269.38140096
 H(0 K) = -1268.980386
 H(298 K) = -1268.952889
 G(298 K) = -1269.039359
 BP86 (D3) = -1269.45482679
 SCF (MeOH) = -1269.43754078
 SCF (DCM) = -1269.43257830
 SCF (BS2) = -1269.39171768
 Lowest Frequencies = 14.1683cm⁻¹,
 33.6199cm⁻¹

51

C 1.81220 0.09858 -2.35702
 C 2.63056 -0.51642 -1.36528

C 2.12245 -1.50994 -0.44562
 C 0.72739 -1.80309 -0.53853
 C -0.12273 -1.18192 -1.51610
 C 0.40607 -0.21579 -2.43232
 Ru 0.92959 0.39322 -0.35973
 N -0.11890 0.45948 1.49340
 C 0.47299 0.59407 2.70441
 C -0.45676 0.38845 3.74152
 C -1.66152 0.12495 3.10012
 N -1.43830 0.16648 1.74977
 C 3.06819 -2.17227 0.54810
 C 2.37059 -2.77160 1.78118
 H -0.27812 0.43990 4.81283
 C -2.44079 0.03994 0.73024
 C -3.24340 -1.11432 0.73551
 C -4.26832 -1.20462 -0.21624
 C -4.49801 -0.19405 -1.15956
 C -3.67662 0.94468 -1.13864
 C -2.64432 1.07869 -0.19500
 C -0.48114 0.49314 -3.41986
 O 2.12080 1.89684 0.58356
 C 1.32367 2.83310 0.18506
 O 0.33596 2.45088 -0.55345
 C 1.52124 4.26535 0.57861
 C 3.90062 -3.24703 -0.19767
 H 1.02304 4.45073 1.54636
 H 2.59272 4.48269 0.69997
 H 1.07537 4.93362 -0.17223
 H 3.76648 -1.38461 0.89277
 H -3.08491 -1.92400 1.45237
 F -5.04553 -2.30460 -0.22156
 H -3.85865 1.75179 -1.85452
 H -5.31326 -0.30358 -1.87919
 H -2.66542 -0.04603 3.48335
 H -2.01254 1.97004 -0.16790
 H 2.22602 0.88587 -2.99338
 H -1.19581 -1.38845 -1.51130
 H 3.66227 -0.16898 -1.24286
 H 0.27183 -2.45682 0.21032
 H 4.64091 -3.69116 0.48765
 H 3.25208 -4.05811 -0.57108
 H 4.44659 -2.82342 -1.05702
 H 3.12691 -3.13864 2.49323
 H 1.74570 -2.02888 2.30534
 H 1.73748 -3.63561 1.51258
 H -0.16849 1.53972 -3.55979
 H -0.41166 -0.01446 -4.39937
 H -1.53310 0.47523 -3.09846
 H 1.53434 0.82979 2.75199

TS(E-F) (R = p-F)

SCF = -1269.35013927
 H(0 K) = -1268.950867
 H(298 K) = -1268.923759
 G(298 K) = -1269.009268
 BP86 (D3) = -1269.42493067
 SCF (MeOH) = -1269.41055503
 SCF (DCM) = -1269.40496516
 SCF (BS2) = -1269.36086508
 Lowest Frequencies = -93.6019cm⁻¹,
 14.6236cm⁻¹

51

C -2.51404 -1.09847 -1.16526
 C -2.73510 0.22225 -0.63532
 C -1.86929 1.32524 -0.97930
 C -0.74253 1.05101 -1.83358
 C -0.49426 -0.27553 -2.27723
 C -1.39041 -1.37904 -1.98940
 Ru -0.74156 -0.35852 -0.08108
 N 0.12602 0.83201 1.43429
 C -0.37150 1.45822 2.51760
 C 0.67147 2.05881 3.25798
 C 1.84039 1.75017 2.57259
 N 1.48576 1.00709 1.47590
 C -2.19542 2.71856 -0.46203
 C -1.00647 3.69451 -0.44786
 H 0.58381 2.62871 4.17993
 C 2.28128 0.34959 0.50151
 C 3.48052 0.92043 0.05606
 C 4.20700 0.22431 -0.92162
 C 3.76435 -0.98990 -1.47197
 C 2.55697 -1.52865 -1.01320
 C 1.79804 -0.87191 -0.02105
 C -1.10687 -2.77014 -2.49299
 O -1.43002 -1.36308 1.62351
 C -0.97263 -2.59815 1.66819
 O -0.17323 -3.05006 0.81637
 C -1.46637 -3.42946 2.83831
 C -3.36562 3.28472 -1.31141
 H -0.62888 -3.58874 3.53828
 H -2.29364 -2.94247 3.37253
 H -1.77875 -4.42057 2.47454
 H -2.56455 2.59772 0.57522
 H 3.84465 1.88273 0.42357
 F 5.36032 0.75743 -1.35559
 H 2.21377 -2.49905 -1.38352
 H 4.37718 -1.49613 -2.22187
 H 2.88444 1.96492 2.78939
 H 1.01944 -1.49045 0.49801
 H -3.14873 -1.92234 -0.82508
 H 0.43308 -0.48571 -2.81887
 H -3.54978 0.38305 0.07738
 H -0.01879 1.83751 -2.05758
 H -3.66093 4.27274 -0.92243
 H -3.06287 3.41081 -2.36479
 H -4.25165 2.62958 -1.28473
 H -1.31057 4.63953 0.02980
 H -0.14674 3.29430 0.11352
 H -0.67366 3.94506 -1.47012
 H -1.39658 -3.52993 -1.75205
 H -1.67715 -2.94950 -3.42255
 H -0.03942 -2.90401 -2.72429
 H -1.44133 1.43223 2.71297

F (R = p-F)

SCF = -1269.37640217
 H(0 K) = -1268.975974
 H(298 K) = -1268.948469
 G(298 K) = -1269.034216
 BP86 (D3) = -1269.45118532
 SCF (MeOH) = -1269.43355603
 SCF (DCM) = -1269.42844787
 SCF (BS2) = -1269.38572674

Lowest Frequencies = 19.0279cm⁻¹,
30.8089cm⁻¹

51

C 1.73591 0.50045 -2.04114
 C 2.38621 1.45555 -1.20636
 C 2.98823 1.00353 0.03196
 C 2.85534 -0.33842 0.44042
 C 2.14438 -1.31461 -0.36674
 C 1.60209 -0.86803 -1.61346
 Ru 0.75625 0.39004 -0.04499
 N -0.13257 -0.36385 1.67295
 C 0.20165 -0.49101 2.97449
 C -0.88297 -1.02483 3.70424
 C -1.90284 -1.21226 2.77533
 N -1.42765 -0.80435 1.55897
 C 2.06427 -2.75951 0.10932
 C 0.89762 -3.56063 -0.49405
 C 2.48018 2.90677 -1.60446
 H -0.91862 -1.24584 4.76835
 C -1.99702 -0.71283 0.26433
 C -3.27876 -1.20844 -0.01016
 C -3.75157 -1.07313 -1.32167
 C -2.98621 -0.47056 -2.32756
 C -1.70189 0.00661 -2.00925
 C -1.15561 -0.08986 -0.70399
 O 0.17964 2.31348 0.78871
 C -0.82938 3.03789 0.58836
 O -1.83214 2.69644 -0.20286
 C -0.97410 4.37930 1.24920
 C 3.42166 -3.45434 -0.16924
 H -1.86390 4.37169 1.90067
 H -0.08075 4.61348 1.84109
 H -1.14215 5.15480 0.48421
 H 1.92376 -2.72106 1.20756
 H -3.90764 -1.69087 0.74236
 F -4.98203 -1.53804 -1.61221
 H -1.11777 0.48118 -2.80514
 H -3.39583 -0.38092 -3.33706
 H -2.91491 -1.59267 2.89032
 H -1.65555 1.76608 -0.55040
 H 1.18922 -0.18727 3.31511
 H 1.28520 0.82611 -2.98268
 H 1.02742 -1.56325 -2.23003
 H 3.25021 -0.64741 1.41434
 H 3.46323 1.73325 0.69399
 H 3.40934 -4.48029 0.23366
 H 3.61485 -3.51715 -1.25392
 H 4.26541 -2.91811 0.29646
 H -0.06888 -3.04836 -0.35428
 H 1.04191 -3.74317 -1.57324
 H 0.83455 -4.54776 -0.00860
 H 2.34576 3.57011 -0.73558
 H 3.48229 3.10847 -2.02431
 H 1.73478 3.16786 -2.37130

F1 (R = p-F)

SCF = -1040.24883222
 H(0 K) = -1039.910459
 H(298 K) = -1039.888351
 G(298 K) = -1039.963335
 BP86 (D3) = -1040.30242348

SCF (MeOH) = -1040.30801890
 SCF (DCM) = -1040.30273837
 SCF (BS2) = -1040.18874671
 Lowest Frequencies = 7.4020cm⁻¹,
 19.5802cm⁻¹

43
 C -1.91322 -1.46295 0.56662
 C -1.68561 -0.89610 1.84896
 C -1.91571 0.51277 2.08073
 C -2.54293 1.28727 1.03614
 C -2.76225 0.72340 -0.23819
 C -2.37731 -0.64055 -0.52869
 Ru -0.59637 0.27318 0.34939
 N 0.53821 1.75174 -0.57361
 N 1.87027 1.44985 -0.71613
 C 2.53273 2.47877 -1.31426
 C 1.60274 3.48909 -1.57133
 C 0.37667 2.99334 -1.09443
 C 2.27647 0.17556 -0.22406
 C 1.22755 -0.61101 0.34558
 C 1.61431 -1.88388 0.83947
 C 2.93531 -2.34491 0.78002
 C 3.90862 -1.51307 0.20588
 C 3.60701 -0.24090 -0.30726
 C -1.58462 1.13619 3.41183
 C -2.58480 -1.19457 -1.93109
 C -1.58890 -2.29827 -2.33109
 C -4.05127 -1.68755 -2.05217
 H 1.79479 4.45039 -2.04153
 H -2.45453 -0.34376 -2.62763
 H 4.40716 0.36326 -0.74204
 F 5.18041 -1.93777 0.13845
 H 0.85948 -2.53771 1.28836
 H 3.22585 -3.32590 1.16466
 H 3.60085 2.42929 -1.51472
 H -0.60894 3.45485 -1.09533
 H -1.22669 -1.49683 2.63978
 H -1.62492 -2.49946 0.37481
 H -3.11682 1.35466 -1.05919
 H -2.72583 2.35301 1.20325
 H -4.24341 -2.03118 -3.08179
 H -4.24030 -2.53437 -1.37038
 H -4.77621 -0.89054 -1.81802
 H -0.54402 -1.97794 -2.18315
 H -1.75416 -3.22847 -1.76005
 H -1.72310 -2.54944 -3.39542
 H -1.34934 2.20712 3.31079
 H -2.45719 1.04534 4.08586
 H -0.73395 0.63103 3.89486

G (R = p-F)

SCF = -1055.52861033
 H(0 K) = -1055.189532
 H(298 K) = -1055.165870
 G(298 K) = -1055.242410
 BP86 (D3) = -1055.59478828
 SCF (MeOH) = -1055.54878904
 SCF (DCM) = -1055.54563274
 SCF (BS2) = -1500.70546783

Lowest Frequencies = 17.6088cm⁻¹,
 42.4738cm⁻¹

44
 C 1.29151 -0.55849 -0.41121
 C 2.16266 0.44083 0.09336
 C 3.51907 0.55752 -0.25047
 C 4.03135 -0.38941 -1.14030
 C 3.23808 -1.41645 -1.66442
 C 1.88427 -1.49029 -1.28985
 N 1.55255 1.33473 1.00775
 N 0.21664 1.13369 1.22842
 C -0.15603 2.02949 2.16564
 C 0.94809 2.82514 2.54276
 C 2.02099 2.35392 1.78869
 Ru -0.65001 -0.47208 0.25335
 Cl 0.13585 -1.74447 2.16266
 C -1.53714 -1.63974 -1.41562
 C -2.15909 -2.08505 -0.21557
 C -2.83931 -1.10265 0.61245
 C -2.82496 0.26199 0.26850
 C -2.11196 0.73586 -0.90558
 C -1.49586 -0.23922 -1.75465
 C -2.12440 -3.53118 0.20801
 C -2.11210 2.22773 -1.21988
 C -3.46345 2.62474 -1.86232
 C -0.92914 2.68607 -2.09084
 H 0.96438 3.63222 3.27129
 H -2.03417 2.75149 -0.24619
 H 4.17221 1.33780 0.14919
 F 5.34064 -0.30579 -1.49851
 H 1.28435 -2.31677 -1.68449
 H 3.68418 -2.14637 -2.34599
 H 3.06542 2.65320 1.75851
 H -1.18120 2.03687 2.52809
 H -1.01506 -2.36445 -2.04720
 H -0.93900 0.07935 -2.63906
 H -3.28571 0.99420 0.94079
 H -3.27537 -1.42209 1.56320
 H -3.50911 3.71523 -2.02488
 H -3.59023 2.12899 -2.84077
 H -4.31845 2.33889 -1.22643
 H 0.03406 2.35969 -1.66563
 H -1.00413 2.29253 -3.12001
 H -0.92041 3.78634 -2.16543
 H -1.71011 -3.61292 1.22755
 H -3.14332 -3.95850 0.20317
 H -1.49304 -4.12980 -0.46679

G^{OAc} (R = p-F)

SCF = -1268.96645353
 H(0 K) = -1268.578643
 H(298 K) = -1268.551337
 G(298 K) = -1268.636805
 BP86 (D3) = -1269.03924040
 SCF (MeOH) = -1268.98179047
 SCF (DCM) = -1268.97943452
 SCF (BS2) = -1268.98555202
 Lowest Frequencies = 17.0359cm⁻¹,
 33.3745cm⁻¹

50

C	2.33886	0.10243	2.90797
N	1.70952	0.11114	1.69427
N	0.35650	-0.02553	1.85092
C	0.13477	-0.13029	3.17685
C	1.35537	-0.04948	3.88333
C	2.16877	0.17925	0.35416
C	1.14508	0.06408	-0.62172
C	1.58289	0.06523	-1.96359
C	2.93812	0.21429	-2.31247
C	3.88810	0.35362	-1.29473
C	3.53229	0.33342	0.05645
Ru	-0.75982	-0.17141	0.10589
O	-0.15414	-2.16874	0.31771
C	-0.22984	-3.05936	-0.65342
C	0.45447	-4.37909	-0.27472
C	-2.19664	1.36529	0.72353
C	-2.95388	0.13757	0.81980
C	-2.97681	-0.76249	-0.27095
C	-2.29130	-0.38633	-1.49308
C	-1.64976	0.87927	-1.60239
C	-1.59994	1.81038	-0.50175
C	-3.64912	-2.10905	-0.18145
C	-0.93436	3.16938	-0.67889
C	-1.92632	4.15414	-1.34368
O	-0.75717	-2.91120	-1.76988
C	-0.35900	3.75870	0.62096
H	0.85497	-0.08464	-2.76714
H	3.26397	0.21256	-3.35658
H	-0.87984	-0.26717	3.54422
H	0.37294	-4.58256	0.80403
H	0.02150	-5.20599	-0.85680
H	1.52772	-4.30654	-0.52300
F	5.20051	0.50387	-1.61906
H	4.30580	0.42740	0.82341
H	1.50281	-0.09669	4.95971
H	3.41916	0.19482	2.98472
H	-1.11729	1.12713	-2.52687
H	-3.41918	-0.14241	1.76974
H	-2.09044	1.98359	1.62039
H	-2.20055	-1.11902	-2.29589
H	-0.09009	3.01251	-1.37840
H	-2.31139	3.75931	-2.29903
H	-2.79161	4.34334	-0.68379
H	-1.43600	5.12178	-1.54729
H	-3.04466	-2.86458	-0.70710
H	-3.79251	-2.42210	0.86477
H	-4.64114	-2.06738	-0.66811
H	-1.15694	4.03163	1.33476
H	0.32180	3.04673	1.11572
H	0.20599	4.67989	0.40064

1-C6H4R-pyrazole (R = p-CF3)
 SCF = -794.290873472
 H(0 K) = -794.139040
 H(298 K) = -794.126959
 G(298 K) = -794.179832
 BP86 (D3) = -794.310370802
 SCF (DCM) = -794.295615336
 SCF (MeOH) = -794.296340981
 SCF (BS2) = -794.523499591
 Lowest Frequencies = 15.7822cm⁻¹,
 32.0589cm⁻¹

22

C	0.79008	1.89418	0.08897
C	-0.48563	2.47118	0.09950
C	-1.63742	1.67223	0.04689
C	-1.49753	0.27606	-0.02854
C	-0.22716	-0.31932	-0.05218
C	0.91870	0.49306	0.01603
H	1.69720	2.50044	0.12857
H	-0.58065	3.56018	0.15144
H	-2.63345	2.12200	0.05120
C	-2.72811	-0.60160	-0.03444
H	-0.14825	-1.40392	-0.15017
N	2.21643	-0.08605	0.00432
N	3.31031	0.70867	-0.21494
C	2.56671	-1.40418	0.20380
C	3.94797	-1.47012	0.10576
C	4.35173	-0.13262	-0.15376
H	4.57067	-2.35583	0.21384
H	5.35913	0.25723	-0.30237
H	1.82741	-2.17152	0.41968
F	-2.49292	-1.80780	-0.62735
F	-3.16175	-0.86092	1.23429
F	-3.76480	-0.01351	-0.69473

D (R = p-CF3)

SCF = -1522.42383791
 H(0 K) = -1522.010795
 H(298 K) = -1521.978204
 G(298 K) = -1522.077387
 BP86 (D3) = -1522.51322415
 SCF (MeOH) = -1522.44418527
 SCF (DCM) = -1522.44090405
 SCF (BS2) = -1967.75410973
 Lowest Frequencies = 15.2148cm⁻¹,
 16.8486cm⁻¹

55

C	3.18016	-0.92612	-0.08012
C	1.97864	-0.87425	-0.80639
C	1.72499	0.16326	-1.72162
C	2.70133	1.15518	-1.90249
C	3.91101	1.11604	-1.19143
C	4.14755	0.07259	-0.28011
N	1.05426	-1.95648	-0.65605
N	-0.30083	-1.81701	-0.44269
C	-0.80329	-3.06742	-0.48205
C	0.21234	-4.01830	-0.71733
C	1.38086	-3.27954	-0.82696
Ru	-1.44376	-0.05657	0.14570
Cl	-1.67488	0.37634	-2.23008

H	4.67437	1.88316	-1.34635
C	-1.10460	-0.08903	2.35948
C	-2.37967	0.47429	2.04365
C	-2.51876	1.58292	1.13877
C	-1.37062	2.17097	0.51509
C	-0.08051	1.60222	0.79259
C	0.02896	0.47191	1.66490
C	-0.95681	-1.25276	3.30798
C	-1.57817	3.34972	-0.42904
C	-1.99520	4.58964	0.40088
O	-2.98990	-1.40782	-0.22606
C	-4.27701	-1.12239	-0.09275
C	-5.16366	-2.22096	-0.68931
O	-4.76848	-0.10491	0.41719
C	-0.37202	3.66780	-1.32634
H	2.51780	1.96074	-2.61990
H	-3.52559	1.88960	0.85038
H	0.80853	1.96993	0.27832
H	1.00784	-0.00589	1.78321
H	-3.29302	-0.00256	2.40844
H	-2.42242	3.06756	-1.08587
H	-0.09190	2.78845	-1.92728
H	-0.63209	4.48492	-2.02009
H	0.50063	4.00385	-0.73684
H	-2.21427	5.43666	-0.27119
H	-2.89506	4.39489	1.00740
H	-1.18447	4.90010	1.08384
H	-0.11749	-1.90499	3.01619
H	-0.76024	-0.89234	4.33476
H	-1.87468	-1.86148	3.33485
H	-5.17778	-2.10530	-1.78665
H	-6.18967	-2.12237	-0.30700
H	-4.76979	-3.22563	-0.46710
H	-1.87660	-3.17899	-0.34268
H	0.10252	-5.09616	-0.81024
H	2.40581	-3.56355	-1.05578
H	0.76960	0.18699	-2.26162
C	5.40875	0.06014	0.55297
H	3.36161	-1.73744	0.63026
F	5.78808	-1.20944	0.87574
F	6.44911	0.65245	-0.09414
F	5.23194	0.73278	1.72857

D^{OAC} (R = p-CF3)

SCF = -1735.85886476
 H(0 K) = -1735.396712
 H(298 K) = -1735.360539
 G(298 K) = -1735.468250
 BP86 (D3) = -1735.95688243
 SCF (MeOH) = -1735.87593592
 SCF (DCM) = -1735.87334384
 SCF (BS2) = -1736.03019669
 Lowest Frequencies = 14.2699cm⁻¹,
 19.0628cm⁻¹

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C	3.62381	0.76963	-0.02007
C	2.38592	0.63563	0.63579
C	2.11113	-0.48862	1.43083
C	3.09024	-1.48622	1.55870
C	4.33488	-1.36246	0.92374
C	4.59847	-0.22783	0.13655

N	1.44972	1.71138	0.51799
N	0.10075	1.58775	0.22886
C	-0.35353	2.85220	0.08877
C	0.67746	3.79322	0.29660
C	1.80632	3.03752	0.56575
Ru	-1.23683	-0.09395	-0.14426
O	-0.82271	-0.65683	1.83168
C	-1.13677	-1.82730	2.36353
C	-0.99469	-1.81467	3.89061
C	-2.16838	0.18955	-2.12936
C	-2.93151	-0.81549	-1.42122
C	-2.23750	-1.92878	-0.86457
C	-0.80998	-2.06360	-1.02781
C	-0.05394	-1.12159	-1.78198
C	-0.76324	0.03465	-2.28686
C	-4.43728	-0.63965	-1.27898
C	-5.11213	-1.16821	-2.56990
C	1.41693	-1.31586	-2.05063
O	-2.60660	0.99778	1.02129
C	-3.38667	1.97203	0.61445
C	-4.29967	2.48934	1.73173
C	-5.03454	-1.30372	-0.02607
O	-3.40126	2.49901	-0.51998
O	-1.52148	-2.84412	1.76394
H	-2.65951	1.11366	-2.44135
H	-2.74361	-2.63381	-0.20565
H	-0.30595	-2.88087	-0.50601
H	-0.18851	0.84525	-2.74842
H	-4.61839	0.44858	-1.22093
H	-4.51154	-0.97387	0.88554
H	-6.10014	-1.03370	0.06538
H	-4.98114	-2.40542	-0.08012
H	-6.20057	-0.99312	-2.52568
H	-4.72317	-0.66507	-3.47135
H	-4.94612	-2.25388	-2.68593
H	1.90322	-1.89237	-1.24845
H	1.54984	-1.87218	-2.99731
H	1.94372	-0.35448	-2.15515
H	-4.68844	1.66106	2.34371
H	-5.12635	3.07229	1.30058
H	-3.71531	3.14579	2.39967
H	-1.86798	-1.29759	4.32395
H	-0.96458	-2.84436	4.27507
H	-0.09892	-1.25882	4.21109
H	-1.39873	3.00615	-0.18947
H	0.59924	4.87727	0.26663
H	2.82545	3.31887	0.82098
H	1.13185	-0.56628	1.91666
H	2.88139	-2.36289	2.17961
H	5.10246	-2.13198	1.04173
C	5.90478	-0.11563	-0.61586
H	3.82635	1.63877	-0.65129
F	6.25112	1.18459	-0.83860
F	6.92822	-0.70696	0.06000
F	5.82938	-0.72192	-1.83715

E (R = p-CF₃)

SCF	=	-1507.18097314
H(0 K)	=	-1506.767787
H(298 K)	=	-1506.737269
G(298 K)	=	-1506.832923
BP86 (D3)	=	-1507.25933067

SCF (MeOH)	=	-1507.23828359
SCF (DCM)	=	-1507.23313673
SCF (BS2)	=	-1507.27082529
Lowest Frequencies	=	8.7175cm ⁻¹ , 15.3800cm ⁻¹

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C	-2.19753	0.49106	-2.38200
C	-2.85415	1.23371	-1.35811
C	-2.12985	1.96138	-0.33979
C	-0.70638	1.84808	-0.37361
C	-0.02194	1.09143	-1.38524
C	-0.75796	0.39493	-2.39734
Ru	-1.53401	-0.20527	-0.39952
N	-0.64145	-0.72476	1.46337
C	-1.29923	-0.77206	2.64645
C	-0.39690	-0.93907	3.71449
C	0.85903	-0.99921	3.12157
N	0.69250	-0.86432	1.76925
C	-2.89503	2.78567	0.68751
C	-2.11616	3.05895	1.98555
H	-0.62979	-1.01908	4.77356
C	1.72755	-0.95693	0.77939
C	2.80989	-0.06775	0.86094
C	3.85773	-0.18271	-0.06788
C	3.82192	-1.17814	-1.05921
C	2.73173	-2.06168	-1.12278
C	1.67491	-1.96003	-0.20525
C	-0.06294	-0.45169	-3.42942
O	-3.15371	-1.36180	0.37721
C	-2.64695	-2.45629	-0.08756
O	-1.55585	-2.32422	-0.76528
C	-3.27437	-3.79286	0.16749
C	-3.35033	4.11030	0.02230
H	-2.90444	-4.19375	1.12746
H	-4.36747	-3.69267	0.23935
H	-3.00430	-4.50092	-0.62928
H	-3.80419	2.20695	0.94310
H	2.83920	0.70265	1.63660
C	4.98387	0.83332	-0.03914
H	2.71386	-2.85064	-1.88052
H	4.65101	-1.26638	-1.76614
H	1.85079	-1.16564	3.53734
H	0.82390	-2.64572	-0.24249
H	-2.78696	-0.08991	-3.09692
H	1.06482	0.98654	-1.34114
H	-3.94671	1.18854	-1.29184
H	-0.11987	2.28238	0.44067
H	-3.96554	4.69247	0.72763
H	-2.48062	4.72752	-0.26140
H	-3.95251	3.93160	-0.88404
H	-2.77046	3.56985	2.70985
H	-1.75430	2.12870	2.45515
H	-1.25136	3.72310	1.81107
H	-0.64024	-1.36180	-3.65590
H	0.03533	0.12735	-4.36589
H	0.94563	-0.74162	-3.09954
H	-2.38370	-0.68177	2.65380
F	6.12427	0.33291	-0.57266
F	4.64013	1.94037	-0.75945
F	5.24805	1.24265	1.23035

TS(E-F) (R = p-CF₃)

SCF = -1507.14801927
H(0 K) = -1506.736647
H(298 K) = -1506.706562
G(298 K) = -1506.801071
BP86 (D3) = -1507.22743741
SCF (MeOH) = -1507.21030804
SCF (DCM) = -1507.20447720
SCF (BS2) = -1507.23832900
Lowest Frequencies = -95.3907cm⁻¹,
7.1920cm⁻¹

54

C -3.13885 -0.38560 -1.49469
C -3.07185 0.90529 -0.86278
C -1.91405 1.75812 -1.01579
C -0.80410 1.24804 -1.77051
C -0.85714 -0.07113 -2.30499
C -2.03700 -0.90682 -2.22921
Ru -1.38392 -0.23352 -0.17063
N -0.59307 0.59742 1.60127
C -1.15238 1.18224 2.67789
C -0.16224 1.48599 3.63881
C 1.03563 1.03910 3.09382
N 0.75010 0.50411 1.86387
C -1.92705 3.14741 -0.39792
C -0.53573 3.75581 -0.15377
H -0.30552 1.95481 4.60945
C 1.57973 -0.15908 0.92248
C 2.91955 0.21516 0.75635
C 3.69432 -0.45518 -0.20411
C 3.13718 -1.47795 -0.99507
C 1.79318 -1.83319 -0.82291
C 0.99631 -1.17738 0.13633
C -2.06746 -2.27881 -2.84987
O -2.49281 -1.29009 1.25240
C -2.22425 -2.58088 1.21932
O -1.35524 -3.06887 0.46176
C -3.03129 -3.43197 2.18258
C -2.78515 4.06844 -1.30741
H -2.36493 -3.78156 2.98913
H -3.86922 -2.87588 2.62475
H -3.40156 -4.32541 1.65655
H -2.44765 3.06000 0.57564
H 3.35921 1.02300 1.34679
C 5.12629 -0.00975 -0.44627
H 1.36229 -2.66092 -1.39395
H 3.76340 -2.00295 -1.72108
H 2.04945 1.02778 3.48782
H 0.03773 -1.70152 0.42097
H -4.00275 -1.02782 -1.29731
H 0.04597 -0.48816 -2.76164
H -3.90073 1.23409 -0.22848
H 0.12104 1.82290 -1.84717
H -2.86242 5.06896 -0.85184
H -2.32161 4.18236 -2.30198
H -3.80664 3.67833 -1.44698
H -0.64018 4.71198 0.38322
H 0.10453 3.09573 0.45386
H -0.01452 3.97575 -1.10157
H -2.72043 -2.96127 -2.28642
H -2.44837 -2.20721 -3.88498
H -1.06208 -2.72429 -2.89135

H -2.22872 1.33683 2.71122
F 5.91264 -1.05414 -0.80353
F 5.17131 0.90704 -1.45192
F 5.65934 0.56858 0.66212

F (R = p-CF3)

SCF = -1507.17656077
H(0 K) = -1506.763720
H(298 K) = -1506.733272
G(298 K) = -1506.827288
BP86 (D3) = -1507.25611158
SCF (MeOH) = -1507.23602138
SCF (DCM) = -1507.23066064
SCF (BS2) = -1507.26558837
Lowest Frequencies = 14.3798cm⁻¹,
16.8930cm⁻¹

54

C 1.98321 0.07904 -2.26906
C 2.95088 0.90592 -1.62810
C 3.66543 0.38004 -0.48135
C 3.34393 -0.88740 0.04041
C 2.31293 -1.71782 -0.55858
C 1.65683 -1.21401 -1.72639
Ru 1.37519 0.25210 -0.13213
N 0.66617 -0.25423 1.75166
C 1.18914 -0.42615 2.98432
C 0.16153 -0.70113 3.91280
C -1.02140 -0.68271 3.17882
N -0.69144 -0.40922 1.87970
C 2.02944 -3.09403 0.02996
C 0.64207 -3.65887 -0.32097
C 3.26300 2.28850 -2.14225
H 0.26699 -0.88949 4.97855
C -1.44589 -0.21818 0.69503
C -2.83082 -0.41560 0.66034
C -3.50643 -0.20603 -0.55258
C -2.79504 0.18990 -1.69726
C -1.40256 0.37479 -1.63348
C -0.67125 0.17902 -0.43489
O 1.37153 2.26896 0.66948
C 0.52912 3.19991 0.59094
O -0.64031 3.08491 -0.01716
C 0.79261 4.54828 1.19787
C 3.15445 -4.06694 -0.40719
H 0.04806 4.74448 1.98756
H 1.80359 4.58690 1.62171
H 0.66517 5.33236 0.43388
H 2.08770 -2.98288 1.13073
H -3.39094 -0.73688 1.54264
C -5.01455 -0.34489 -0.60336
H -0.87769 0.68637 -2.54302
H -3.32766 0.34495 -2.63967
H -2.05454 -0.83551 3.48153
H -0.73892 2.13918 -0.34235
H 2.26218 -0.33514 3.13874
H 1.44578 0.45679 -3.14327
H 0.85345 -1.79536 -2.18506
H 3.84205 -1.23902 0.95032
H 4.38955 1.01672 0.03524
H 3.00637 -5.05063 0.06755
H 3.14450 -4.21222 -1.50104

H 4.15468 -3.70074 -0.12127
H -0.16662 -2.95299 -0.06828
H 0.56216 -3.91053 -1.39289
H 0.46817 -4.59110 0.23991
H 3.43311 2.99534 -1.31491
H 4.18807 2.25596 -2.74592
H 2.45624 2.67647 -2.78291
F -5.42917 -0.79316 -1.81632
F -5.46499 -1.21126 0.34554
F -5.61944 0.85420 -0.38059

F1 (R = p-CF3)

SCF = -1278.04650166
H(0 K)= -1277.695861
H(298 K)= -1277.670844
G(298 K)= -1277.753233
BP86 (D3) = -1278.10522058
SCF (MeOH) = -1278.10907568
SCF (DCM) = -1278.10326925
SCF (BS2) = -1278.06650547
Lowest Frequencies = 13.2200cm⁻¹,
15.8449cm⁻¹

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C -2.16237 -1.81010 0.24836
C -2.14138 -1.48750 1.63224
C -2.72157 -0.25280 2.10067
C -3.48438 0.55207 1.17451
C -3.50715 0.22632 -0.19658
C -2.78107 -0.91851 -0.70940
Ru -1.32187 0.19073 0.45876
N -0.56361 1.93505 -0.35976
N 0.80040 1.96027 -0.52099
C 1.20160 3.16748 -1.00477
C 0.06166 3.96189 -1.16305
C -1.01217 3.15574 -0.75208
C 1.49389 0.77473 -0.14040
C 0.65806 -0.27316 0.34663
C 1.32293 -1.45930 0.73858
C 2.71697 -1.59008 0.65657
C 3.49267 -0.52474 0.16509
C 2.88396 0.67663 -0.23792
C -2.59362 0.15506 3.54548
C -2.80475 -1.21502 -2.20176
C -1.55796 -1.95142 -2.72402
C -4.10147 -2.00624 -2.52070
H 0.02387 4.98430 -1.53098
H -2.86955 -0.23709 -2.71689
H 3.50528 1.49875 -0.60281
C 4.99319 -0.68917 0.00876
H 0.74212 -2.30189 1.12780
H 3.20821 -2.51280 0.97726
H 2.25007 3.38275 -1.19980
H -2.07680 3.37820 -0.71493
H -1.57893 -2.11149 2.33268
H -1.61269 -2.68379 -0.11087
H -3.98235 0.90757 -0.90990
H -3.93670 1.48400 1.52627
H -4.17517 -2.17355 -3.60772
H -4.09413 -2.99204 -2.02497
H -5.00668 -1.46621 -2.19721
H -0.62793 -1.42997 -2.44296

H -1.50483 -2.98828 -2.34900
H -1.59838 -2.01201 -3.82334
H -2.61116 1.24997 3.66171
H -3.44705 -0.25643 4.11679
H -1.66888 -0.23556 3.99743
F 5.50909 -1.46216 0.99714
F 5.28712 -1.28448 -1.17837
F 5.62868 0.51386 0.03390

G (R = p-CF3)

SCF = -1293.33317352
H(0 K)= -1292.981757
H(298 K)= -1292.955132
G(298 K)= -1293.040128
BP86 (D3) = -1293.40408799
SCF (MeOH) = -1293.35327145
SCF (DCM) = -1293.35018332
SCF (BS2) = -1738.59039623
Lowest Frequencies = 13.4797cm⁻¹,
17.6775cm⁻¹

47

C 0.72148 -0.52836 -0.09935
C 1.47996 0.49774 0.52545
C 2.86727 0.63530 0.40143
C 3.56169 -0.30362 -0.37711
C 2.86081 -1.35398 -0.99871
C 1.46926 -1.46036 -0.85179
N 0.70976 1.38448 1.31875
N -0.63909 1.15245 1.32135
C -1.18029 2.04514 2.17523
C -0.17063 2.87001 2.71841
C 1.02133 2.42024 2.15438
Ru -1.29671 -0.47666 0.23035
Cl -0.81941 -1.72047 2.25437
C -1.87875 -1.68454 -1.54507
C -2.69011 -2.11825 -0.45940
C -3.51326 -1.13228 0.22128
C -3.45273 0.22672 -0.13813
C -2.55615 0.69217 -1.18289
C -1.79540 -0.28919 -1.89653
C -2.71190 -3.55641 -0.00907
C -2.51890 2.17843 -1.52033
C -3.74827 2.54756 -2.38579
C -1.21187 2.63702 -2.19070
H -0.29168 3.68201 3.43140
H -2.60928 2.71904 -0.55698
H 3.41501 1.43782 0.90318
C 5.04283 -0.14640 -0.59686
H 0.95890 -2.30798 -1.32037
H 3.41089 -2.09618 -1.58489
H 2.04951 2.74526 2.29092
H -2.25065 2.02904 2.36621
H -1.25136 -2.41261 -2.06737
H -1.10024 0.02257 -2.67981
H -4.02960 0.96318 0.43219
H -4.10318 -1.44247 1.08842
H -3.77642 3.63455 -2.57337
H -3.70558 2.03454 -3.36259
H -4.69458 2.26180 -1.89596
H -0.32952 2.32986 -1.60566
H -1.11065 2.22639 -3.21087

H	-1.20120	3.73590	-2.28238
H	-2.46379	-3.61578	1.06466
H	-3.71388	-3.99417	-0.16700
H	-1.97683	-4.15974	-0.56388
F	5.67312	-1.35043	-0.70942
F	5.31542	0.54577	-1.74675
F	5.64326	0.53884	0.42139

G^{oAc} (R = p-CF₃)

SCF = -1506.77086505
H(0 K) = -1506.370667
H(298 K) = -1506.340421
G(298 K) = -1506.433953
BP86 (D3) = -1506.84844817
SCF (MeOH) = -1506.78629081
SCF (DCM) = -1506.78397801
SCF (BS2) = -1506.87023413
Lowest Frequencies = 14.6776cm⁻¹,
17.7372cm⁻¹

H	-2.07368	4.02075	-2.43155
H	-2.76697	4.60782	-0.89662
H	-1.21189	5.26257	-1.48161
H	-3.72382	-2.52868	-1.29273
H	-4.68586	-2.05375	0.14677
H	-5.21498	-1.56970	-1.49081
H	-1.54636	4.07206	1.35425
H	-0.15695	2.94324	1.34628
H	0.01569	4.59780	0.69559
F	5.62770	-0.41515	0.51883
F	5.49957	-0.56446	-1.67420
F	5.41642	1.39584	-0.69939

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C	1.18048	-0.25033	3.35184
N	0.78783	-0.13865	2.04701
N	-0.57756	-0.14892	1.95081
C	-1.04761	-0.27734	3.20792
C	0.02508	-0.33989	4.12518
C	1.48861	-0.06971	0.81544
C	0.65071	-0.05470	-0.33235
C	1.32275	-0.06078	-1.57437
C	2.72383	-0.03278	-1.66220
C	3.50740	-0.01396	-0.49354
C	2.88704	-0.03980	0.76590
Ru	-1.36102	-0.11651	0.02851
O	-1.01008	-2.17323	0.23665
C	-0.97378	-3.00896	-0.78558
C	-0.52132	-4.41177	-0.36199
C	-2.72654	1.55042	0.45187
C	-3.60539	0.40551	0.36116
C	-3.52594	-0.45722	-0.75633
C	-2.59932	-0.12473	-1.82209
C	-1.82599	1.06790	-1.76219
C	-1.88091	1.96035	-0.62967
C	-4.33226	-1.72804	-0.84409
C	-1.06341	3.24613	-0.62894
C	-1.82338	4.34683	-1.40791
O	-1.24067	-2.75413	-1.97262
C	-0.66760	3.73588	0.77513
H	0.74116	-0.12211	-2.49936
H	3.21450	-0.04325	-2.64005
H	-2.12047	-0.32817	3.37953
H	-0.83749	-4.64665	0.66584
H	-0.91347	-5.15982	-1.06667
H	0.58141	-4.45340	-0.39283
C	5.00627	0.09435	-0.58694
H	3.49831	-0.05286	1.67264
H	-0.03233	-0.43882	5.20658
H	2.23225	-0.26544	3.62599
H	-1.11678	1.28227	-2.56872
H	-4.25687	0.15185	1.20284
H	-2.72229	2.13199	1.37894
H	-2.43965	-0.84124	-2.62871
H	-0.13021	3.02133	-1.18141

1-C6H4R-pyrazole (R = p-NO2)
 SCF = -661.778898052
 H(0 K) = -661.629300
 H(298 K) = -661.618316
 G(298 K) = -661.669435
 BP86 (D3) = -661.797100112
 SCF (DCM) = -661.785728829
 SCF (MeOH) = -661.786746122
 SCF (BS2) = -661.960871253
 Lowest Frequencies = 4.4667cm⁻¹,
 55.5425cm⁻¹

21

C	-0.52609	-0.45598	-0.00230
C	-1.81606	0.08612	0.00016
C	-2.06499	1.46371	0.00496
C	-0.95827	2.32510	0.00749
C	0.34895	1.82110	0.00615
C	0.56744	0.42606	0.00160
H	-0.42274	-1.54182	-0.00856
N	-2.96482	-0.85235	-0.00367
H	-3.09455	1.82546	0.00631
H	-1.11428	3.40797	0.01107
H	1.21824	2.48145	0.00814
N	1.89774	-0.06810	0.00066
N	2.94509	0.81638	-0.01877
C	2.32830	-1.37822	0.01798
C	3.71315	-1.34335	0.00920
C	4.03675	0.04079	-0.01358
H	4.38918	-2.19578	0.01863
H	5.02130	0.50906	-0.02673
H	1.63633	-2.21626	0.03682
O	-4.10625	-0.36059	-0.00222
O	-2.71309	-2.07111	-0.00817

D (R = p-NO2)

SCF = -1389.91078943
 H(0 K) = -1389.499940
 H(298 K) = -1389.468516
 G(298 K) = -1389.564099
 BP86 (D3) = -1389.99863685
 SCF (MeOH) = -1389.93363896
 SCF (DCM) = -1389.93007272
 SCF (BS2) = -1835.19109011
 Lowest Frequencies = 19.2591cm⁻¹,
 23.8591cm⁻¹

54

C	3.44056	-0.88932	0.05793
C	2.24543	-0.82469	-0.67591
C	1.98934	0.24370	-1.55830
C	2.95350	1.25575	-1.70077
C	4.16245	1.21006	-0.99047
C	4.38183	0.13211	-0.12326
N	1.33147	-1.91823	-0.56941
N	-0.03552	-1.79694	-0.42804
C	-0.51761	-3.05357	-0.49921
C	0.52163	-3.99037	-0.68504
C	1.68425	-3.23709	-0.72932
Ru	-1.23496	-0.06475	0.13836
Cl	-1.35882	0.42964	-2.23276
H	4.93217	1.97781	-1.09303

C	-0.99291	-0.15279	2.36485
C	-2.26620	0.38902	2.00910
C	-2.39341	1.51890	1.12864
C	-1.23496	2.15319	0.57413
C	0.05565	1.60770	0.89382
C	0.15580	0.45503	1.73696
C	-0.85617	-1.33826	3.28755
C	-1.43053	3.35501	-0.34304
C	-1.91502	4.55828	0.50424
O	-2.73653	-1.42757	-0.34782
C	-4.03461	-1.17305	-0.26076
C	-4.87063	-2.26827	-0.93112
O	-4.56851	-0.18374	0.26126
C	-0.19476	3.73077	-1.17561
H	2.76042	2.08309	-2.38999
H	-3.39417	1.80969	0.80502
H	0.95672	2.01455	0.43251
H	1.14035	-0.00204	1.88748
H	-3.18236	-0.11879	2.32123
H	-2.23787	3.07311	-1.04486
H	0.13322	2.87924	-1.79224
H	-0.44503	4.56392	-1.85360
H	0.64269	4.06841	-0.53795
H	-2.12649	5.41972	-0.15164
H	-2.83503	4.32313	1.06435
H	-1.14291	4.86750	1.23102
H	0.00256	-1.96967	3.00680
H	-0.69771	-1.00066	4.32850
H	-1.76446	-1.96140	3.27049
H	-4.83779	-2.11792	-2.02381
H	-5.91441	-2.20132	-0.59273
H	-4.46685	-3.27191	-0.72264
H	-1.59508	-3.18025	-0.41541
H	0.43090	-5.06899	-0.78874
H	2.72290	-3.50815	-0.90595
H	1.03965	0.27352	-2.10979
N	5.64846	0.06594	0.64386
H	3.65348	-1.70059	0.75762
O	5.80645	-0.90582	1.40478
O	6.46743	0.98520	0.47614

D^{OAC} (R = p-NO2)

SCF = -1603.34619509
 H(0 K) = -1602.886257
 H(298 K) = -1602.851261
 G(298 K) = -1602.955365
 BP86 (D3) = -1603.44282209
 SCF (MeOH) = -1603.36581714
 SCF (DCM) = -1603.36293837
 SCF (BS2) = -1603.46739426
 Lowest Frequencies = 18.2016cm⁻¹,
 23.1335cm⁻¹

60

C	3.85791	0.76148	-0.11542
C	2.63309	0.58889	0.55275
C	2.36347	-0.59229	1.26756
C	3.33028	-1.61109	1.30169
C	4.56634	-1.45915	0.65715
C	4.80521	-0.26582	-0.03678
N	1.70249	1.67291	0.52939
N	0.34143	1.56952	0.28913

C	-0.11110	2.84113	0.24552
C	0.93251	3.76563	0.46749
C	2.06786	2.99351	0.64275
Ru	-1.01399	-0.08079	-0.16015
O	-0.54448	-0.78285	1.75827
C	-0.84350	-1.98964	2.21403
C	-0.66525	-2.08438	3.73407
C	-2.02098	0.34389	-2.08174
C	-2.75303	-0.71732	-1.42405
C	-2.03329	-1.86379	-0.97931
C	-0.61247	-1.97641	-1.20632
C	0.10950	-0.97502	-1.91578
C	-0.62276	0.21136	-2.30440
C	-4.25291	-0.56306	-1.21231
C	-4.97408	-1.00356	-2.51129
C	1.56822	-1.13855	-2.26006
O	-2.34381	0.92608	1.12079
C	-3.13256	1.92813	0.80756
C	-4.01269	2.36231	1.98468
C	-4.79901	-1.31809	0.01207
O	-3.17713	2.53515	-0.28514
O	-1.23962	-2.96213	1.55235
H	-2.52670	1.28604	-2.30289
H	-2.51096	-2.62055	-0.35752
H	-0.08561	-2.82893	-0.77053
H	-0.06999	1.05817	-2.72594
H	-4.43706	0.51701	-1.07081
H	-4.24442	-1.04844	0.92478
H	-5.86191	-1.06377	0.16127
H	-4.74179	-2.41282	-0.12101
H	-6.06068	-0.83943	-2.41360
H	-4.62189	-0.43518	-3.38874
H	-4.80811	-2.07711	-2.71012
H	2.08311	-1.79655	-1.54309
H	1.66151	-1.59349	-3.26385
H	2.09341	-0.17075	-2.28683
H	-4.40509	1.49001	2.52969
H	-4.83673	2.99438	1.62366
H	-3.40285	2.94621	2.69568
H	-1.52944	-1.60293	4.22311
H	-0.62354	-3.13849	4.04390
H	0.23618	-1.54859	4.07226
H	-1.16563	3.01526	0.01868
H	0.85825	4.84964	0.50658
H	3.09777	3.25772	0.87170
H	1.39297	-0.69579	1.76804
H	3.11792	-2.53014	1.85608
H	5.33999	-2.22932	0.67980
N	6.10032	-0.08191	-0.73482
H	4.08699	1.65571	-0.69877
O	6.27766	0.98996	-1.34126
O	6.92311	-1.01066	-0.66754

E (R = p-NO₂)

SCF	=	-1374.66415291
H(0 K)	=	-1374.253262
H(298 K)	=	-1374.223910
G(298 K)	=	-1374.315685
BP86 (D3)	=	-1374.74070931
SCF (MeOH)	=	-1374.72705921
SCF (DCM)	=	-1374.72126208
SCF (BS2)	=	-1374.70474344

Lowest Frequencies = 9.9077cm⁻¹,
24.6558cm⁻¹

53

C	-2.09763	0.08145	-2.39193
C	-2.82174	0.85493	-1.43940
C	-2.17301	1.77322	-0.52967
C	-0.74715	1.82280	-0.59060
C	0.00624	1.03927	-1.53064
C	-0.65693	0.15213	-2.43836
Ru	-1.32491	-0.30364	-0.36467
N	-0.33397	-0.50385	1.51188
C	-0.96297	-0.46256	2.71047
C	-0.03141	-0.39150	3.76426
C	1.21366	-0.39792	3.14784
N	1.01254	-0.46057	1.79364
C	-3.01470	2.61599	0.41979
C	-2.25467	3.12499	1.65651
H	-0.23769	-0.35541	4.83124
C	2.04029	-0.59220	0.80268
C	3.08142	0.34801	0.79685
C	4.12009	0.16662	-0.12373
C	4.14835	-0.90175	-1.02737
C	3.09001	-1.82470	-1.00368
C	2.03317	-1.68235	-0.08975
C	0.11668	-0.71731	-3.39262
O	-2.78475	-1.53248	0.59489
C	-2.17066	-2.61200	0.23764
O	-1.11688	-2.44072	-0.48976
C	-2.63891	-3.97033	0.66177
C	-3.63194	3.79394	-0.37798
H	-2.20132	-4.21831	1.64473
H	-3.73405	-3.98020	0.76479
H	-2.31355	-4.73104	-0.06254
H	-3.84602	1.96988	0.76374
H	3.10577	1.20434	1.47525
N	5.22806	1.16414	-0.13939
H	3.09907	-2.67793	-1.68814
H	4.98978	-0.99431	-1.71789
H	2.22342	-0.40633	3.55339
H	1.21387	-2.40629	-0.05943
H	-2.62496	-0.64104	-3.02123
H	1.09834	1.06715	-1.50712
H	-3.90019	0.69173	-1.33756
H	-0.20422	2.41286	0.15289
H	-4.30137	4.37817	0.27421
H	-2.84503	4.47076	-0.75275
H	-4.22172	3.44412	-1.24156
H	-2.95413	3.63689	2.33649
H	-1.77894	2.30319	2.21799
H	-1.47671	3.85996	1.38468
H	-0.35580	-1.70534	-3.50824
H	0.13589	-0.23463	-4.38689
H	1.15648	-0.85528	-3.06092
H	-2.05066	-0.48525	2.73874
O	6.13638	0.98298	-0.96183
O	5.15077	2.10149	0.67117

TS (E-F) (R = p-NO₂)

SCF	=	-1374.63166592
H(0 K)	=	-1374.222513
H(298 K)	=	-1374.193702

G(298 K) = -1374.283647
 BP86 (D3) = -1374.70984053
 SCF (MeOH) = -1374.69872611
 SCF (DCM) = -1374.69230343
 SCF (BS2) = -1374.67254442
 Lowest Frequencies = -101.3585cm⁻¹,
 11.5023cm⁻¹

53

C	-3.05847	1.32240	-0.04809
C	-1.98697	2.00469	0.61499
C	-0.74175	2.31371	-0.05939
C	-0.58971	1.78479	-1.36771
C	-1.65724	1.06685	-2.02995
C	-2.92429	0.86757	-1.41730
Ru	-1.30128	0.08543	-0.07241
N	-0.36294	-0.43348	1.74267
C	-0.80742	-0.53370	3.01000
C	0.21978	-1.01293	3.85382
C	1.31813	-1.21178	3.02716
N	0.94269	-0.85831	1.75594
C	0.31757	3.13571	0.65944
C	1.72462	3.03221	0.04890
H	0.16186	-1.20223	4.92303
C	1.66162	-0.89896	0.53437
C	3.05049	-0.71706	0.51549
C	3.69013	-0.73596	-0.72932
C	3.00392	-0.90768	-1.93908
C	1.61435	-1.08388	-1.89413
C	0.93014	-1.08472	-0.66191
C	-4.04127	0.12916	-2.10300
O	-2.53097	-1.50718	0.52251
C	-2.43288	-2.50232	-0.33452
O	-1.65279	-2.46086	-1.31557
C	-3.30722	-3.70622	-0.04351
C	-0.15891	4.61209	0.70554
H	-2.66425	-4.53598	0.29568
H	-4.05736	-3.49524	0.73090
H	-3.79804	-4.03452	-0.97265
H	0.35761	2.76411	1.70247
H	3.64434	-0.54192	1.41560
N	5.16930	-0.54126	-0.75598
H	1.05337	-1.27572	-2.81330
H	3.56644	-0.92017	-2.87528
H	2.31498	-1.59662	3.23080
H	-0.10511	-1.53727	-0.68228
H	-3.95897	1.06089	0.51574
H	-1.46528	0.61194	-3.00637
H	-2.10335	2.27752	1.66947
H	0.37705	1.86465	-1.87046
H	0.55994	5.21725	1.28130
H	-0.22388	5.03555	-0.31111
H	-1.14718	4.71629	1.18352
H	2.44222	3.58584	0.67498
H	2.07326	1.98811	-0.01867
H	1.76402	3.48089	-0.95902
H	-4.61091	-0.48298	-1.38657
H	-4.74022	0.85760	-2.55247
H	-3.66093	-0.52296	-2.90300
H	-1.83846	-0.27669	3.24369
O	5.71434	-0.54051	-1.86808
O	5.73493	-0.39266	0.33875

F (R = p-NO₂)

SCF = -1374.66110817
 H(0 K) = -1374.250585
 H(298 K) = -1374.221274
 G(298 K) = -1374.311863
 BP86 (D3) = -1374.73935027
 SCF (MeOH) = -1374.72684450
 SCF (DCM) = -1374.72065750
 SCF (BS2) = -1374.70056322
 Lowest Frequencies = 15.5557cm⁻¹,
 24.7612cm⁻¹

53

C	1.82680	0.12826	-2.23226
C	2.76637	0.95061	-1.54534
C	3.44710	0.40841	-0.38553
C	3.11856	-0.86985	0.10326
C	2.11416	-1.69696	-0.54391
C	1.49445	-1.17705	-1.72439
Ru	1.14555	0.25953	-0.11244
N	0.38332	-0.28514	1.73948
C	0.86713	-0.47444	2.98522
C	-0.18743	-0.77985	3.87366
C	-1.34563	-0.76246	3.10177
N	-0.97572	-0.45949	1.81982
C	1.82446	-3.08656	0.00890
C	0.45485	-3.65744	-0.39760
C	3.08604	2.34368	-2.02490
H	-0.11474	-0.98693	4.93870
C	-1.69225	-0.25815	0.61464
C	-3.07118	-0.46835	0.53310
C	-3.68265	-0.23631	-0.70498
C	-2.96214	0.18918	-1.82646
C	-1.57554	0.38587	-1.70546
C	-0.88426	0.16961	-0.48464
O	1.10848	2.25835	0.72900
C	0.26677	3.18882	0.63648
O	-0.87676	3.08178	-0.02119
C	0.49990	4.52489	1.28056
C	2.97284	-4.04023	-0.41025
H	-0.28355	4.70807	2.03494
H	1.48853	4.55456	1.75476
H	0.41137	5.32284	0.52532
H	1.84636	-2.99624	1.11288
H	-3.68867	-0.80137	1.37109
N	-5.14703	-0.45061	-0.81660
H	-1.02242	0.72570	-2.58740
H	-3.49191	0.35847	-2.76695
H	-2.38638	-0.93450	3.36618
H	-0.95511	2.14464	-0.37096
H	1.93315	-0.37309	3.17742
H	1.31688	0.51669	-3.11818
H	0.71244	-1.75707	-2.22028
H	3.59026	-1.23455	1.02201
H	4.14917	1.04074	0.16574
H	2.81902	-5.03397	0.04105
H	2.99940	-4.16485	-1.50633
H	3.95972	-3.67055	-0.08513
H	-0.36935	-2.96630	-0.15418
H	0.41053	-3.88629	-1.47665
H	0.27398	-4.60355	0.13712
H	3.22516	3.03699	-1.18052

H 4.03059 2.32653 -2.59830
H 2.29860 2.73826 -2.68521
O -5.66674 -0.23632 -1.92222
O -5.74136 -0.82964 0.20695

F1 (R = p-NO2)

SCF = -1145.53022685
H(0 K)= -1145.181867
H(298 K)= -1145.158039
G(298 K)= -1145.236561
BP86 (D3) = -1145.58779845
SCF (MeOH) = -1145.59948564
SCF (DCM) = -1145.59277066
SCF (BS2) = -1145.50084799
Lowest Frequencies = 15.4105cm-1,
22.7354cm-1

45

C 1.96470 -1.78153 -0.00500
C 1.93528 -1.66762 -1.42171
C 2.47069 -0.49582 -2.06703
C 3.20402 0.46325 -1.27164
C 3.23906 0.34237 0.13149
C 2.55284 -0.73988 0.81023
Ru 1.05546 0.13655 -0.49659
N 0.23868 1.92758 0.13425
N -1.12400 1.92203 0.31252
C -1.56603 3.16143 0.65997
C -0.45498 4.00946 0.70846
C 0.64457 3.20148 0.37760
C -1.77608 0.67763 0.07977
C -0.90514 -0.38931 -0.29808
C -1.52273 -1.64010 -0.53974
C -2.90932 -1.82066 -0.42169
C -3.69700 -0.72572 -0.04582
C -3.15874 0.54187 0.21199
C 2.32662 -0.30475 -3.55445
C 2.58843 -0.81488 2.32949
C 1.37661 -1.52346 2.96096
C 3.92004 -1.49227 2.75138
H -0.45228 5.06841 0.95513
H 2.60868 0.22948 2.69665
H -3.83543 1.35136 0.49685
N -5.16883 -0.89933 0.08922
H -0.91118 -2.49846 -0.83526
H -3.39170 -2.78266 -0.61007
H -2.62011 3.35890 0.84410
H 1.69942 3.45743 0.29974
H 1.39717 -2.40748 -2.02109
H 1.44510 -2.61133 0.48078
H 3.69277 1.13529 0.73500
H 3.62424 1.34835 -1.75839
H 4.00049 -1.49597 3.85067
H 3.95767 -2.53902 2.40440
H 4.80008 -0.96483 2.34763
H 0.42335 -1.09035 2.61505
H 1.37063 -2.60499 2.74022
H 1.42038 -1.42254 4.05712
H 2.29197 0.76197 -3.82586
H 3.20104 -0.75142 -4.06436
H 1.42357 -0.80036 -3.94267
O -5.62612 -2.02766 -0.14196

O -5.82438 0.10128 0.42385

G (R = p-NO2)

SCF = -1160.82339760
H(0 K)= -1160.474064
H(298 K)= -1160.448616
G(298 K)= -1160.530029
BP86 (D3) = -1160.89298536
SCF (MeOH) = -1160.84654346
SCF (DCM) = -1160.84317128
SCF (BS2) = -1606.03027467
Lowest Frequencies = 15.0174cm-1,
34.0883cm-1

46

C 0.95283 -0.53842 -0.14757
C 1.74371 0.51226 0.40359
C 3.12108 0.63884 0.21597
C 3.75512 -0.34375 -0.55706
C 3.04460 -1.42066 -1.11069
C 1.66261 -1.50730 -0.89609
N 1.00981 1.43684 1.18596
N -0.33859 1.21114 1.25317
C -0.84150 2.14294 2.08769
C 0.19241 2.98660 2.55195
C 1.35909 2.50696 1.96159
Ru -1.04151 -0.46031 0.26034
Cl -0.49773 -1.61430 2.31760
C -1.71201 -1.74972 -1.43002
C -2.48032 -2.12076 -0.29129
C -3.26648 -1.09368 0.37193
C -3.20829 0.24496 -0.05541
C -2.35332 0.64942 -1.15892
C -1.63309 -0.37474 -1.85355
C -2.49894 -3.53526 0.22798
C -2.32375 2.11559 -1.57553
C -3.59277 2.44794 -2.39796
C -1.04984 2.52765 -2.33396
H 0.10261 3.82984 3.23251
H -2.36374 2.70688 -0.63897
H 3.72086 1.44849 0.63806
N 5.20265 -0.23491 -0.78179
H 1.12548 -2.36624 -1.30985
H 3.58873 -2.16880 -1.69170
H 2.39319 2.83251 2.04081
H -1.90308 2.14105 2.32315
H -1.11671 -2.50987 -1.94396
H -0.97038 -0.10967 -2.68092
H -3.75577 1.01439 0.50000
H -3.82311 -1.35466 1.27648
H -3.62371 3.52359 -2.64146
H -3.60127 1.88366 -3.34693
H -4.51538 2.19672 -1.84778
H -0.13996 2.24782 -1.77809
H -1.00164 2.06176 -3.33405
H -1.03928 3.61971 -2.48590
H -2.21128 -3.54690 1.29328
H -3.51086 -3.96728 0.12897
H -1.79214 -4.17328 -0.32456
O 5.75089 -1.11753 -1.46988
O 5.79679 0.73777 -0.27272

G^o_{Ac} (R = p-NO₂)

SCF = -1374.26119158
H(0 K) = -1373.863103
H(298 K) = -1373.834005
G(298 K) = -1373.924303
BP86 (D3) = -1374.33748111
SCF (MeOH) = -1374.27994750
SCF (DCM) = -1374.27730419
SCF (BS2) = -1374.31008893
Lowest Frequencies = 15.2260cm⁻¹,
27.9278cm⁻¹

H	0.19227	4.62059	0.65480
O	5.82829	0.16880	0.24660
O	5.61812	0.19797	-1.95167

52

C	1.53899	-0.23430	3.27433
N	1.09516	-0.12344	1.98572
N	-0.27259	-0.16086	1.93937
C	-0.69257	-0.30483	3.21196
C	0.41506	-0.35025	4.08852
C	1.74746	-0.03503	0.73040
C	0.86306	-0.02968	-0.38858
C	1.48510	-0.00985	-1.65969
C	2.87791	0.05172	-1.80784
C	3.68570	0.07966	-0.66007
C	3.13829	0.02732	0.63000
Ru	-1.12349	-0.12764	0.04670
O	-0.74835	-2.18001	0.23189
C	-0.73104	-3.00634	-0.80022
C	-0.26136	-4.40985	-0.40042
C	-2.49780	1.52284	0.52793
C	-3.36130	0.36373	0.47354
C	-3.32111	-0.49468	-0.64871
C	-2.44335	-0.14962	-1.75084
C	-1.68598	1.05392	-1.72257
C	-1.70794	1.94613	-0.58868
C	-4.11357	-1.77565	-0.70520
C	-0.91314	3.24566	-0.62257
C	-1.72392	4.32978	-1.37342
O	-1.02673	-2.73948	-1.97711
C	-0.47132	3.74671	0.76363
H	0.86635	-0.07440	-2.55944
H	3.35526	0.07013	-2.79032
H	-1.75686	-0.37799	3.42401
H	-0.55181	-4.65606	0.63225
H	-0.66614	-5.15310	-1.10290
H	0.84048	-4.44530	-0.45785
N	5.14633	0.15310	-0.79919
H	3.81164	0.03125	1.49034
H	0.39949	-0.45594	5.17066
H	2.60058	-0.22961	3.50838
H	-1.01765	1.28074	-2.55991
H	-3.97300	0.10085	1.34176
H	-2.46472	2.10536	1.45367
H	-2.31138	-0.86033	-2.56743
H	0.00102	3.03643	-1.21171
H	-2.00840	3.99652	-2.38570
H	-2.65091	4.57523	-0.82554
H	-1.13227	5.25585	-1.47312
H	-3.51289	-2.56957	-1.17576
H	-4.42668	-2.10481	0.29793
H	-5.02094	-1.62915	-1.31963
H	-1.33244	4.06896	1.37609
H	0.07632	2.96602	1.31684

2. ortho-substituted species

D (R = o-NMe₂)

SCF = -1319.36230058
H(0 K) = -1318.882474
H(298 K) = -1318.849292
G(298 K) = -1318.947368
BP86 (D3) = -1319.45943127
SCF (MeOH) = -1319.38283801
SCF (DCM) = -1319.37953048
SCF (BS2) = -1764.60803293
Lowest Frequencies = 19.3197cm⁻¹,
31.8159cm⁻¹

60

C	2.62605	-2.22124	1.48066
C	1.94455	-1.82943	0.31366
C	2.44614	-0.86089	-0.56102
C	3.68129	-0.21566	-0.27235
C	4.38060	-0.61921	0.90334
C	3.85333	-1.59727	1.75445
N	0.74012	-2.53080	-0.04045
N	-0.46190	-1.93331	-0.34799
C	-1.26760	-2.93009	-0.77116
C	-0.59781	-4.17060	-0.74024
C	0.67832	-3.87956	-0.27550
Ru	-1.15233	0.07240	0.13120
Cl	-0.23734	0.77765	-2.00765
C	-1.97907	1.90904	1.01119
C	-0.55505	2.07311	1.00057
C	0.25366	1.03766	1.58356
C	-0.36946	-0.11776	2.15519
C	-1.80175	-0.26779	2.24232
C	-2.58352	0.75671	1.62195
C	0.03100	3.31355	0.33383
C	-0.40408	4.57356	1.12242
C	-2.43393	-1.47798	2.88400
O	-2.72235	-0.58743	-1.07550
C	-3.79311	0.13778	-1.35828
C	-4.63320	-0.50387	-2.46869
C	1.55759	3.27887	0.16706
O	-4.12245	1.21886	-0.84715
H	-2.62231	2.59350	0.45552
H	1.34192	1.07628	1.51444
H	0.27139	-0.93734	2.49820
H	-3.66304	0.62764	1.50920
H	-0.42134	3.35607	-0.67530
H	1.88308	2.39111	-0.39655
H	1.89017	4.17292	-0.38707
H	2.07352	3.28754	1.14472
H	-0.03715	5.48142	0.61391
H	-1.50042	4.65161	1.20549
H	0.01530	4.56545	2.14438
H	-1.80026	-2.37201	2.76478
H	-2.57929	-1.31086	3.96755
H	-3.41992	-1.69175	2.44124
H	-4.15162	-0.29552	-3.43951
H	-5.64384	-0.07091	-2.47166
H	-4.68798	-1.59834	-2.35472
H	-2.27926	-2.66492	-1.07082
H	-0.98897	-5.14296	-1.03043
H	1.56292	-4.49571	-0.12986

H	1.84944	-0.59912	-1.43787
N	4.18236	0.76828	-1.11697
H	5.34669	-0.17420	1.15017
H	4.41705	-1.88281	2.64870
H	2.21091	-2.99072	2.13750
C	5.55031	1.23659	-0.92156
C	3.60098	0.93059	-2.45275
H	2.51059	1.08495	-2.39267
H	4.04049	1.82336	-2.92210
H	3.79429	0.05644	-3.10943
H	5.75819	2.03742	-1.64603
H	5.68102	1.66193	0.08897
H	6.30870	0.43665	-1.05997

D^{OAc} (R = o-NMe₂)

SCF = -1532.79582440
H(0 K) = -1532.266836
H(298 K) = -1532.230208
G(298 K) = -1532.335901
BP86 (D3) = -1532.90293462
SCF (MeOH) = -1532.81326763
SCF (DCM) = -1532.81057385
SCF (BS2) = -1532.88172821
Lowest Frequencies = 21.4202cm⁻¹,
31.6682cm⁻¹

66

C	3.61607	2.07869	-0.67159
C	2.62044	1.41938	0.07801
C	2.72933	0.06931	0.42942
C	3.85476	-0.68896	-0.00702
C	4.86814	-0.01544	-0.74863
C	4.74002	1.34111	-1.06620
N	1.49846	2.21339	0.51046
N	0.16834	1.97114	0.20403
C	-0.49272	3.10829	0.50718
C	0.38775	4.08807	1.01106
C	1.63798	3.48880	0.99503
Ru	-0.85187	0.13876	-0.27662
O	-0.07317	-0.37138	1.60695
C	-0.16857	-1.53936	2.20608
C	0.05090	-1.42707	3.71923
C	-2.34465	0.03088	-1.86194
C	-2.30758	-1.27846	-1.23752
C	-1.03677	-1.90793	-1.11299
C	0.15949	-1.29715	-1.64233
C	0.10298	-0.03918	-2.31140
C	-1.17603	0.62756	-2.40521
C	-3.60146	-1.86648	-0.68537
C	-4.56700	-2.17323	-1.85623
C	1.32955	0.58726	-2.92414
O	-2.33354	0.74521	1.09176
C	-3.30073	1.60034	0.84879
C	-4.27034	1.73576	2.02926
C	-3.40307	-3.10712	0.20092
O	-3.44378	2.29821	-0.17818
O	-0.40678	-2.64212	1.67597
H	-3.26476	0.61986	-1.83064
H	-0.93498	-2.80022	-0.49352
H	1.12870	-1.78015	-1.48815
H	-1.22978	1.64251	-2.81007
H	-4.05999	-1.07146	-0.06566

H	-2.67790	-2.92348	1.00957
H	-4.36725	-3.40144	0.64886
H	-3.04193	-3.96697	-0.39248
H	-5.53398	-2.53409	-1.46624
H	-4.76394	-1.28319	-2.47750
H	-4.15082	-2.95970	-2.51064
H	2.25694	0.17934	-2.49595
H	1.33194	0.38525	-4.01168
H	1.33360	1.68044	-2.78959
H	-4.41482	0.77365	2.54382
H	-5.23289	2.13566	1.67792
H	-3.84640	2.44461	2.76194
H	0.85479	-0.71185	3.95427
H	-0.87413	-1.03961	4.17983
H	0.27475	-2.41518	4.14702
H	-1.56674	3.15242	0.31805
H	0.13843	5.09089	1.34940
H	2.62163	3.84983	1.28657
H	1.92829	-0.36559	1.03010
N	3.95935	-2.04550	0.28446
H	5.76334	-0.54974	-1.07268
H	5.53215	1.83044	-1.64255
H	3.49657	3.12847	-0.95107
C	5.21926	-2.72981	0.01278
C	3.06933	-2.63882	1.28425
H	2.00960	-2.53245	1.00248
H	3.28130	-3.71585	1.35207
H	3.20499	-2.19401	2.29184
H	5.10987	-3.79270	0.27227
H	5.47502	-2.67565	-1.06043
H	6.07332	-2.31672	0.59063

E (R = o-NMe2)

SCF = -1304.12633261
H(0 K) = -1303.646482
H(298 K) = -1303.615211
G(298 K) = -1303.711448
BP86 (D3) = -1304.21094373
SCF (MeOH) = -1304.17908522
SCF (DCM) = -1304.17447094
SCF (BS2) = -1304.13285226
Lowest Frequencies = 3.3147cm⁻¹,
23.0670cm⁻¹

59

C	1.32231	1.91325	-1.00267
C	2.63840	1.36867	-0.98131
C	2.90530	0.05287	-1.50888
C	1.88222	-0.73338	-2.12302
C	0.54746	-0.18049	-2.13448
C	0.26928	1.09646	-1.57510
Ru	1.28871	-0.12060	-0.05633
O	2.45221	-0.46341	1.70147
C	1.54873	0.06921	2.45536
O	0.52194	0.55918	1.84489
C	2.16610	-2.10273	-2.68518
C	0.97162	3.27756	-0.42734
C	0.78929	4.27378	-1.60222
N	0.42818	-1.98587	0.47475
N	-0.84900	-2.43575	0.23083
C	-0.95557	-3.75551	0.57025
C	0.28212	-4.18112	1.04329

C	1.11116	-3.04681	0.96953
C	-1.91658	-1.60333	-0.26012
C	-2.28111	-0.46565	0.47104
C	-3.36251	0.34767	0.02204
C	-4.05679	-0.07017	-1.15417
C	-3.67440	-1.22029	-1.84949
C	-2.59224	-2.00995	-1.42308
C	1.67610	0.08682	3.94935
C	1.97861	3.81330	0.60406
H	2.33766	-2.02865	-3.77431
H	1.31906	-2.78840	-2.52666
H	0.54480	-5.17263	1.40406
H	1.23638	-0.83764	4.36302
H	2.73590	0.12120	4.24153
H	1.13254	0.94445	4.37169
H	3.06660	-2.54685	-2.23324
H	-2.28978	-2.91176	-1.96210
H	-4.23494	-1.51159	-2.74311
N	-3.72618	1.49421	0.70744
H	-4.91267	0.50149	-1.51751
H	-1.91245	-4.26482	0.47752
H	-1.73018	-0.22852	1.38203
H	3.43995	1.90291	-0.46587
H	-0.76810	1.43852	-1.51844
H	3.90376	-0.37783	-1.38171
H	-0.28685	-0.79621	-2.48412
H	-0.00858	3.16129	0.07430
H	2.15789	-2.92428	1.24106
H	0.46161	5.25236	-1.21497
H	1.73989	4.42252	-2.14236
H	0.03531	3.92551	-2.32765
H	1.60104	4.75435	1.03523
H	2.13514	3.10238	1.43173
H	2.95610	4.04047	0.14400
C	-4.97044	2.17886	0.35217
C	-3.15216	1.75767	2.02735
H	-2.04988	1.77926	1.98258
H	-3.49282	2.74381	2.37334
H	-3.45332	1.00177	2.78131
H	-5.07531	3.07491	0.97956
H	-4.95195	2.51108	-0.70035
H	-5.86560	1.54282	0.50197

TS (E-F) (R = o-NMe2)

SCF = -1304.09909088
H(0 K) = -1303.620309
H(298 K) = -1303.589604
G(298 K) = -1303.682179
BP86 (D3) = -1304.19066363
SCF (MeOH) = -1304.15587588
SCF (DCM) = -1304.15061495
SCF (BS2) = -1304.10593524
Lowest Frequencies = -92.4950cm⁻¹,
17.6992cm⁻¹

59

C	2.34463	0.38071	-1.02655
C	2.30620	-0.99498	-1.43227
C	1.18560	-1.53869	-2.14513
C	0.07318	-0.69912	-2.54579
C	0.09287	0.66370	-2.13529
C	1.17948	1.16260	-1.33798

Ru	0.45981	-0.63843	-0.33193
O	1.28204	-1.80949	1.15867
C	0.92439	-1.51280	2.39813
O	0.21910	-0.52885	2.69189
C	-1.08443	-1.27800	-3.31562
C	3.51688	1.00046	-0.27649
C	4.41676	1.75596	-1.28710
N	-1.27177	-1.76944	0.11210
N	-2.48881	-1.15238	0.23007
C	-3.46570	-2.06996	0.50103
C	-2.85747	-3.32103	0.55953
C	-1.48730	-3.08574	0.31573
C	-2.55845	0.26702	0.08750
C	-1.53615	1.01903	0.71505
C	-1.53353	2.44593	0.54959
C	-2.56701	3.03119	-0.24818
C	-3.55635	2.24277	-0.83266
C	-3.56895	0.83859	-0.68566
C	1.43520	-2.48674	3.44629
C	4.33208	-0.00916	0.55162
H	-0.82830	-1.31183	-4.39011
H	-1.99157	-0.66548	-3.20128
H	-3.33787	-4.27424	0.76705
H	0.68024	-3.27796	3.59704
H	2.37272	-2.96714	3.13056
H	1.57238	-1.96421	4.40374
H	-1.30695	-2.30832	-2.99542
H	-4.32671	0.22100	-1.17440
H	-4.33770	2.72569	-1.42752
N	-0.57858	3.22814	1.15996
H	-2.60955	4.11332	-0.38332
H	-4.49379	-1.75439	0.66414
H	-0.91858	0.52784	1.48734
H	3.08430	-1.67953	-1.08407
H	1.09949	2.17290	-0.92027
H	1.16246	-2.60947	-2.37164
H	-0.77843	1.29820	-2.31903
H	3.08651	1.74870	0.41746
H	-0.64860	-3.77844	0.28348
H	5.24067	2.25903	-0.75467
H	4.86224	1.05673	-2.01564
H	3.85546	2.52163	-1.84848
H	5.06699	0.52735	1.17297
H	3.68629	-0.60826	1.21360
H	4.90284	-0.69811	-0.09573
C	-0.69068	4.69001	1.11956
C	0.33480	2.62443	2.13087
H	0.88236	1.77412	1.68379
H	1.06024	3.38075	2.46033
H	-0.19823	2.22807	3.01482
H	0.18240	5.12641	1.62302
H	-0.70077	5.06051	0.08019
H	-1.60347	5.05107	1.63060

F (R = o-NMe2)

SCF	=	-1304.10541740
H(0 K)	=	-1303.626788
H(298 K)	=	-1303.595649
G(298 K)	=	-1303.689330
BP86 (D3)	=	-1304.19897765
SCF (MeOH)	=	-1304.16286301
SCF (DCM)	=	-1304.15748777

SCF (BS2) = -1304.11103542
 Lowest Frequencies = 10.7316cm⁻¹,
 27.3743cm⁻¹

59

C	2.44754	0.04328	-1.00587
C	2.12538	-1.32106	-1.35355
C	0.95148	-1.62428	-2.10476
C	0.05505	-0.59131	-2.57782
C	0.34859	0.74421	-2.17925
C	1.52521	1.05479	-1.40224
Ru	0.32845	-0.48874	-0.34709
O	1.07771	-1.09658	1.51041
C	0.46921	-1.03995	2.67770
O	-0.62489	-0.47783	2.90340
C	-1.15918	-0.93129	-3.40400
C	3.70993	0.41832	-0.23934
C	4.76371	0.93695	-1.25219
N	-1.27891	-1.76422	0.09464
N	-2.49950	-1.14840	0.15851
C	-3.48868	-2.05820	0.41611
C	-2.87971	-3.30508	0.51958
C	-1.49951	-3.07461	0.31294
C	-2.50031	0.26296	-0.00508
C	-1.33255	0.91966	0.52210
C	-1.28698	2.36821	0.39599
C	-2.32866	3.02406	-0.33839
C	-3.41217	2.30974	-0.83682
C	-3.52923	0.90652	-0.67385
C	1.23354	-1.74430	3.79332
C	4.28484	-0.71533	0.62907
H	-0.87863	-0.99578	-4.47079
H	-1.94063	-0.16182	-3.30598
H	-3.36504	-4.25440	0.73344
H	1.23523	-2.83197	3.61054
H	2.28455	-1.41517	3.81290
H	0.75582	-1.54039	4.76090
H	-1.58479	-1.90538	-3.11410
H	-4.37806	0.35710	-1.08849
H	-4.19952	2.84926	-1.37262
N	-0.30327	3.10072	1.00017
H	-2.30798	4.10637	-0.47553
H	-4.52323	-1.74467	0.53521
H	-0.97835	0.45280	1.49771
H	2.74244	-2.13791	-0.97293
H	1.68945	2.08595	-1.07449
H	0.69866	-2.67280	-2.29600
H	-0.36134	1.54114	-2.42010
H	3.43818	1.26132	0.42541
H	-0.66531	-3.77350	0.31701
H	5.67046	1.25993	-0.71469
H	5.05593	0.14069	-1.95827
H	4.38950	1.79279	-1.83829
H	5.11284	-0.32547	1.24310
H	3.51701	-1.13614	1.29706
H	4.70329	-1.52785	0.00899
C	-0.34516	4.56897	0.97018
C	0.63955	2.45401	1.91797
H	1.11495	1.58572	1.42782
H	1.41729	3.17630	2.20095
H	0.13470	2.08899	2.83004
H	0.54500	4.95868	1.48104
H	-0.33526	4.94799	-0.06598

H -1.24123 4.96377 1.48344

F1 (R = o-NMe2)

SCF = -1074.98481048
H(0 K)= -1074.567142
H(298 K)= -1074.541802
G(298 K)= -1074.621853
BP86 (D3) = -1075.05445535
SCF (MeOH) = -1075.04006465
SCF (DCM) = -1075.03517562
SCF (BS2) = -1074.92019455
Lowest Frequencies = 21.9491cm⁻¹,
31.7588cm⁻¹

51

C -1.62286 -1.62763 -0.19261
C -0.77086 -2.03758 0.87759
C -0.73433 -1.27873 2.09502
C -1.68148 -0.19680 2.25269
C -2.59118 0.13914 1.21836
C -2.54634 -0.52265 -0.05050
Ru -0.43028 0.09077 0.40348
N -0.19315 2.11784 0.03415
N 1.09869 2.47449 -0.23012
C 1.19981 3.82093 -0.42183
C -0.07951 4.35972 -0.27102
C -0.91529 3.26408 0.01605
C 2.04078 1.40559 -0.26282
C 1.46899 0.08523 -0.31676
C 2.43615 -0.98436 -0.47808
C 3.82536 -0.71588 -0.29617
C 4.29010 0.58830 -0.14691
C 3.40166 1.68213 -0.15957
C 0.23053 -1.61854 3.20237
C -3.49752 -0.11612 -1.16820
C -2.88390 -0.19598 -2.57909
C -4.78521 -0.97300 -1.06666
H -0.36365 5.40494 -0.36497
H -3.77787 0.93817 -0.97848
H 3.77594 2.70360 -0.04991
H 5.36538 0.76947 -0.05751
N 2.03090 -2.27391 -0.81595
H 4.55381 -1.52675 -0.35868
H 2.15087 4.29330 -0.65653
H -1.98594 3.23511 0.20742
H -0.04085 -2.83569 0.72276
H -1.56424 -2.14432 -1.15311
H -3.24435 1.00890 1.34189
H -1.64524 0.41134 3.16170
H -5.51489 -0.64784 -1.82654
H -4.56429 -2.03982 -1.24431
H -5.26007 -0.88327 -0.07581
H -1.94441 0.37746 -2.64701
H -2.68017 -1.23837 -2.88068
H -3.59198 0.21574 -3.31639
H 0.53558 -0.71928 3.76064
H -0.25425 -2.30911 3.91708
H 1.13283 -2.11309 2.81198
C 2.98062 -3.38563 -0.70680
C 1.08465 -2.45008 -1.92786
H 0.49462 -1.53513 -2.06077
H 1.63713 -2.66126 -2.86568

H 0.41284 -3.30443 -1.73340
H 2.41718 -4.33003 -0.77259
H 3.73616 -3.38476 -1.51901
H 3.49594 -3.36047 0.26485

G (R = o-NMe2)

SCF = -1090.26009957
H(0 K)= -1089.841964
H(298 K)= -1089.815265
G(298 K)= -1089.897251
BP86 (D3) = -1090.34348683
SCF (MeOH) = -1090.27705224
SCF (DCM) = -1090.27426361
SCF (BS2) = -1535.43170756
Lowest Frequencies = 23.9372cm⁻¹,
40.9425cm⁻¹

52

C 0.74172 -1.91451 0.63648
C 1.46565 -2.02696 -0.59218
C 2.65406 -1.24007 -0.83447
C 3.04854 -0.29756 0.14672
C 2.23737 -0.11770 1.32315
C 1.13563 -0.98058 1.65618
Ru 0.78879 0.07606 -0.29544
Cl 0.65953 0.75887 -2.61728
C 3.37742 -1.35578 -2.15088
C 0.47303 -0.87311 3.02492
C -0.97978 -1.37731 3.06440
C -1.28943 0.23407 -0.24488
C -1.76639 1.51967 0.11860
C -3.11048 1.84901 0.36681
C -4.06330 0.84023 0.21442
C -3.66377 -0.43624 -0.20884
C -2.30575 -0.75232 -0.45720
N -0.75794 2.51066 0.25487
N 0.52701 2.08088 0.10111
C 1.31631 3.17142 0.19526
C 0.52617 4.31848 0.42396
C -0.79119 3.86300 0.45353
C 1.34065 -1.61230 4.07392
H 0.86652 5.34431 0.54375
H 0.46833 0.20263 3.29125
H -3.40310 2.85660 0.67764
H -5.12114 1.04957 0.40215
N -1.95448 -2.07227 -0.90129
H -4.43110 -1.19918 -0.36684
H -1.73130 4.39281 0.58059
H 2.39221 3.07142 0.07263
H 1.10761 -2.70829 -1.36680
H -0.17575 -2.49662 0.74299
H 2.49250 0.68963 2.02031
H 3.90368 0.35886 -0.03800
H 0.91021 -1.49571 5.08359
H 1.38923 -2.69239 3.84848
H 2.37364 -1.22550 4.09552
H -1.59994 -0.88310 2.29969
H -1.03080 -2.46868 2.90119
H -1.42044 -1.17646 4.05560
H 4.32799 -0.80024 -2.13800
H 3.58565 -2.41216 -2.39186
H 2.74182 -0.93212 -2.95042

C	-2.92657	-3.13047	-0.62996
C	-1.51106	-2.12156	-2.30672
H	-0.78490	-1.31960	-2.50718
H	-1.04256	-3.10216	-2.50945
H	-2.36739	-2.00210	-3.00877
H	-2.44640	-4.10508	-0.82752
H	-3.23735	-3.10238	0.42717
H	-3.84123	-3.08263	-1.26654

D (R = o-OMe)

SCF = -1299.91697810
H(0 K) = -1299.476604
H(298 K) = -1299.445201
G(298 K) = -1299.539407
BP86 (D3) = -1300.00885556
SCF (MeOH) = -1299.93720222
SCF (DCM) = -1299.93402141
SCF (BS2) = -1745.16300262
Lowest Frequencies = 21.2769cm⁻¹,
31.4590cm⁻¹

56

C	-2.44217	0.64812	1.62931
C	-1.93791	1.81786	0.96510
C	-0.53030	2.09247	0.92742
C	0.36412	1.14765	1.53554
C	-0.16044	-0.03212	2.15660
C	-1.57456	-0.28887	2.27486
Ru	-0.98262	0.01869	0.14144
O	-2.51106	-0.84761	-0.98356
C	-3.64351	-0.22821	-1.28171
O	-4.04913	0.85026	-0.82357
C	-0.05234	3.35050	0.21072
C	1.46700	3.41589	-0.00456
C	-2.10174	-1.51769	2.97340
N	-0.11097	-1.92852	-0.27672
N	1.15739	-2.38431	0.00637
C	1.22364	-3.74525	-0.14703
C	-0.03545	-4.18873	-0.53005
C	-0.82871	-3.02448	-0.60016
C	2.29430	-1.54014	0.24877
C	3.05870	-1.75766	1.40636
C	4.21829	-0.98286	1.59557
C	4.60041	-0.02411	0.65296
C	3.82194	0.17330	-0.51245
C	2.65650	-0.59084	-0.72111
O	4.28175	1.11658	-1.38430
C	3.60637	1.23238	-2.65166
Cl	-0.20727	0.72836	-2.04950
C	-0.55041	4.59782	0.98234
C	-4.44884	-0.99794	-2.33444
H	-2.63884	2.42947	0.39439
H	1.44514	1.27084	1.45109
H	0.54569	-0.78677	2.52004
H	-3.50961	0.43139	1.53865
H	-0.53797	3.33492	-0.78353
H	1.83277	2.53166	-0.54850
H	1.72088	4.30903	-0.59975
H	2.01274	3.49391	0.95341
H	-0.26372	5.51500	0.44029
H	-1.64655	4.60128	1.09870
H	-0.10037	4.64574	1.98998
H	-1.40220	-2.36428	2.87828
H	-2.24486	-1.31918	4.05189
H	-3.07416	-1.82445	2.55606
H	-4.01243	-0.79540	-3.32761
H	-5.49422	-0.65737	-2.32893
H	-4.40121	-2.08579	-2.16719
H	-1.87442	-2.87960	-0.86343
H	-0.33808	-5.21127	-0.74342
H	2.17157	-4.26135	-0.01089

H	2.00264	-0.43848	-1.58442
H	5.50295	0.57899	0.78669
H	4.82967	-1.13328	2.49088
H	2.75256	-2.51330	2.13564
H	2.54231	1.50160	-2.52740
H	4.13547	2.02921	-3.19281
H	3.67661	0.28678	-3.22087

D^{OAc} (R = o-OMe)

SCF = -1513.34988993
H(0 K) = -1512.860407
H(298 K) = -1512.825507
G(298 K) = -1512.927847
BP86 (D3) = -1513.44856063
SCF (MeOH) = -1513.36958189
SCF (DCM) = -1513.36656887
SCF (BS2) = -1513.43664919
Lowest Frequencies = 20.0861cm⁻¹,
21.2629cm⁻¹

62

C	3.73909	1.89298	-0.87318
C	2.75354	1.35681	-0.01389
C	2.89133	0.08687	0.54831
C	4.03369	-0.68065	0.23529
C	5.03509	-0.16276	-0.61203
C	4.87416	1.12453	-1.15364
N	1.63604	2.18999	0.32282
N	0.30235	1.82007	0.31022
C	-0.38654	2.94798	0.59403
C	0.48235	4.03914	0.80386
C	1.75609	3.52355	0.62487
Ru	-0.78607	-0.00283	-0.21326
O	0.22460	-0.88527	1.39082
C	0.27094	-2.18522	1.63394
C	0.98558	-2.48938	2.95627
C	-2.21730	0.51025	-1.82036
C	-2.60880	-0.76774	-1.26682
C	-1.63076	-1.80150	-1.18055
C	-0.28510	-1.58239	-1.65337
C	0.10143	-0.35371	-2.26169
C	-0.88799	0.70263	-2.28986
C	-4.03916	-0.95957	-0.78070
C	-4.92345	-1.32328	-1.99986
C	1.47548	-0.15576	-2.84975
O	-1.96603	0.46381	1.46596
C	-2.97619	1.29950	1.51214
C	-3.62934	1.34442	2.89848
C	-4.18788	-1.99817	0.34493
O	-3.38259	2.04115	0.58981
O	-0.15723	-3.09916	0.91058
H	-2.91149	1.35169	-1.76883
H	-1.83754	-2.72749	-0.64486
H	0.45785	-2.36377	-1.47456
H	-0.58169	1.70148	-2.62008
H	-4.37081	0.02258	-0.39914
H	-3.50622	-1.77703	1.18139
H	-5.22344	-1.98864	0.72508
H	-3.98090	-3.02270	-0.01164
H	-5.97938	-1.40434	-1.69003
H	-4.85977	-0.56049	-2.79441
H	-4.62001	-2.29324	-2.43229

H	2.22753	-0.77637	-2.33847
H	1.46663	-0.44060	-3.91875
H	1.79920	0.89466	-2.78625
H	-3.67750	0.34125	3.34892
H	-4.63440	1.78483	2.82566
H	-3.01578	1.97580	3.56454
H	0.68066	-1.78294	3.74366
H	0.77222	-3.52310	3.26437
H	2.07471	-2.38214	2.80791
H	-1.47824	2.91037	0.59595
H	0.21198	5.05983	1.06344
H	2.74268	3.97182	0.71611
H	2.10565	-0.31434	1.19809
O	4.07701	-1.91690	0.82450
H	5.92858	-0.74319	-0.85264
H	5.64627	1.52559	-1.81797
H	3.60349	2.88125	-1.32092
C	5.22126	-2.73564	0.56849
H	5.05315	-3.66566	1.12924
H	5.32060	-2.97173	-0.50796
H	6.15297	-2.25560	0.92368

E (R = o-OMe)

SCF	=	-1284.67892973
H(0 K)	=	-1284.238297
H(298 K)	=	-1284.209025
G(298 K)	=	-1284.299040
BP86 (D3)	=	-1284.75835225
SCF (MeOH)	=	-1284.73262147
SCF (DCM)	=	-1284.72781943
SCF (BS2)	=	-1284.68525365
Lowest Frequencies = 20.0953cm ⁻¹ , 31.3606cm ⁻¹		

55

C	2.50987	0.36706	0.46977
C	1.84103	1.59311	0.38153
C	2.27655	2.62175	-0.47633
C	3.41889	2.39519	-1.25656
C	4.10466	1.17038	-1.20465
C	3.64473	0.14932	-0.34393
N	0.70517	1.84468	1.22367
N	-0.38814	1.01400	1.30974
C	-1.20348	1.56771	2.23957
C	-0.64389	2.75312	2.75213
C	0.56971	2.89604	2.08838
Ru	-0.89215	-0.65918	0.09446
O	0.22014	-1.79018	1.54726
C	-0.80518	-1.84541	2.32902
C	-0.74135	-2.47555	3.68727
C	-1.40478	-2.23869	-1.35460
C	-2.49099	-1.31986	-1.21894
C	-2.34438	0.09741	-1.44646
C	-1.02179	0.55310	-1.75154
C	0.09058	-0.34278	-1.86817
C	-0.08394	-1.75333	-1.65605
C	-3.56106	1.01025	-1.35978
C	-4.36571	0.89532	-2.67989
C	1.09076	-2.69443	-1.69267
O	-1.88707	-1.30197	1.87607
C	-3.22847	2.47841	-1.04184
H	-1.06055	3.40875	3.51288

H	-0.48486	-1.70505	4.43534
H	-1.71913	-2.90134	3.95666
H	0.03747	-3.25145	3.71224
H	-4.19571	0.61462	-0.54278
H	1.73214	3.56855	-0.52809
H	3.78029	3.18196	-1.92545
O	4.21743	-1.08350	-0.22071
H	4.98939	1.02192	-1.82741
H	1.36688	3.63031	2.18316
H	2.17502	-0.41703	1.15400
H	-1.55329	-3.29602	-1.11854
H	1.09304	0.05802	-2.03559
H	-3.45473	-1.69423	-0.85631
H	-0.83007	1.62802	-1.81158
H	-5.28735	1.49641	-2.61326
H	-3.77589	1.27001	-3.53421
H	-4.65534	-0.14648	-2.89616
H	-4.16131	3.04782	-0.90193
H	-2.63089	2.57631	-0.12004
H	-2.67987	2.96161	-1.86958
H	0.91059	-3.58412	-1.07036
H	1.24977	-3.03356	-2.73287
H	2.01495	-2.20655	-1.34604
H	-2.14367	1.07561	2.48046
C	5.45100	-1.32516	-0.92108
H	5.75497	-2.34182	-0.63818
H	5.31138	-1.27439	-2.01634
H	6.23154	-0.60728	-0.61219

TS (E-F) (R = o-OMe)

SCF	=	-1284.64904838
H(0 K)	=	-1284.209934
H(298 K)	=	-1284.181127
G(298 K)	=	-1284.270216
BP86 (D3)	=	-1284.73000222
SCF (MeOH)	=	-1284.70740557
SCF (DCM)	=	-1284.70190825
SCF (BS2)	=	-1284.65537879
Lowest Frequencies = -110.2600cm ⁻¹ , 8.9672cm ⁻¹		

55

C	1.22277	-1.29495	0.25099
C	1.88947	-0.62650	1.29746
C	3.28911	-0.59992	1.39753
C	4.03377	-1.27932	0.42104
C	3.41223	-1.93620	-0.65237
C	2.00427	-1.93505	-0.75066
N	1.08934	0.07266	2.24153
N	-0.10155	0.62101	1.83715
C	-0.63536	1.21491	2.92294
C	0.22208	1.06546	4.03474
C	1.30792	0.33330	3.56893
Ru	-0.87047	0.26142	-0.09808
O	-2.41059	-0.55047	1.08758
C	-2.41350	-1.85701	0.95118
C	-3.47711	-2.60379	1.73273
C	-2.38691	1.51263	-0.96260
C	-1.26175	2.31688	-0.58547
C	0.06171	2.07928	-1.12719
C	0.21208	0.93253	-1.95080
C	-0.91404	0.09226	-2.29528

C	-2.23722	0.38953	-1.86524
C	1.19763	3.02478	-0.76488
C	0.98782	4.35862	-1.52923
C	-3.41190	-0.48018	-2.22469
C	2.60307	2.45875	-1.02434
O	-1.57565	-2.44632	0.22742
H	0.06270	1.43069	5.04644
H	-2.99339	-3.14038	2.56645
H	-4.24095	-1.92668	2.13950
H	-3.94420	-3.36149	1.08498
H	1.09985	3.23966	0.31762
H	3.78640	-0.04297	2.19544
H	5.12605	-1.27611	0.48309
O	1.30201	-2.53698	-1.74678
H	4.02462	-2.44484	-1.39965
H	2.19463	-0.04433	4.07268
H	0.15325	-1.62552	0.32896
H	-3.35554	1.68743	-0.48476
H	-0.72569	-0.84194	-2.83182
H	-1.40155	3.11588	0.15065
H	1.20985	0.62713	-2.27245
H	1.76047	5.08575	-1.23072
H	1.06852	4.20340	-2.61864
H	0.00256	4.80773	-1.32051
H	3.36139	3.17033	-0.66007
H	2.76693	1.49766	-0.50915
H	2.78829	2.31555	-2.10342
H	-4.12170	-0.55417	-1.38600
H	-3.94959	-0.03871	-3.08318
H	-3.08824	-1.49385	-2.50378
H	-1.60942	1.69406	2.85238
C	2.01869	-3.38913	-2.66260
H	1.25014	-3.84058	-3.30370
H	2.72475	-2.80951	-3.28405
H	2.56058	-4.18341	-2.12062

F (R = o-OMe)

SCF = -1284.67494589
H(0 K) = -1284.234981
H(298 K) = -1284.205652
G(298 K) = -1284.295371
BP86 (D3) = -1284.75706875
SCF (MeOH) = -1284.72870683
SCF (DCM) = -1284.72398395
SCF (BS2) = -1284.68038648
Lowest Frequencies = 17.6434cm⁻¹,
30.8560cm⁻¹

55

C	-0.94103	-0.85826	-0.38286
C	-1.38314	-1.64569	0.71727
C	-2.20099	-2.78180	0.61416
C	-2.61363	-3.16892	-0.66568
C	-2.21957	-2.44100	-1.79833
C	-1.38649	-1.30788	-1.66380
N	-0.93193	-1.18078	1.98073
N	-0.06899	-0.11645	1.95871
C	0.18935	0.19673	3.24676
C	-0.50860	-0.67847	4.10644
C	-1.21259	-1.54129	3.27023
Ru	0.44076	0.64604	0.10156
O	-1.05758	2.15766	0.53522

C	-2.30326	2.16535	0.35508
C	-3.13521	3.36842	0.70064
C	2.19893	2.13087	0.25136
C	2.58520	0.82283	0.64839
C	2.41823	-0.33355	-0.20599
C	1.76932	-0.10957	-1.46392
C	1.33789	1.19759	-1.87023
C	1.53427	2.32298	-1.00869
C	2.96272	-1.68557	0.23880
C	4.49419	-1.71135	0.00191
C	1.03661	3.68948	-1.40272
C	2.28041	-2.89240	-0.42832
O	-2.97609	1.14593	-0.14582
H	-0.50102	-0.68288	5.19379
H	-3.91479	3.08213	1.42547
H	-2.50532	4.16283	1.11939
H	-3.65229	3.73096	-0.20320
H	2.78973	-1.75240	1.33100
H	-2.50487	-3.35345	1.49500
H	-3.25183	-4.04874	-0.78698
O	-0.97430	-0.56291	-2.74325
H	-2.55737	-2.76872	-2.78366
H	-1.88596	-2.36450	3.49505
H	-2.31510	0.39563	-0.31923
H	2.31907	2.97354	0.93761
H	0.79474	1.31855	-2.80836
H	3.00122	0.67121	1.65105
H	1.53978	-0.95805	-2.11123
H	4.91978	-2.65557	0.37969
H	4.72582	-1.64112	-1.07494
H	5.00608	-0.87982	0.51475
H	2.65318	-3.82601	0.02314
H	1.18520	-2.86511	-0.30519
H	2.50968	-2.94428	-1.50723
H	0.65982	4.24700	-0.53148
H	1.87132	4.26839	-1.83816
H	0.23934	3.62724	-2.15895
H	0.84858	1.02940	3.48289
C	-1.48426	-0.91701	-4.04131
H	-1.06546	-0.17578	-4.73611
H	-1.15545	-1.92738	-4.34444
H	-2.58722	-0.86253	-4.06895

F1 (R = o-OMe)

SCF = -1055.54987401
H(0 K) = -1055.171572
H(298 K) = -1055.147798
G(298 K) = -1055.225073
BP86 (D3) = -1055.61030157
SCF (MeOH) = -1055.60562115
SCF (DCM) = -1055.60069781
SCF (BS2) = -1055.48577597
Lowest Frequencies = 18.2924cm⁻¹,
26.7900cm⁻¹

47

C	1.88851	1.22771	0.15288
C	1.54297	1.09886	1.52441
C	1.62207	-0.18382	2.18582
C	2.21067	-1.28862	1.46852
C	2.55469	-1.15805	0.10462
C	2.32886	0.07865	-0.60609

Ru	0.42005	-0.38231	0.36689	Cl	-0.09369	0.88990	-2.60708
N	-0.77240	-2.00559	-0.12091	C	3.19885	-0.10863	-2.70004
N	-2.07015	-1.69163	-0.42881	C	1.21986	-0.71717	2.88228
C	-2.77480	-2.81735	-0.73157	C	0.01791	-1.65478	3.09294
C	-1.90533	-3.90534	-0.61685	C	-1.31710	-0.36401	-0.14204
C	-0.67062	-3.35359	-0.23517	C	-2.24107	0.61411	0.29026
C	-2.41494	-0.30744	-0.37184	C	-3.61426	0.39119	0.50155
C	-1.34266	0.56205	-0.00031	C	-4.10832	-0.88929	0.24400
C	-1.68905	1.95103	0.06024	C	-3.25082	-1.90149	-0.22194
C	-2.99731	2.40334	-0.23076	C	-1.87930	-1.63849	-0.42114
C	-3.99071	1.48596	-0.58828	N	-1.67356	1.90211	0.47480
C	-3.71510	0.10967	-0.66446	N	-0.33478	2.00605	0.22240
C	1.16944	-0.34233	3.61446	C	-0.01146	3.30600	0.38419
C	2.65899	0.16137	-2.08999	C	-1.15465	4.04603	0.75641
C	1.77479	1.14232	-2.88138	C	-2.19701	3.12159	0.80248
C	4.16286	0.50972	-2.24230	C	2.42892	-1.16647	3.73961
H	-2.14250	-4.95237	-0.78852	H	-1.21629	5.11239	0.96041
H	2.50195	-0.85317	-2.50481	H	0.92408	0.29518	3.22266
H	-4.50312	-0.59455	-0.94370	H	-4.27891	1.19072	0.84190
H	-4.99930	1.84554	-0.81187	H	-5.16971	-1.10764	0.39675
O	-0.68816	2.80906	0.41507	O	-1.00827	-2.60176	-0.89765
H	-3.24822	3.46461	-0.18140	H	-3.66400	-2.89167	-0.42890
H	-3.82701	-2.77605	-1.00342	H	-3.25330	3.24035	1.02824
H	0.28077	-3.84307	-0.03661	H	1.01014	3.63418	0.20693
H	1.08378	1.94190	2.04504	H	1.71075	-2.18632	-1.66141
H	1.68738	2.17005	-0.35893	H	0.84344	-2.46322	0.65138
H	2.88332	-2.03680	-0.45943	H	2.37218	1.46956	1.68141
H	2.27235	-2.26595	1.95694	H	3.43406	1.67435	-0.59235
H	4.43978	0.50834	-3.30939	H	2.15160	-1.21370	4.80696
H	4.37804	1.51317	-1.83653	H	2.77233	-2.17054	3.43352
H	4.80927	-0.21583	-1.72136	H	3.28099	-0.47318	3.63753
H	0.70216	0.93739	-2.72756	H	-0.83398	-1.36467	2.45682
H	1.97343	2.19147	-2.60170	H	0.27882	-2.70391	2.86600
H	1.99168	1.05054	-3.95784	H	-0.30507	-1.62244	4.14726
H	0.83148	-1.36965	3.82186	H	2.32606	0.05949	-3.35804
H	2.01387	-0.12152	4.29414	H	3.87640	0.75342	-2.80068
H	0.35230	0.35434	3.85754	H	3.72467	-1.01746	-3.03876
C	-0.98701	4.21706	0.49545	C	-1.56646	-3.84368	-1.32608
H	-0.04713	4.70054	0.79495	H	-0.72677	-4.42568	-1.73420
H	-1.30893	4.61455	-0.48301	H	-2.02243	-4.40681	-0.48802
H	-1.76228	4.41874	1.25526	H	-2.32591	-3.69687	-2.11702

G (R = o-OMe)

SCF = -1070.82114424
H(0 K) = -1070.442481
H(298 K) = -1070.417065
G(298 K) = -1070.497283
BP86 (D3) = -1070.89359970
SCF (MeOH) = -1070.84173613
SCF (DCM) = -1070.83832512
SCF (BS2) = -1515.99331010
Lowest Frequencies = 21.9102cm⁻¹,
37.7751cm⁻¹

48

C	1.44869	-1.58400	0.42472
C	1.94732	-1.43119	-0.90904
C	2.71691	-0.26763	-1.28155
C	2.91393	0.75324	-0.31511
C	2.30532	0.62687	0.98250
C	1.65242	-0.57566	1.42778
Ru	0.63068	0.28054	-0.38108

D (R = o-Me)

SCF = -1224.70674914
H(0 K) = -1224.271330
H(298 K) = -1224.240616
G(298 K) = -1224.334609
BP86 (D3) = -1224.79484590
SCF (MeOH) = -1224.72750585
SCF (DCM) = -1224.72417493
SCF (BS2) = -1669.92783485
Lowest Frequencies = 12.8022cm⁻¹,
26.5440cm⁻¹

55

C	-2.17484	0.43234	1.79788
C	-2.01253	1.61627	0.99611
C	-0.71110	2.13679	0.70799
C	0.43359	1.42672	1.21507
C	0.25041	0.23666	1.98745
C	-1.05534	-0.26632	2.34451
Ru	-0.85391	-0.03983	0.12653
O	-2.37076	-1.15670	-0.77567
C	-3.62614	-0.75681	-0.90136
O	-4.15165	0.24027	-0.38309
C	-0.60348	3.39671	-0.14421
C	0.80595	3.67662	-0.68693
C	-1.22004	-1.50695	3.18709
N	0.21642	-1.88634	-0.29397
N	1.55556	-2.17695	-0.14868
C	1.77505	-3.52062	-0.31872
C	0.54988	-4.12054	-0.57417
C	-0.38584	-3.06574	-0.55190
C	2.60506	-1.21075	0.01295
C	3.52167	-1.39610	1.06306
C	4.61363	-0.52033	1.16982
C	4.78011	0.51659	0.24074
C	3.86259	0.70068	-0.81742
C	2.76339	-0.17411	-0.92237
C	4.08152	1.78514	-1.85144
Cl	-0.38936	0.57637	-2.17453
C	-1.13352	4.60301	0.67026
C	-4.42268	-1.67996	-1.83077
H	-2.89740	2.03710	0.51573
H	1.44403	1.73621	0.94320
H	1.13624	-0.33741	2.27992
H	-3.18117	0.01759	1.89737
H	-1.27370	3.23652	-1.00973
H	1.17163	2.82054	-1.27499
H	0.78096	4.55951	-1.34773
H	1.52172	3.89548	0.12666
H	-1.12174	5.51341	0.04706
H	-2.16712	4.44230	1.01864
H	-0.50076	4.79110	1.55601
H	-0.40190	-2.22417	3.01002
H	-1.21320	-1.24828	4.26231
H	-2.17486	-2.01117	2.96845
H	-4.15374	-1.44636	-2.87519
H	-5.50030	-1.51161	-1.69257
H	-4.17776	-2.73991	-1.65612
H	-1.46206	-3.05389	-0.71076
H	0.35759	-5.17355	-0.76595
H	2.78889	-3.91356	-0.28558
H	2.01541	-0.05049	-1.71503

H	5.63882	1.19172	0.33075
H	5.33381	-0.64884	1.98420
H	3.37602	-2.21075	1.77958
H	4.37254	2.73982	-1.38124
H	4.89499	1.50544	-2.54559
H	3.17524	1.95594	-2.45274

D^{OAc} (R = o-Me)

SCF = -1438.14282066
H(0 K) = -1437.658091
H(298 K) = -1437.623956
G(298 K) = -1437.724973
BP86 (D3) = -1438.24155962
SCF (MeOH) = -1438.15972169
SCF (DCM) = -1438.15715970
SCF (BS2) = -1438.20428545
Lowest Frequencies = 19.2790cm⁻¹,
27.2279cm⁻¹

61

C	4.12541	1.24053	-0.75852
C	3.03322	0.89026	0.06055
C	2.94059	-0.38469	0.63343
C	3.93344	-1.35308	0.37611
C	5.02613	-0.99888	-0.44204
C	5.12565	0.28812	-0.99496
N	2.04034	1.89180	0.32421
N	0.67123	1.72913	0.19620
C	0.14268	2.96089	0.36666
C	1.14843	3.91793	0.61529
C	2.33763	3.20643	0.58103
Ru	-0.62111	0.02646	-0.21989
O	0.06300	-0.74779	1.60663
C	0.16339	-2.02597	1.91593
C	0.35774	-2.23209	3.42346
C	-2.00553	0.38822	-1.89420
C	-2.41304	-0.83124	-1.22289
C	-1.43788	-1.85123	-1.03215
C	-0.08624	-1.68769	-1.51559
C	0.30737	-0.51415	-2.21611
C	-0.67527	0.53864	-2.36631
C	-3.84728	-0.95734	-0.72616
C	-4.72775	-1.48267	-1.88713
C	1.68929	-0.36657	-2.79987
O	-1.86640	0.86985	1.25655
C	-2.76666	1.81082	1.09190
C	-3.54015	2.10122	2.38420
C	-4.00389	-1.82569	0.53428
O	-2.98814	2.46980	0.05245
O	0.11976	-2.99501	1.13444
H	-2.69007	1.23899	-1.91836
H	-1.65533	-2.72743	-0.42043
H	0.64953	-2.45470	-1.26555
H	-0.36545	1.50039	-2.78863
H	-4.18269	0.06817	-0.48509
H	-3.35114	-1.46435	1.34475
H	-5.04923	-1.78812	0.88485
H	-3.76561	-2.88546	0.33551
H	-5.78674	-1.51168	-1.57868
H	-4.65108	-0.84056	-2.78099
H	-4.42843	-2.50583	-2.17553
H	2.42842	-0.97596	-2.25811

H 1.67642 -0.69998 -3.85464
H 2.02691 0.68141 -2.78719
H -3.82685 1.16650 2.89073
H -4.43035 2.70696 2.16156
H -2.89022 2.66206 3.07783
H -0.58467 -1.99310 3.94490
H 0.63236 -3.27618 3.63109
H 1.12554 -1.54827 3.82001
H -0.93645 3.08841 0.26470
H 1.01815 4.98036 0.80644
H 3.37037 3.50729 0.74138
H 2.07882 -0.60658 1.26805
C 3.82910 -2.72905 0.99930
H 5.80690 -1.73999 -0.64724
H 5.97734 0.54636 -1.63259
H 4.17280 2.23155 -1.21985
H 4.43709 -3.46619 0.44962
H 4.19396 -2.71666 2.04293
H 2.78353 -3.07956 1.02282

E (R = o-Me)

SCF = -1209.46920243
H(0 K) = -1209.033655
H(298 K) = -1209.005046
G(298 K) = -1209.094449
BP86 (D3) = -1209.54641468
SCF (MeOH) = -1209.52312121
SCF (DCM) = -1209.51837491
SCF (BS2) = -1209.45095248
Lowest Frequencies = 11.8620cm⁻¹,
33.6510cm⁻¹

54

C 2.85835 0.04187 0.27022
C 2.22174 1.29261 0.34680
C 2.61311 2.37008 -0.46505
C 3.66313 2.17432 -1.37667
C 4.30068 0.92782 -1.46568
C 3.91531 -0.15354 -0.64144
N 1.18887 1.50922 1.32356
N 0.04550 0.75001 1.41170
C -0.61679 1.19932 2.50532
C 0.09250 2.24658 3.12263
C 1.23668 2.41298 2.34939
Ru -0.75265 -0.61429 -0.01197
O 0.40376 -2.09500 1.03570
C -0.52124 -2.22404 1.92651
C -0.36301 -3.11413 3.12192
C -1.44924 -1.84530 -1.70231
C -2.51012 -1.02010 -1.22706
C -2.39697 0.41889 -1.14153
C -1.13155 0.97604 -1.50204
C -0.04004 0.16475 -1.96429
C -0.18099 -1.25801 -2.05942
C -3.59267 1.24509 -0.68519
C -4.58715 1.37660 -1.86740
C 0.97321 -2.12941 -2.47586
O -1.58716 -1.51803 1.73604
C -3.22553 2.62612 -0.11566
H -0.18377 2.79755 4.01837
H 0.05015 -2.52831 3.96166
H -1.34032 -3.51218 3.43245

H 0.33362 -3.93512 2.89864
H -4.09338 0.66286 0.11299
H 2.10435 3.33554 -0.38433
H 3.98294 2.99992 -2.01956
C 4.65555 -1.47262 -0.69526
H 5.12169 0.79174 -2.17792
H 2.09947 3.06646 2.46070
H 2.53200 -0.77157 0.92573
H -1.56032 -2.93324 -1.69579
H 0.93024 0.62532 -2.16624
H -3.41655 -1.49754 -0.83899
H -0.95616 2.04314 -1.34039
H -5.49262 1.91278 -1.53927
H -4.13679 1.94534 -2.69908
H -4.89853 0.39269 -2.25601
H -4.12896 3.11546 0.28210
H -2.49144 2.55310 0.70440
H -2.81627 3.29353 -0.89451
H 0.96883 -3.08722 -1.93265
H 0.88912 -2.35225 -3.55532
H 1.93583 -1.62560 -2.30358
H -1.56450 0.73888 2.77752
H 4.04817 -2.29860 -0.29269
H 4.95500 -1.72784 -1.72505
H 5.58183 -1.42204 -0.09499

TS(E-F) (R = o-Me)

SCF = -1209.43856255
H(0 K) = -1209.004228
H(298 K) = -1208.976323
G(298 K) = -1209.062862
BP86 (D3) = -1209.51935894
SCF (MeOH) = -1209.49663698
SCF (DCM) = -1209.49129363
SCF (BS2) = -1209.42071760
Lowest Frequencies = -89.7768cm⁻¹,
15.3683cm⁻¹

54

C 0.95403 -1.44837 -0.83968
C 1.85902 -1.52650 0.24359
C 3.22945 -1.73565 0.04087
C 3.69324 -1.88041 -1.27736
C 2.80917 -1.79668 -2.36323
C 1.42845 -1.57978 -2.16791
N 1.34150 -1.35445 1.55633
N 0.24560 -0.55226 1.74307
C -0.04200 -0.59733 3.05921
C 0.88370 -1.42290 3.73344
C 1.74760 -1.89119 2.74998
Ru -0.73711 0.33097 0.10536
O -2.28779 -0.86226 0.87521
C -2.64860 -1.77045 -0.00584
C -3.78117 -2.68424 0.42336
C -1.95288 2.05344 0.50513
C -0.60139 2.31773 0.90641
C 0.50323 2.25556 -0.02798
C 0.19221 1.77937 -1.32930
C -1.16613 1.49467 -1.73953
C -2.26517 1.67226 -0.85772
C 1.89975 2.65367 0.42816
C 1.94320 4.19677 0.58398

C	-3.68025	1.37068	-1.26942
C	3.03034	2.16439	-0.49142
O	-2.07978	-1.88465	-1.11693
H	0.90851	-1.65873	4.79460
H	-3.36598	-3.68266	0.64218
H	-4.29790	-2.31008	1.31795
H	-4.49235	-2.80208	-0.40855
H	2.04691	2.21130	1.43331
H	3.92401	-1.76139	0.88507
H	4.75968	-2.04915	-1.45426
C	0.47740	-1.54487	-3.34265
H	3.19131	-1.92163	-3.38186
H	2.59020	-2.57723	2.79565
H	-0.15126	-1.57943	-0.69279
H	-2.74979	2.06212	1.25472
H	-1.34388	1.06535	-2.72937
H	-0.39550	2.54415	1.95836
H	1.00365	1.56682	-2.02943
H	2.92533	4.50503	0.97787
H	1.79552	4.69384	-0.38994
H	1.16988	4.56743	1.27730
H	4.00520	2.42776	-0.05065
H	3.00975	1.07132	-0.63424
H	2.98398	2.65001	-1.48204
H	-4.23949	0.89833	-0.44673
H	-4.19504	2.31360	-1.52839
H	-3.71172	0.70784	-2.14665
H	-0.90451	-0.05691	3.44329
H	-0.56934	-1.62663	-3.01431
H	0.59682	-0.60929	-3.92029
H	0.69037	-2.37119	-4.04100

F (R = o-Me)

SCF = -1209.45841220
H(0 K) = -1209.023143
H(298 K) = -1208.994845
G(298 K) = -1209.081837
BP86 (D3) = -1209.54018859
SCF (MeOH) = -1209.51339623
SCF (DCM) = -1209.50855381
SCF (BS2) = -1209.43929766
Lowest Frequencies = 19.5693cm⁻¹,
35.8968cm⁻¹

54

C	-0.83413	-0.87915	-0.80369
C	-1.20498	-1.91198	0.11228
C	-1.80890	-3.12217	-0.25532
C	-2.09341	-3.32869	-1.61075
C	-1.79774	-2.32724	-2.54443
C	-1.17737	-1.11157	-2.17182
N	-0.94617	-1.61515	1.47656
N	-0.32087	-0.42186	1.72093
C	-0.24952	-0.28956	3.06390
C	-0.83388	-1.41118	3.68965
C	-1.26830	-2.23421	2.65320
Ru	0.30261	0.66390	0.07693
O	-1.38694	1.95532	0.47576
C	-2.62073	1.81290	0.26911
C	-3.60894	2.86348	0.69041
C	1.88009	2.21939	0.73809
C	2.32143	0.88779	0.96645

C	2.39174	-0.10682	-0.08151
C	1.91430	0.29545	-1.37084
C	1.43193	1.62348	-1.61726
C	1.39197	2.58860	-0.55937
C	3.00092	-1.47290	0.21180
C	4.54357	-1.33161	0.26642
C	0.83901	3.96941	-0.79888
C	2.58430	-2.57676	-0.77566
O	-3.14787	0.75922	-0.32728
H	-0.92970	-1.59766	4.75665
H	-4.35067	2.41811	1.37367
H	-3.09555	3.69748	1.18439
H	-4.16090	3.22657	-0.19229
H	2.65377	-1.76419	1.22277
H	-2.05760	-3.88509	0.48824
H	-2.56514	-4.26135	-1.93271
C	-0.93485	-0.08353	-3.25930
H	-2.05537	-2.48365	-3.59769
H	-1.78353	-3.19128	2.66849
H	-2.39574	0.12787	-0.57733
H	1.82411	2.93188	1.56544
H	1.06156	1.89645	-2.60718
H	2.59665	0.58655	1.98373
H	1.88010	-0.44066	-2.17762
H	5.00179	-2.29533	0.54306
H	4.94553	-1.03464	-0.71764
H	4.86474	-0.57925	1.00619
H	2.97908	-3.54737	-0.43454
H	1.48865	-2.66428	-0.86032
H	3.00037	-2.39924	-1.78306
H	0.27627	4.33316	0.07455
H	1.67512	4.66988	-0.97678
H	0.18256	3.99764	-1.68181
H	0.20497	0.59717	3.50084
H	-1.07649	0.94350	-2.88657
H	0.09089	-0.14943	-3.66635
H	-1.62161	-0.24029	-4.10624

F1 (R = o-Me)

SCF = -980.328581520
H(0 K) = -979.955181
H(298 K) = -979.932292
G(298 K) = -980.008076
BP86 (D3) = -980.387972520
SCF (MeOH) = -980.386595745
SCF (DCM) = -980.381365676
SCF (BS2) = -980.240393073
Lowest Frequencies = 14.8992cm⁻¹,
19.3493cm⁻¹

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C	-1.96867	-1.30326	-0.01700
C	-1.71702	-1.35073	1.37818
C	-1.70792	-0.13785	2.16091
C	-2.15350	1.08413	1.53653
C	-2.41978	1.12393	0.15101
C	-2.24490	-0.04589	-0.67722
Ru	-0.37636	0.14727	0.43915
N	0.82892	1.76341	0.01755
N	2.11892	1.46009	-0.31590
C	2.82799	2.59686	-0.55973
C	1.96575	3.68244	-0.37617

C	0.73140	3.11788	-0.01813	C	3.66042	0.36443	-0.10563
C	2.45844	0.07353	-0.31759	C	3.97862	0.79124	-1.39925
C	1.39480	-0.82859	0.02203	C	2.98509	0.78829	-2.39037
C	1.75813	-2.21650	0.03746	C	1.65057	0.41350	-2.11717
C	3.07700	-2.60891	-0.28014	N	1.95877	-0.54758	1.41288
C	4.06842	-1.67904	-0.61584	N	0.64844	-0.91293	1.53361
C	3.76425	-0.31085	-0.63379	C	0.51940	-1.50227	2.74090
C	-1.33264	-0.16571	3.61990	C	1.76300	-1.50862	3.40921
C	-2.48625	0.04800	-2.17732	C	2.65905	-0.89560	2.53438
C	-1.64059	-0.92793	-3.01607	C	-1.96697	3.82143	1.45616
C	-4.00210	-0.14467	-2.44546	H	1.98354	-1.91313	4.39424
H	2.20819	4.73611	-0.49036	H	-0.33368	2.51660	2.00078
H	-2.21748	1.07969	-2.47596	H	4.43077	0.30491	0.67008
H	4.53534	0.42192	-0.88803	H	5.00249	1.09242	-1.64139
H	5.08002	-2.01494	-0.86136	C	0.67723	0.32885	-3.27617
C	0.79170	-3.31792	0.41106	H	3.25163	1.06738	-3.41693
H	3.32939	-3.67428	-0.26251	H	3.72495	-0.70092	2.61750
H	3.87790	2.56640	-0.84130	H	-0.44554	-1.90021	3.04642
H	-0.21524	3.60074	0.21536	H	-2.24173	-0.02479	-2.53351
H	-1.42322	-2.29050	1.85035	H	-1.08196	2.00902	-1.64434
H	-1.86804	-2.20859	-0.61929	H	-1.82713	0.63770	2.40257
H	-2.63315	2.08216	-0.33366	H	-3.17664	-1.29790	1.53004
H	-2.16048	2.00792	2.12296	H	-1.54405	4.71293	1.95066
H	-4.20903	-0.01368	-3.52027	H	-2.51623	4.15942	0.55961
H	-4.32823	-1.15907	-2.15832	H	-2.69589	3.36149	2.14479
H	-4.61589	0.58283	-1.88897	H	0.98373	2.80258	-0.15457
H	-0.56651	-0.84222	-2.78138	H	-0.26276	3.94723	-0.73591
H	-1.94937	-1.97676	-2.86329	H	0.68654	4.34018	0.71052
H	-1.77688	-0.70867	-4.08723	H	-2.72001	-2.70359	-1.50438
H	-0.90978	0.79656	3.94819	H	-4.07952	-2.56009	-0.35240
H	-2.23623	-0.36138	4.22743	H	-4.18224	-1.77000	-1.95850
H	-0.60478	-0.96321	3.83509	H	1.21769	0.32293	-4.23731
H	1.25464	-4.30790	0.27966	H	0.08435	-0.59775	-3.20274
H	0.48705	-3.23699	1.46874	H	-0.02723	1.18008	-3.30979
H	-0.12025	-3.29385	-0.20560				

G (R = o-Me)

SCF = -995.608936315
H(0 K) = -995.234976
H(298 K) = -995.210578
G(298 K) = -995.288096
BP86 (D3) = -995.681370025
SCF (MeOH) = -995.627323549
SCF (DCM) = -995.624331141
SCF (BS2) = -1440.75652604
Lowest Frequencies = 23.5965cm⁻¹,
41.8937cm⁻¹

47

C	-1.55623	1.31767	-0.94368
C	-2.22146	0.15825	-1.45660
C	-2.85349	-0.78706	-0.56567
C	-2.75932	-0.56693	0.83206
C	-1.98913	0.54494	1.32181
C	-1.45661	1.57176	0.46615
Ru	-0.59310	-0.43981	-0.04482
Cl	-0.09942	-2.62955	-0.93318
C	-3.50619	-2.02436	-1.12474
C	-0.84213	2.83032	1.06739
C	0.20320	3.51149	0.16616
C	1.27435	0.06318	-0.79039
C	2.33140	-0.00530	0.15462

D (R = o-F)

SCF = -1284.62288800
H(0 K) = -1284.222212
H(298 K) = -1284.192589
G(298 K) = -1284.283236
BP86 (D3) = -1284.70752523
SCF (MeOH) = -1284.64419332
SCF (DCM) = -1284.64076112
SCF (BS2) = -1729.87192406
Lowest Frequencies = 20.3699cm-1,
32.2201cm-1

52

C	-2.17199	0.56408	1.77291
C	-1.93411	1.71095	0.93912
C	-0.59951	2.15670	0.66490
C	0.49307	1.40401	1.21575
C	0.23289	0.23852	2.00665
C	-1.10184	-0.18200	2.35791
Ru	-0.85586	-0.02641	0.13756
O	-2.40766	-1.14769	-0.69370
C	-3.64193	-0.69734	-0.86377
O	-4.12076	0.35812	-0.42335
C	-0.40584	3.38081	-0.22340
C	1.03562	3.59442	-0.70986
C	-1.34980	-1.38655	3.23175
N	0.18479	-1.89695	-0.26982
N	1.52460	-2.20443	-0.16436
C	1.72234	-3.55317	-0.32972
C	0.48262	-4.13793	-0.54138
C	-0.43884	-3.07043	-0.49830
C	2.58516	-1.25121	-0.03331
C	3.57276	-1.48407	0.94392
C	4.67425	-0.61754	1.02462
C	4.78796	0.47599	0.15285
C	3.78051	0.67535	-0.80096
C	2.67290	-0.16950	-0.92496
F	3.88787	1.72676	-1.64926
Cl	-0.43139	0.52442	-2.18396
C	-0.92619	4.63372	0.52474
C	-4.47401	-1.64485	-1.73503
H	-2.78685	2.16256	0.42948
H	1.52290	1.66069	0.96386
H	1.08137	-0.37602	2.32807
H	-3.20074	0.20625	1.86420
H	-1.04284	3.21296	-1.11238
H	1.41062	2.71913	-1.26138
H	1.07006	4.45968	-1.39303
H	1.72132	3.81476	0.12891
H	-0.85503	5.51907	-0.12959
H	-1.97873	4.52302	0.83355
H	-0.32457	4.83275	1.42958
H	-0.55732	-2.14270	3.10753
H	-1.37082	-1.09420	4.29811
H	-2.31689	-1.85730	2.99313
H	-4.19803	-1.48500	-2.79146
H	-5.54410	-1.42632	-1.60911
H	-4.27035	-2.70079	-1.49552
H	-1.51930	-3.04585	-0.62453
H	0.27103	-5.18954	-0.71984
H	2.73132	-3.95964	-0.32811
H	1.88878	0.01633	-1.67102

H	5.63492	1.16537	0.19848
H	5.44705	-0.79158	1.77933
H	3.47244	-2.33103	1.62886

D^{OAc} (R = o-F)

SCF = -1498.05838795
H(0 K) = -1497.608358
H(298 K) = -1497.575319
G(298 K) = -1497.673445
BP86 (D3) = -1498.15188087
SCF (MeOH) = -1498.07626655
SCF (DCM) = -1498.07351478
SCF (BS2) = -1498.14850579
Lowest Frequencies = 23.7827cm-1,
24.3480cm-1

58

C	4.12675	1.27184	-0.84572
C	3.04916	0.92486	-0.00388
C	2.99913	-0.32071	0.63685
C	4.04814	-1.21323	0.40078
C	5.14253	-0.90485	-0.41692
C	5.17091	0.35471	-1.03597
N	2.03460	1.90526	0.23424
N	0.66803	1.68107	0.23606
C	0.10626	2.89575	0.42441
C	1.08857	3.89967	0.56009
C	2.29908	3.23796	0.43592
Ru	-0.62785	-0.03288	-0.20057
O	0.26442	-0.96061	1.45056
C	0.15373	-2.24665	1.74951
C	0.87163	-2.58954	3.06024
C	-1.96907	0.57674	-1.85097
C	-2.52617	-0.61212	-1.24396
C	-1.68757	-1.75521	-1.09197
C	-0.32118	-1.73332	-1.55537
C	0.22480	-0.59549	-2.21580
C	-0.62176	0.57491	-2.30931
C	-3.97583	-0.59753	-0.77804
C	-4.88004	-0.89473	-2.00102
C	1.62004	-0.60199	-2.78800
O	-1.74030	0.66012	1.44173
C	-2.64807	1.60760	1.43635
C	-3.29602	1.79832	2.81221
C	-4.27767	-1.56106	0.38304
O	-2.96265	2.34169	0.47293
O	-0.40983	-3.12446	1.07749
H	-2.55132	1.50061	-1.85239
H	-2.01511	-2.62010	-0.51620
H	0.31339	-2.59419	-1.32957
H	-0.18787	1.50926	-2.68265
H	-4.18316	0.43426	-0.44247
H	-3.59573	-1.39097	1.23113
H	-5.31293	-1.40814	0.73198
H	-4.19112	-2.61753	0.07336
H	-5.94222	-0.82603	-1.71045
H	-4.70557	-0.18017	-2.82327
H	-4.69812	-1.91282	-2.38859
H	2.28250	-1.28195	-2.23026
H	1.58973	-0.94342	-3.83972
H	2.07036	0.40287	-2.77659
H	-3.46722	0.83114	3.30904

H	-4.24001	2.35277	2.70863
H	-2.61315	2.38189	3.45391
H	0.70854	-1.81068	3.82084
H	0.52551	-3.56570	3.42889
H	1.95722	-2.65348	2.86695
H	-0.98354	2.97687	0.41629
H	0.92989	4.96031	0.73930
H	3.32769	3.58292	0.51058
H	2.14269	-0.58482	1.27038
F	4.00700	-2.42787	1.00540
H	5.94137	-1.63723	-0.55810
H	6.00969	0.61885	-1.68709
H	4.13556	2.23902	-1.35589

E (R = o-F)

SCF = -1269.38278658
H(0 K) = -1268.981715
H(298 K) = -1268.954290
G(298 K) = -1269.040021
BP86 (D3) = -1269.45715781
SCF (MeOH) = -1269.43826604
SCF (DCM) = -1269.43335535
SCF (BS2) = -1269.39221742
Lowest Frequencies = 23.4185cm⁻¹,
37.4753cm⁻¹

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C	2.71885	-0.08998	0.18178
C	2.25299	1.21664	0.40447
C	2.78449	2.31954	-0.28792
C	3.80806	2.10466	-1.22588
C	4.27793	0.80910	-1.49125
C	3.71687	-0.26240	-0.78339
N	1.23428	1.44521	1.38674
N	0.05213	0.74092	1.43773
C	-0.60556	1.20109	2.52860
C	0.14263	2.20007	3.18040
C	1.30709	2.32632	2.43196
Ru	-0.76441	-0.61686	0.00956
O	-1.64923	-1.48070	1.75531
C	-0.60334	-2.20709	1.97436
C	-0.48400	-3.08747	3.18057
C	-1.59963	-1.83757	-1.62360
C	-2.55355	-0.86175	-1.19932
C	-2.26821	0.55239	-1.19034
C	-0.93880	0.92888	-1.56508
C	0.04442	-0.03087	-1.97310
C	-0.26997	-1.43234	-1.99728
C	-3.35612	1.54504	-0.80065
C	-4.29700	1.75517	-2.01490
C	0.77185	-2.45906	-2.35377
C	-2.82480	2.88944	-0.27417
O	0.33945	-2.10855	1.09719
H	-0.12273	2.74484	4.08320
H	-1.47195	-3.47818	3.46610
H	0.21511	-3.91298	2.98375
H	-0.09306	-2.49648	4.02734
H	-3.94714	1.06698	0.00489
H	2.39825	3.32518	-0.09955
H	4.23414	2.95500	-1.76576
F	4.14290	-1.52004	-1.04423
H	5.06562	0.62094	-2.22510

H	2.19839	2.93392	2.57403
H	2.31856	-0.94555	0.73138
H	-1.84509	-2.90143	-1.56255
H	1.06303	0.29683	-2.19365
H	-3.51286	-1.20435	-0.79587
H	-0.63267	1.97330	-1.45876
H	-5.13093	2.41920	-1.73440
H	-3.75657	2.22372	-2.85541
H	-4.72631	0.80462	-2.37278
H	-3.66577	3.50884	0.07649
H	-2.12798	2.75555	0.57025
H	-2.31218	3.46454	-1.06540
H	0.58778	-3.41347	-1.83721
H	0.73076	-2.65027	-3.44193
H	1.78861	-2.11802	-2.10866
H	-1.57860	0.78186	2.77702

TS (E-F) (R = o-F)

SCF = -1269.35248297
H(0 K) = -1268.953123
H(298 K) = -1268.926131
G(298 K) = -1269.011330
BP86 (D3) = -1269.42779940
SCF (MeOH) = -1269.41223356
SCF (DCM) = -1269.40666578
SCF (BS2) = -1269.36099841
Lowest Frequencies = -119.6278cm⁻¹,
10.2831cm⁻¹

51

C	-1.98104	-0.02693	-0.32200
C	-2.07812	-1.33761	0.19917
C	-2.92218	-2.30378	-0.36684
C	-3.70328	-1.94921	-1.48012
C	-3.61906	-0.66698	-2.04675
C	-2.75474	0.26253	-1.46043
N	-1.22912	-1.65697	1.29064
N	-0.01523	-1.02354	1.39056
C	0.56124	-1.48334	2.51813
C	-0.27481	-2.43435	3.14383
C	-1.40578	-2.52034	2.34059
Ru	0.52939	0.51945	0.04476
O	0.64122	1.54178	1.87222
C	-0.34767	2.40256	1.97655
C	-0.35638	3.24378	3.23835
C	2.17612	1.81942	-0.61467
C	2.65802	0.51290	-0.25600
C	2.14740	-0.67848	-0.89941
C	1.10498	-0.51719	-1.87304
C	0.57810	0.78009	-2.14059
C	1.12367	1.98802	-1.56001
C	2.74075	-2.03065	-0.53644
C	4.09883	-2.17553	-1.27465
C	0.55092	3.33940	-1.89863
C	1.82417	-3.23148	-0.82530
O	-1.23085	2.51326	1.09375
H	-0.08495	-2.97457	4.06825
H	-1.21075	2.93589	3.86428
H	0.57220	3.13314	3.81492
H	-0.51430	4.30008	2.97067
H	2.95110	-2.00511	0.55058
H	-2.95230	-3.32128	0.03158

H -4.36941 -2.69231 -1.92737
 F -2.66422 1.50241 -1.99630
 H -4.21424 -0.38173 -2.91774
 H -2.32458 -3.09307 2.44429
 H -1.60320 0.85260 0.27582
 H 2.53141 2.68690 -0.04994
 H -0.30817 0.87342 -2.77512
 H 3.40085 0.41651 0.54188
 H 0.63462 -1.39267 -2.32509
 H 4.58121 -3.12180 -0.98048
 H 3.95278 -2.19346 -2.36803
 H 4.79096 -1.35186 -1.03439
 H 2.28793 -4.15217 -0.43683
 H 0.83698 -3.12181 -0.34729
 H 1.67514 -3.37972 -1.90895
 H 0.73408 4.06770 -1.09483
 H 1.02351 3.72003 -2.82249
 H -0.53410 3.27804 -2.07006
 H 1.52893 -1.09389 2.82684

F (R = o-F)

SCF = -1269.38321747
 H(0 K) = -1268.982746
 H(298 K) = -1268.955185
 G(298 K) = -1269.041187
 BP86 (D3) = -1269.45897704
 SCF (MeOH) = -1269.43857104
 SCF (DCM) = -1269.43367830
 SCF (BS2) = -1269.39094869
 Lowest Frequencies = 17.8184cm⁻¹,
 31.5196cm⁻¹

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C -0.82765 -0.83936 -0.80828
 C -1.36399 -1.84124 0.05390
 C -2.06796 -2.97159 -0.38686
 C -2.26313 -3.13632 -1.76710
 C -1.76122 -2.19105 -2.67408
 C -1.05513 -2.108713 -2.17708
 N -1.12278 -1.59345 1.42965
 N -0.34782 -0.49689 1.71530
 C -0.28371 -0.41352 3.06127
 C -1.01658 -1.46778 3.64820
 C -1.53788 -2.19883 2.58417
 Ru 0.33344 0.62843 0.10811
 O -1.33296 1.93805 0.58612
 C -2.53972 1.91971 0.22996
 C -3.50151 2.98801 0.66629
 C 1.89684 2.21107 0.71330
 C 2.36341 0.90058 0.98883
 C 2.42403 -0.13195 -0.02508
 C 1.93539 0.21751 -1.32570
 C 1.43368 1.53098 -1.61901
 C 1.39106 2.52946 -0.59711
 C 3.03234 -1.48722 0.31329
 C 4.57699 -1.35771 0.30463
 C 0.81451 3.89323 -0.87534
 C 2.56868 -2.63407 -0.60152
 O -3.06019 0.98558 -0.54660
 H -1.14841 -1.67109 4.70826
 H -4.35265 2.52608 1.19282
 H -3.00018 3.71117 1.32112

H -3.91041 3.49929 -0.22105
 H 2.71947 -1.72420 1.34928
 H -2.45280 -3.71442 0.31727
 H -2.81012 -4.00752 -2.13730
 F -0.57917 -0.18913 -3.08957
 H -1.90081 -2.29902 -3.75295
 H -2.16780 -3.08474 2.56470
 H -2.33152 0.32191 -0.76313
 H 1.83282 2.95240 1.51448
 H 1.02696 1.74800 -2.60820
 H 2.66024 0.64330 2.01197
 H 1.89316 -0.54548 -2.10590
 H 5.03745 -2.31013 0.61455
 H 4.94487 -1.11584 -0.70738
 H 4.93029 -0.57112 0.99230
 H 2.96393 -3.59149 -0.22565
 H 1.46947 -2.70975 -0.64153
 H 2.94772 -2.51342 -1.63146
 H 0.24557 4.27239 -0.01242
 H 1.63926 4.60226 -1.07163
 H 0.16036 3.88420 -1.76036
 H 0.27265 0.39507 3.53070

F1 (R = o-F)

SCF = -1040.25610477
 H(0 K) = -1039.917475
 H(298 K) = -1039.895464
 G(298 K) = -1039.969168
 BP86 (D3) = -1040.31068877
 SCF (MeOH) = -1040.31392768
 SCF (DCM) = -1040.30881354
 SCF (BS2) = -1040.19461039
 Lowest Frequencies = 15.0759cm⁻¹,
 26.9702cm⁻¹

43

C -1.96899 -1.18795 0.30165
 C -1.64539 -0.91838 1.65742
 C -1.61989 0.43971 2.15026
 C -2.09050 1.49451 1.28369
 C -2.40967 1.22412 -0.06453
 C -2.27974 -0.10938 -0.60907
 Ru -0.36575 0.30777 0.36122
 N 1.00421 1.71172 -0.31350
 N 2.26743 1.22628 -0.54943
 C 3.08920 2.22359 -0.97697
 C 2.33925 3.40279 -1.02210
 C 1.04997 3.03762 -0.60213
 C 2.46177 -0.16629 -0.30730
 C 1.29167 -0.85009 0.14403
 C 1.48717 -2.22651 0.38074
 C 2.70610 -2.89315 0.20286
 C 3.81242 -2.15653 -0.24182
 C 3.70329 -0.77730 -0.50372
 C -1.17978 0.73664 3.56001
 C -2.57602 -0.35129 -2.08189
 C -1.77065 -1.50404 -2.70890
 C -4.10299 -0.57702 -2.24249
 H 2.68843 4.38809 -1.32098
 H -2.31301 0.58302 -2.61473
 H 4.57577 -0.21625 -0.84942
 H 4.77345 -2.65736 -0.38798

F	0.43346	-2.97032	0.81157	H	1.00460	-2.58526	1.60581
H	2.77514	-3.96407	0.41035	H	1.11295	-0.25582	2.53003
H	4.13368	2.03745	-1.21711	H	3.01005	1.09872	-1.17037
H	0.15470	3.64609	-0.49005	H	2.81978	-1.20474	-2.10858
H	-1.28758	-1.72712	2.29897	H	3.74266	3.36799	2.08987
H	-1.85199	-2.20267	-0.08257	H	3.85793	1.68120	2.66443
H	-2.64357	2.04955	-0.74450	H	4.38408	2.09749	1.01211
H	-2.07619	2.52657	1.64707	H	0.12692	2.16819	2.01600
H	-4.35091	-0.68781	-3.31086	H	1.33502	1.86561	3.29930
H	-4.42248	-1.49608	-1.72212	H	1.19961	3.48252	2.57991
H	-4.69010	0.26589	-1.84192	H	1.24332	-3.38919	-1.86311
H	-0.68715	-1.38071	-2.54446	H	2.77376	-3.91193	-1.08465
H	-2.07518	-2.48579	-2.30699	H	1.21003	-4.12740	-0.23863
H	-1.95130	-1.53257	-3.79541				
H	-0.75236	1.74757	3.64866				
H	-2.05477	0.68054	4.23474				
H	-0.43744	0.00457	3.91364				

G (R = o-F)

SCF = -1055.53476161
H(0 K) = -1055.195530
H(298 K) = -1055.171827
G(298 K) = -1055.249120
BP86 (D3) = -1055.60168825
SCF (MeOH) = -1055.55469954
SCF (DCM) = -1055.55152858
SCF (BS2) = -1500.70932573
Lowest Frequencies = 9.8717cm⁻¹,
37.1169cm⁻¹

44

C	1.54128	-0.45953	1.54581
C	1.48917	-1.80153	1.02255
C	1.93171	-2.08903	-0.29728
C	2.52890	-1.01477	-1.07156
C	2.61564	0.28979	-0.54526
C	2.08832	0.61172	0.76919
Ru	0.44673	-0.37922	-0.35463
Cl	-0.61654	-1.35153	-2.30604
C	1.78149	-3.46103	-0.90243
C	2.19212	2.04396	1.28041
C	1.14944	2.40437	2.35328
C	-1.42534	-0.46052	0.50183
C	-2.28983	0.62919	0.22209
C	-3.60299	0.75869	0.70458
C	-4.11583	-0.26620	1.51023
C	-3.32187	-1.38547	1.80725
C	-2.01815	-1.45169	1.29956
N	-1.71410	1.60733	-0.62945
N	-0.42321	1.37435	-1.01684
C	-0.09177	2.36750	-1.86791
C	-1.17678	3.25819	-2.01883
C	-2.19501	2.74259	-1.21926
C	3.62972	2.31265	1.78785
H	-1.21703	4.15479	-2.63275
H	2.01403	2.70129	0.40591
H	-4.21762	1.62875	0.45462
H	-5.13476	-0.19748	1.90201
F	-1.30248	-2.57864	1.61423
H	-3.69726	-2.20770	2.42316
H	-3.21036	3.08532	-1.03865
H	0.88926	2.37213	-2.33674

D (R = o-CF₃)

SCF = -1522.42417743
H(0 K) = -1522.010969
H(298 K) = -1521.978493
G(298 K) = -1522.076280
BP86 (D3) = -1522.51533752
SCF (MeOH) = -1522.44573592
SCF (DCM) = -1522.44222410
SCF (BS2) = -1967.75034082
Lowest Frequencies = 22.2460cm⁻¹,
24.9998cm⁻¹

55

C	-2.39523	0.52105	1.89965
C	-2.15154	1.72591	1.14531
C	-0.82857	2.14253	0.81357
C	0.26714	1.29812	1.23125
C	0.01652	0.10433	1.96948
C	-1.32088	-0.30174	2.34492
Ru	-1.19019	0.02506	0.13430
O	-2.85563	-0.62365	-0.94986
C	-4.07380	-0.11057	-0.91277
O	-4.50147	0.76182	-0.14024
C	-0.64122	3.42876	0.01220
C	0.78162	3.64388	-0.52681
C	-1.56144	-1.57064	3.12509
N	-0.56676	-2.00783	-0.38148
N	0.65786	-2.63334	-0.26447
C	0.55915	-3.95465	-0.62880
C	-0.75735	-4.19584	-0.98794
C	-1.41493	-2.95914	-0.82044
C	1.88498	-2.00507	0.11599
C	2.69240	-2.66058	1.06567
C	3.94920	-2.12957	1.39184
C	4.38703	-0.94186	0.79147
C	3.56139	-0.29087	-0.14412
C	2.30936	-0.81678	-0.50269
C	4.01519	1.02908	-0.72727
Cl	-0.40004	0.59107	-2.09116
C	-1.08631	4.63360	0.87860
C	-4.97007	-0.70861	-2.00418
H	-3.01587	2.25100	0.73530
H	1.28821	1.53662	0.92790
H	0.85756	-0.55283	2.21315
H	-3.43091	0.20117	2.03635
H	-1.32596	3.35164	-0.85373
H	1.10392	2.80257	-1.15869
H	0.80550	4.55859	-1.14305
H	1.51144	3.78133	0.29062
H	-1.01400	5.56557	0.29267
H	-2.12713	4.53110	1.22770
H	-0.43766	4.74200	1.76615
H	-0.83665	-2.35480	2.85179
H	-1.45607	-1.37983	4.20919
H	-2.57660	-1.95972	2.94799
H	-4.66601	-0.29678	-2.98152
H	-6.02010	-0.44629	-1.81192
H	-4.85801	-1.80342	-2.06291
H	-2.44529	-2.66303	-1.00425
H	-1.18463	-5.13115	-1.34150
H	1.44589	-4.58448	-0.64202
H	1.66197	-0.32254	-1.24063

H	5.36518	-0.52090	1.03875
H	4.58229	-2.64176	2.12251
H	2.33178	-3.57665	1.54366
F	3.70096	2.06160	0.12378
F	5.36617	1.06678	-0.89964
F	3.43213	1.30015	-1.91977

D^{OAc} (R = o-CF₃)

SCF = -1735.86037006
H(0 K) = -1735.398177
H(298 K) = -1735.362173
G(298 K) = -1735.468553
BP86 (D3) = -1735.96098724
SCF (MeOH) = -1735.87846134
SCF (DCM) = -1735.87567208
SCF (BS2) = -1736.02861753
Lowest Frequencies = 13.5679cm⁻¹,
18.7668cm⁻¹

61

C	3.46803	2.35726	-0.69923
C	2.48219	1.66606	0.03727
C	2.65819	0.31913	0.38107
C	3.82947	-0.33628	-0.03914
C	4.82733	0.34132	-0.75869
C	4.64199	1.69475	-1.08027
N	1.32333	2.39597	0.45419
N	0.00850	1.98630	0.29520
C	-0.74567	3.05565	0.62650
C	0.05897	4.15026	1.01033
C	1.36256	3.69963	0.88772
Ru	-0.93236	0.11484	-0.26276
O	0.10314	-0.64896	1.38868
C	-0.16312	-1.81477	1.96223
C	0.61949	-1.99190	3.26801
C	-2.41829	0.37028	-1.87069
C	-2.59438	-0.96191	-1.32552
C	-1.45368	-1.80892	-1.23179
C	-0.16279	-1.36170	-1.70299
C	0.00333	-0.08483	-2.31323
C	-1.15006	0.78876	-2.35141
C	-3.97922	-1.37540	-0.84559
C	-4.86484	-1.65626	-2.08629
C	1.31653	0.34648	-2.91546
O	-2.21023	0.51743	1.34791
C	-3.29818	1.25255	1.32213
C	-4.05999	1.19603	2.65101
C	-3.98620	-2.56952	0.12291
O	-3.70210	1.96126	0.37459
O	-0.92629	-2.69523	1.54064
H	-3.24167	1.08513	-1.81025
H	-1.51489	-2.74398	-0.67474
H	0.71439	-1.99597	-1.54431
H	-1.02127	1.82275	-2.68918
H	-4.40259	-0.49329	-0.33084
H	-3.27276	-2.42930	0.95005
H	-4.99927	-2.70409	0.53826
H	-3.72075	-3.50785	-0.39713
H	-5.89345	-1.89598	-1.76739
H	-4.91349	-0.78793	-2.76518
H	-4.47738	-2.51754	-2.65888
H	2.16590	-0.19535	-2.47297

H	1.30749	0.13613	-4.00141
H	1.48753	1.42737	-2.78956
H	-4.28541	0.15046	2.91621
H	-4.99040	1.77659	2.57694
H	-3.43177	1.60565	3.45966
H	0.40238	-1.15964	3.95721
H	0.34825	-2.94788	3.73748
H	1.70290	-1.98004	3.06327
H	-1.83196	2.97530	0.54495
H	-0.27331	5.12975	1.34558
H	2.31785	4.17615	1.09556
H	1.87291	-0.19604	0.95417
C	3.98784	-1.80002	0.30728
H	5.73362	-0.18697	-1.06406
H	5.40737	2.23263	-1.64777
H	3.30325	3.40066	-0.98447
F	5.17205	-2.30891	-0.12964
F	3.92593	-2.00894	1.65333
F	2.99251	-2.55342	-0.25448

E (R = o-CF₃)

SCF = -1507.18488926
H(0 K) = -1506.771347
H(298 K) = -1506.741007
G(298 K) = -1506.834061
BP86 (D3) = -1507.26521841
SCF (MeOH) = -1507.24126413
SCF (DCM) = -1507.23618099
SCF (BS2) = -1507.27194202
Lowest Frequencies = 17.8691cm⁻¹,
28.4001cm⁻¹

54

C	1.11184	2.04429	-0.95198
C	2.47535	1.63813	-1.02348
C	2.84915	0.38698	-1.63791
C	1.87952	-0.47515	-2.23407
C	0.49519	-0.06907	-2.14343
C	0.11889	1.14618	-1.50925
Ru	1.34684	-0.02296	-0.10588
O	2.62989	-0.25475	1.58463
C	1.69879	0.12516	2.39626
O	0.58626	0.47997	1.84456
C	2.27196	-1.77739	-2.88343
C	0.65325	3.33785	-0.29670
C	0.36580	4.37245	-1.41725
N	0.77904	-2.01653	0.40141
N	-0.43740	-2.64999	0.26270
C	-0.32374	-3.97231	0.60326
C	0.99582	-4.20967	0.96721
C	1.64287	-2.96654	0.83018
C	-1.64050	-1.98602	-0.14228
C	-2.01410	-0.77797	0.46535
C	-3.20172	-0.15387	0.04927
C	-4.02708	-0.74641	-0.92196
C	-3.65264	-1.97123	-1.49578
C	-2.45006	-2.59015	-1.12311
C	1.89073	0.12890	3.88210
C	1.62956	3.90573	0.74677
H	2.38439	-1.62893	-3.97268
H	1.50610	-2.55390	-2.73055
H	1.42837	-5.14962	1.30130

H	1.24922	0.89073	4.34844
H	1.60509	-0.85695	4.28919
H	2.94713	0.30834	4.13028
H	3.23257	-2.15016	-2.49537
H	-2.13780	-3.52926	-1.59017
H	-4.29238	-2.44098	-2.24817
C	-3.53842	1.21002	0.61347
H	-4.95695	-0.25488	-1.21898
H	-1.19993	-4.61727	0.59698
H	-1.39589	-0.33666	1.25146
H	3.24470	2.22873	-0.52025
H	-0.94033	1.38396	-1.37638
H	3.89353	0.06219	-1.59025
H	-0.28567	-0.75281	-2.48987
H	-0.30551	3.11180	0.20642
H	2.67952	-2.69372	1.01818
H	-0.04148	5.29549	-0.97369
H	1.29049	4.63335	-1.96002
H	-0.36786	3.99678	-2.14968
H	1.17738	4.78428	1.23404
H	1.86317	3.16933	1.53287
H	2.57444	4.24415	0.28673
F	-2.85929	2.18729	-0.08729
F	-4.85591	1.49661	0.51581
F	-3.16444	1.33061	1.91117

TS(E-F) (R = o-CF₃)

SCF = -1507.15253661
H(0 K) = -1506.740656
H(298 K) = -1506.710665
G(298 K) = -1506.802762
BP86 (D3) = -1507.23519231
SCF (MeOH) = -1507.21422114
SCF (DCM) = -1507.20827598
SCF (BS2) = -1507.23864032
Lowest Frequencies = -76.8064cm⁻¹,
24.6862cm⁻¹

54

C	1.96664	-1.35398	-0.88580
C	1.23063	-2.57073	-0.87883
C	-0.04225	-2.67545	-1.54290
C	-0.56517	-1.58626	-2.34584
C	0.18111	-0.36918	-2.38196
C	1.37232	-0.24491	-1.60483
Ru	-0.17147	-0.99700	-0.23633
O	-0.29664	-2.01468	1.52289
C	-0.56041	-1.33237	2.64022
O	-0.66287	-0.09693	2.68487
C	-1.87355	-1.73521	-3.07332
C	3.29098	-1.16500	-0.16016
C	4.44093	-1.31658	-1.19011
N	-2.20778	-0.50728	0.10503
N	-2.67868	0.77962	0.04959
C	-4.02120	0.80799	0.32328
C	-4.42896	-0.50008	0.55524
C	-3.26468	-1.28549	0.41395
C	-1.77791	1.85785	-0.18275
C	-0.47969	1.76158	0.35858
C	0.42229	2.81496	0.12006
C	0.03072	3.94276	-0.62321
C	-1.27101	4.01777	-1.14230

C -2.18319 2.97032 -0.93666
 C -0.69873 -2.21967 3.86418
 C 3.48443 -2.10537 1.04207
 H -1.68787 -2.21835 -4.05008
 H -2.35019 -0.76163 -3.26261
 H -5.43006 -0.83995 0.80935
 H -0.94932 -1.60653 4.73994
 H -1.47615 -2.98376 3.70217
 H 0.24779 -2.75468 4.04742
 H -2.57753 -2.37425 -2.51745
 H -3.18786 3.01407 -1.36743
 H -1.57714 4.89347 -1.72146
 C 1.83501 2.75140 0.66250
 H 0.73430 4.76512 -0.77972
 H -4.56010 1.75175 0.36838
 H -0.27129 0.98953 1.13608
 H 1.54903 -3.39181 -0.23112
 H 1.84994 0.73589 -1.52048
 H -0.63130 -3.59141 -1.43256
 H -0.22513 0.50463 -2.89833
 H 3.30353 -0.12289 0.20768
 H -3.12749 -2.35925 0.52681
 H 5.40731 -1.11638 -0.69947
 H 4.47173 -2.34119 -1.59900
 H 4.33749 -0.61316 -2.03322
 H 4.40085 -1.82558 1.58560
 H 2.63800 -2.04686 1.74605
 H 3.60693 -3.15644 0.72627
 F 2.72630 2.50497 -0.36237
 F 2.21057 3.91383 1.23671
 F 1.99652 1.74985 1.56822

F (R = o-CF3)

SCF = -1507.17899685
 H(0 K) = -1506.766107
 H(298 K) = -1506.735820
 G(298 K) = -1506.827185
 BP86 (D3) = -1507.26486154
 SCF (MeOH) = -1507.23457381
 SCF (DCM) = -1507.22965638
 SCF (BS2) = -1507.26217904
 Lowest Frequencies = 21.1991cm⁻¹,
 38.7535cm⁻¹

54

C 0.78742 0.98201 -0.19176
 C 0.40048 2.17731 0.49201
 C 0.92991 3.45190 0.23984
 C 1.93617 3.57901 -0.72358
 C 2.41352 2.43740 -1.37901
 C 1.86009 1.16667 -1.11565
 N -0.56750 1.99090 1.51331
 N -1.03702 0.71323 1.66434
 C -1.85112 0.72551 2.74207
 C -1.90566 2.02541 3.29023
 C -1.07766 2.80572 2.48818
 Ru -0.46182 -0.66599 0.23891
 O 0.80797 -1.53319 1.75834
 C 1.85643 -1.11735 2.31550
 C 2.54137 -1.91182 3.38984
 C -1.87426 -2.48215 0.26594
 C -2.58134 -1.28769 -0.02501

C -2.21931 -0.41403 -1.12136
 C -1.06304 -0.78640 -1.87717
 C -0.32694 -1.98505 -1.59149
 C -0.70953 -2.82848 -0.50558
 C -3.08959 0.79543 -1.44057
 C -4.37945 0.30919 -2.14986
 C 0.09273 -4.05437 -0.15782
 C -2.38182 1.88031 -2.27064
 O 2.44846 0.02321 2.00286
 H -2.47179 2.35311 4.15891
 H 2.78682 -1.25919 4.24232
 H 1.90693 -2.74611 3.71381
 H 3.49439 -2.30403 2.99510
 H -3.38652 1.23925 -0.46965
 H 0.57163 4.33123 0.78336
 H 2.36550 4.56030 -0.94190
 C 2.48708 0.00277 -1.86083
 H 3.23403 2.52334 -2.09508
 H -0.81102 3.85784 2.54811
 H 1.95058 0.42438 1.22588
 H -2.15749 -3.09271 1.12769
 H 0.56281 -2.22204 -2.17415
 H -3.41169 -0.98863 0.62480
 H -0.70057 -0.12789 -2.66872
 H -5.05456 1.16147 -2.33161
 H -4.14147 -0.14991 -3.12475
 H -4.92820 -0.43468 -1.54821
 H -3.03870 2.75947 -2.36955
 H -1.43895 2.20984 -1.80371
 H -2.15929 1.52930 -3.29342
 H 0.17978 -4.17881 0.93275
 H -0.41956 -4.94813 -0.55816
 H 1.10149 -4.01606 -0.59473
 H -2.34109 -0.19056 3.06538
 F 2.61453 -1.11216 -1.07380
 F 1.74203 -0.37049 -2.95524
 F 3.72505 0.29776 -2.32310

F1 (R = o-CF3)

SCF = -1278.04672256
 H(0 K) = -1277.695530
 H(298 K) = -1277.670851
 G(298 K) = -1277.749974
 BP86 (D3) = -1278.11106308
 SCF (MeOH) = -1278.10758027
 SCF (DCM) = -1278.10181018
 SCF (BS2) = -1278.06156403
 Lowest Frequencies = 21.3164cm⁻¹,
 26.7998cm⁻¹

46

C 0.98599 -1.79791 0.76268
 C 0.62126 -2.33597 -0.50107
 C 1.27377 -1.88323 -1.69732
 C 2.43238 -1.02903 -1.57503
 C 2.82167 -0.53508 -0.31193
 C 2.06302 -0.83998 0.88206
 Ru 0.61465 -0.09383 -0.55349
 N 0.83340 1.94345 -0.67997
 N -0.23474 2.69117 -0.27068
 C 0.03468 4.02064 -0.40522
 C 1.32650 4.13999 -0.92455

C	1.78902	2.82279	-1.07794	C	-1.85207	3.12877	0.40896
C	-1.39651	1.96238	0.11792	C	-3.11025	2.70965	0.84894
C	-1.28924	0.53824	0.03565	C	-3.40173	1.34146	0.86820
C	-2.51125	-0.14329	0.32630	C	-2.43966	0.38217	0.48325
C	-3.67762	0.53933	0.72015	N	0.34379	2.55941	-0.48346
C	-3.68996	1.93518	0.83935	N	1.19688	1.55201	-0.82403
C	-2.54141	2.66427	0.51862	C	2.28235	2.13107	-1.37738
C	0.79490	-2.33204	-3.05295	C	2.12948	3.53479	-1.37971
C	2.48707	-0.25009	2.21866	C	0.88257	3.77485	-0.80724
C	1.33145	-0.04964	3.21599	C	3.42143	-0.69235	3.23529
C	3.59861	-1.15229	2.81772	H	2.83037	4.27622	-1.75579
H	1.85527	5.06152	-1.15551	H	2.88648	0.91946	1.89982
H	2.93381	0.73968	2.00248	H	-1.61104	4.19522	0.35389
H	-2.55023	3.75653	0.57597	H	-3.86261	3.44223	1.15436
H	-4.59758	2.45335	1.16008	C	-2.90816	-1.05726	0.52942
C	-2.65194	-1.64668	0.17157	H	-4.39364	1.00306	1.17498
H	-4.58563	-0.03012	0.92749	H	0.34441	4.70090	-0.62462
H	-0.69209	4.78241	-0.13347	H	3.08968	1.51293	-1.76210
H	2.74307	2.45770	-1.45219	H	-0.74346	-2.98054	0.40353
H	-0.24455	-2.99217	-0.57918	H	-0.05278	-1.40281	2.20981
H	0.38909	-2.04862	1.64050	H	3.52046	-0.38683	-0.05487
H	3.63184	0.19858	-0.24348	H	2.80898	-1.92572	-1.89512
H	2.93848	-0.68109	-2.48054	H	3.86177	-0.03189	4.00199
H	3.96873	-0.71033	3.75729	H	2.95736	-1.55108	3.75155
H	3.20884	-2.15894	3.04630	H	4.24142	-1.07972	2.60692
H	4.45568	-1.26356	2.13296	H	0.48685	1.16448	2.70101
H	0.50577	0.53132	2.77257	H	0.78031	-0.12414	3.90391
H	0.92593	-1.01148	3.57420	H	1.69949	1.39170	3.99624
H	1.69801	0.49337	4.10181	H	0.32126	-2.82402	-2.89239
H	1.00037	-1.57687	-3.82801	H	1.29041	-4.20322	-2.27657
H	1.33052	-3.25719	-3.33817	H	-0.41296	-3.99236	-1.75981
H	-0.28216	-2.55533	-3.04588	F	-4.26032	-1.16003	0.68864
F	-3.92137	-2.07496	0.35929	F	-2.60067	-1.76504	-0.58978
F	-2.28032	-2.06016	-1.08275	F	-2.36216	-1.74832	1.59808
F	-1.87415	-2.33912	1.06670				

G (R = o-CF₃)

SCF = -1293.33134283
H(0 K) = -1292.979668
H(298 K) = -1292.953241
G(298 K) = -1293.035890
BP86 (D3) = -1293.40706729
SCF (MeOH) = -1293.35052128
SCF (DCM) = -1293.34745995
SCF (BS2) = -1738.58214001
Lowest Frequencies = 23.9487cm⁻¹,
37.4812cm⁻¹

47

C	0.61318	-1.54796	1.35748
C	0.20790	-2.45738	0.31766
C	0.98618	-2.60192	-0.86601
C	2.22566	-1.87384	-0.97209
C	2.61809	-0.99673	0.07339
C	1.84735	-0.82795	1.28439
Ru	0.55504	-0.36756	-0.49138
Cl	-0.34980	-0.19842	-2.72923
C	0.51702	-3.46130	-2.01170
C	2.36969	0.07384	2.39617
C	1.26588	0.65894	3.29517
C	-1.12157	0.74562	0.08008
C	-0.91570	2.15592	0.02918

D (R = o-NO2)

SCF = -1389.90770491
H(0 K) = -1389.497086
H(298 K) = -1389.465663
G(298 K) = -1389.561102
BP86 (D3) = -1389.99701438
SCF (MeOH) = -1389.93378689
SCF (DCM) = -1389.92947919
SCF (BS2) = -1835.18675334
Lowest Frequencies = 16.1836cm-1,
29.7397cm-1

54

C	-2.44346	0.71445	1.73665
C	-1.97482	1.86811	1.01533
C	-0.57512	2.12461	0.86267
C	0.35123	1.17395	1.41726
C	-0.13632	0.01322	2.09822
C	-1.54241	-0.22234	2.32722
Ru	-1.10335	0.04654	0.14392
O	-2.73502	-0.69664	-0.92548
C	-3.86932	-0.04151	-1.12263
O	-4.22347	1.01987	-0.58840
C	-0.13982	3.36940	0.09724
C	1.34357	3.39030	-0.30037
C	-2.02935	-1.43239	3.08530
N	-0.39163	-1.95004	-0.33898
N	0.85799	-2.50487	-0.16425
C	0.83547	-3.84703	-0.46080
C	-0.45931	-4.17181	-0.83416
C	-1.18225	-2.96292	-0.74546
C	2.04949	-1.78619	0.17052
C	2.82922	-2.26910	1.24032
C	4.06475	-1.67006	1.53422
C	4.52206	-0.59129	0.76735
C	3.72077	-0.13617	-0.29019
C	2.48267	-0.70453	-0.61601
N	4.23707	0.97951	-1.13022
Cl	-0.32353	0.63982	-2.06575
C	-0.50710	4.62308	0.93073
C	-4.75293	-0.74218	-2.16058
H	-2.71114	2.48115	0.49310
H	1.42377	1.29189	1.25500
H	0.58444	-0.74193	2.43129
H	-3.51792	0.51433	1.73491
H	-0.74017	3.37934	-0.83210
H	1.60357	2.52089	-0.92389
H	1.55495	4.29680	-0.89163
H	2.00384	3.42124	0.58621
H	-0.25977	5.53620	0.36343
H	-1.58128	4.65565	1.17719
H	0.06126	4.64919	1.87757
H	-1.35185	-2.29146	2.95002
H	-2.08345	-1.21495	4.16822
H	-3.03595	-1.73073	2.75154
H	-4.35786	-0.52068	-3.16683
H	-5.78334	-0.36554	-2.09040
H	-4.73851	-1.83651	-2.03342
H	-2.22364	-2.72922	-0.95713
H	-0.83140	-5.14511	-1.14512
H	1.75270	-4.43072	-0.42151
H	1.86895	-0.31580	-1.44003

H	5.47817	-0.10015	0.95903
H	4.66893	-2.04652	2.36469
H	2.46185	-3.11170	1.83444
O	5.31365	1.49754	-0.78508
O	3.56419	1.30916	-2.11882

D^{OAc} (R = o-NO2)

SCF = -1603.34436605
H(0 K) = -1602.884605
H(298 K) = -1602.849684
G(298 K) = -1602.953301
BP86 (D3) = -1603.44325926
SCF (MeOH) = -1603.36630223
SCF (DCM) = -1603.36295651
SCF (BS2) = -1603.46453313
Lowest Frequencies = 17.3830cm-1,
27.6285cm-1

60

C	3.81441	1.93122	-0.66672
C	2.73557	1.34617	0.03172
C	2.77484	-0.00624	0.40729
C	3.92128	-0.73455	0.06604
C	5.02307	-0.17736	-0.59814
C	4.95671	1.17268	-0.96436
N	1.63161	2.19002	0.37433
N	0.29247	1.90513	0.14865
C	-0.36689	3.05915	0.37815
C	0.52054	4.08857	0.76219
C	1.77598	3.50668	0.74679
Ru	-0.78782	0.08129	-0.26799
O	0.14952	-0.56862	1.48434
C	-0.22260	-1.63966	2.17510
C	0.55544	-1.76204	3.48863
C	-2.22887	0.25603	-1.92614
C	-2.49245	-1.00436	-1.25802
C	-1.40372	-1.89853	-1.05446
C	-0.08105	-1.57409	-1.53915
C	0.16787	-0.37376	-2.26643
C	-0.93243	0.55420	-2.41930
C	-3.90838	-1.28703	-0.77342
C	-4.79525	-1.60291	-2.00481
C	1.51211	-0.07092	-2.87906
O	-2.07953	0.74165	1.24173
C	-3.09120	1.56683	1.09734
C	-3.89958	1.71705	2.39066
C	-4.01037	-2.39862	0.28349
O	-3.38800	2.21580	0.07066
O	-1.06967	-2.47942	1.84291
H	-3.00906	1.01976	-1.95349
H	-1.52968	-2.77054	-0.41222
H	0.75226	-2.24242	-1.30072
H	-0.73992	1.53976	-2.85657
H	-4.27788	-0.34156	-0.33463
H	-3.30464	-2.23867	1.11362
H	-5.03775	-2.43609	0.68345
H	-3.79706	-3.38933	-0.15761
H	-5.84178	-1.74669	-1.68674
H	-4.77557	-0.78956	-2.75001
H	-4.46097	-2.53093	-2.50153
H	2.31976	-0.64321	-2.39843
H	1.49561	-0.34334	-3.95085

H 1.75683 1.00161 -2.81459
H -4.14504 0.72870 2.81016
H -4.81768 2.28934 2.19574
H -3.29361 2.24796 3.14456
H 0.53304 -0.81125 4.04484
H 0.12704 -2.56887 4.09965
H 1.61004 -1.99996 3.26748
H -1.45018 3.07866 0.23689
H 0.26961 5.11208 1.02984
H 2.75975 3.89989 0.99245
H 1.93130 -0.45716 0.95331
N 3.97817 -2.17516 0.42851
H 5.89004 -0.80331 -0.81833
H 5.78970 1.63561 -1.50137
H 3.74928 2.97491 -0.98789
O 5.05617 -2.76719 0.24722
O 2.94338 -2.69758 0.87812

E (R = o-NO₂)

SCF = -1374.66557869
H(0 K) = -1374.254611
H(298 K) = -1374.225372
G(298 K) = -1374.316133
BP86 (D3) = -1374.74410842
SCF (MeOH) = -1374.72746638
SCF (DCM) = -1374.72160044
SCF (BS2) = -1374.70533945
Lowest Frequencies = 18.0496cm⁻¹,
29.7842cm⁻¹

53

C 2.35475 0.48802 0.38623
C 1.66905 1.70676 0.51311
C 2.11821 2.86899 -0.14550
C 3.28225 2.81962 -0.92874
C 3.98565 1.61562 -1.07582
C 3.49594 0.47506 -0.42549
N 0.52864 1.81067 1.37303
N -0.52181 0.91935 1.38176
C -1.35085 1.33706 2.36663
C -0.84660 2.49324 2.99326
C 0.34952 2.76419 2.34225
Ru -0.96241 -0.69405 0.05767
O -1.82406 -1.53425 1.82316
C -0.68924 -2.03809 2.18374
C -0.53442 -2.83891 3.43963
C -1.68062 -2.16422 -1.42161
C -2.66635 -1.14156 -1.21609
C -2.38660 0.25361 -1.41271
C -1.02860 0.58412 -1.74745
C -0.02267 -0.41337 -1.92846
C -0.33521 -1.81254 -1.76528
C -3.50138 1.28307 -1.27411
C -4.32428 1.30340 -2.58812
C 0.74067 -2.85718 -1.88507
C -3.01817 2.69685 -0.90582
O 0.29461 -1.83207 1.37306
H -1.28724 3.04609 3.81934
H 0.50909 -2.81317 3.78475
H -1.21277 -2.46500 4.22069
H -0.80361 -3.88963 3.23249
H -4.16690 0.92326 -0.46527

H 1.55705 3.80287 -0.04428
H 3.63505 3.72311 -1.43353
N 4.22254 -0.81263 -0.59863
H 4.89366 1.54023 -1.67819
H 1.10997 3.52339 2.51267
H 2.03279 -0.41952 0.90399
H -1.93000 -3.20820 -1.21289
H 1.00814 -0.11284 -2.13051
H -3.65166 -1.42998 -0.83346
H -0.73218 1.63604 -1.78792
H -5.17665 1.99517 -2.48812
H -3.70575 1.64633 -3.43548
H -4.72339 0.30659 -2.83855
H -3.88750 3.35297 -0.73930
H -2.41198 2.69989 0.01535
H -2.42681 3.15160 -1.72015
H 0.43795 -3.80530 -1.41642
H 0.93823 -3.05234 -2.95508
H 1.68275 -2.52337 -1.42040
H -2.26139 0.77552 2.56557
O 3.66985 -1.83758 -0.15734
O 5.31551 -0.77479 -1.17810

TS(E-F) (R = o-NO₂)

SCF = -1374.63367515
H(0 K) = -1374.224431
H(298 K) = -1374.195510
G(298 K) = -1374.285452
BP86 (D3) = -1374.71455848
SCF (MeOH) = -1374.70008072
SCF (DCM) = -1374.69349377
SCF (BS2) = -1374.67396092
Lowest Frequencies = -75.2459cm⁻¹,
13.4376cm⁻¹

53

C 2.44476 -0.01398 -0.84149
C 2.38088 -1.43112 -0.94936
C 1.31884 -2.07809 -1.67465
C 0.34508 -1.31195 -2.43050
C 0.41177 0.11047 -2.34530
C 1.38950 0.72478 -1.50311
Ru 0.39253 -0.78027 -0.26238
O 0.79143 -1.80661 1.44467
C 0.18988 -1.42986 2.57798
O -0.56160 -0.44714 2.66531
C -0.72020 -2.01046 -3.23076
C 3.50809 0.72863 -0.04752
C 4.55917 1.29198 -1.04009
N -1.61582 -1.41083 0.02785
N -2.68110 -0.54621 0.05008
C -3.84654 -1.23063 0.28160
C -3.52402 -2.57581 0.40584
C -2.12272 -2.64074 0.24566
C -2.46494 0.85387 -0.07723
C -1.28296 1.38900 0.46936
C -1.07639 2.76887 0.31879
C -1.99877 3.61083 -0.31494
C -3.16861 3.04349 -0.84436
C -3.40442 1.66289 -0.74117
C 0.54928 -2.30468 3.76472
C 4.17001 -0.11719 1.05341

H	-0.30585	-2.28452	-4.21823
H	-1.59600	-1.36571	-3.39852
H	-4.20687	-3.39891	0.60215
H	-0.11297	-2.07160	4.60930
H	0.48280	-3.37263	3.50519
H	1.59245	-2.10407	4.06278
H	-1.05127	-2.94069	-2.74258
H	-4.30196	1.22012	-1.18291
H	-3.89753	3.67910	-1.35451
N	0.15822	3.36614	0.88949
H	-1.79251	4.68160	-0.37788
H	-4.79323	-0.70346	0.37645
H	-0.68178	0.79238	1.19545
H	3.05140	-2.04839	-0.34560
H	1.33544	1.80364	-1.33055
H	1.24341	-3.17000	-1.65554
H	-0.36027	0.72166	-2.82042
H	2.99944	1.58605	0.43217
H	-1.45437	-3.49878	0.28603
H	5.30082	1.89382	-0.49034
H	5.09532	0.47609	-1.55489
H	4.10180	1.93949	-1.80712
H	4.83669	0.52031	1.65542
H	3.42224	-0.56210	1.73040
H	4.79229	-0.92722	0.63303
O	0.24981	4.59975	0.89438
O	1.02709	2.57405	1.30843

F (R = o-NO2)

SCF = -1374.67026766
H(0 K) = -1374.259336
H(298 K) = -1374.230384
G(298 K) = -1374.318905
BP86 (D3) = -1374.75393988
SCF (MeOH) = -1374.72839649
SCF (DCM) = -1374.72315362
SCF (BS2) = -1374.70762021
Lowest Frequencies = 17.1802cm⁻¹,
36.5205cm⁻¹

53

C	0.81725	0.95034	-0.58734
C	0.46116	2.27142	-0.18558
C	0.96346	3.44824	-0.76153
C	1.87467	3.35539	-1.82417
C	2.27578	2.09655	-2.27600
C	1.77401	0.94768	-1.63154
N	-0.47968	2.32810	0.87416
N	-0.97316	1.12417	1.29706
C	-1.77953	1.38481	2.34696
C	-1.81307	2.77431	2.59646
C	-0.97520	3.34596	1.64335
Ru	-0.29091	-0.56414	0.31324
O	1.02926	-0.56568	2.01507
C	2.28091	-0.56325	2.16989
C	2.86714	-0.44761	3.55196
C	-1.18997	-2.55909	0.90359
C	-2.23582	-1.70070	0.60475
C	-2.26388	-0.95508	-0.64102
C	-1.21163	-1.20067	-1.57729
C	-0.16737	-2.14952	-1.29468
C	-0.11247	-2.81855	-0.04147

C	-3.42754	-0.01346	-0.92145
C	-4.66032	-0.85654	-1.33743
C	1.00134	-3.78026	0.28610
C	-3.12326	1.07469	-1.96570
O	3.16923	-0.65418	1.20863
H	-2.37374	3.29356	3.37006
H	3.44955	0.48652	3.62127
H	2.07337	-0.44767	4.30910
H	3.56922	-1.27782	3.73036
H	-3.66804	0.48688	0.03712
H	0.64448	4.43072	-0.40109
H	2.27049	4.26119	-2.28990
N	2.33329	-0.31705	-2.12443
H	2.98929	1.98200	-3.09582
H	-0.69481	4.38156	1.46809
H	2.76876	-0.77311	0.27602
H	-1.14682	-3.07269	1.88695
H	0.62604	-2.32160	-2.02448
H	-3.01184	-1.50826	1.35311
H	-1.18326	-0.64038	-2.51477
H	-5.53512	-0.20042	-1.47615
H	-4.47372	-1.38100	-2.29018
H	-4.92147	-1.61240	-0.57800
H	-3.96628	1.78192	-2.02104
H	-2.21472	1.64622	-1.71232
H	-2.99577	0.64849	-2.97600
H	1.27098	-3.73754	1.35351
H	0.66706	-4.81224	0.07378
H	1.89693	-3.58225	-0.32106
H	-2.27732	0.57095	2.86927
O	2.66033	-1.19802	-1.27421
O	2.48367	-0.47449	-3.33763

F1 (R = o-NO2)

SCF = -1145.52967933
H(0 K) = -1145.181148
H(298 K) = -1145.157240
G(298 K) = -1145.235451
BP86 (D3) = -1145.59275022
SCF (MeOH) = -1145.59287921
SCF (DCM) = -1145.58688254
SCF (BS2) = -1145.49975172
Lowest Frequencies = 18.2174cm⁻¹,
25.4979cm⁻¹

45

C	1.71019	-1.26272	0.58264
C	1.44059	-1.87328	-0.67441
C	1.65583	-1.14436	-1.89282
C	2.32990	0.13446	-1.82526
C	2.64929	0.71186	-0.57811
C	2.27265	0.06853	0.66052
Ru	0.45133	0.12463	-0.53795
N	-0.38482	2.01065	-0.51746
N	-1.69545	2.08374	-0.11810
C	-2.14510	3.36741	-0.18929
C	-1.09234	4.16020	-0.65438
C	-0.01743	3.27641	-0.84430
C	-2.31105	0.84834	0.23355
C	-1.44855	-0.28700	0.15112
C	-2.10005	-1.49805	0.46753
C	-3.44804	-1.61819	0.82871

C	-4.22391	-0.45334	0.91067
C	-3.65938	0.79582	0.60730
C	1.23367	-1.71890	-3.21928
C	2.57674	0.74362	1.98912
C	1.56724	0.42452	3.10730
C	4.02158	0.36040	2.40695
H	-1.10931	5.23363	-0.82648
H	2.55559	1.83511	1.80436
H	-4.27525	1.69815	0.65724
H	-5.27544	-0.51775	1.20273
N	-1.32455	-2.75974	0.38749
H	-3.87895	-2.59975	1.04419
H	-3.16334	3.63173	0.08717
H	0.99314	3.47408	-1.19579
H	0.95296	-2.85043	-0.71325
H	1.40385	-1.77645	1.49622
H	3.06926	1.72236	-0.53978
H	2.49789	0.69685	-2.74883
H	4.29117	0.89094	3.33485
H	4.10210	-0.72304	2.59955
H	4.76095	0.62804	1.63400
H	0.53134	0.63612	2.79450
H	1.62388	-0.63030	3.42579
H	1.79180	1.04038	3.99290
H	0.95932	-0.92871	-3.93604
H	2.07926	-2.28472	-3.65409
H	0.38700	-2.41281	-3.10676
O	-1.42164	-3.41305	-0.66231
O	-0.62747	-3.06247	1.36836

C	1.54124	2.43732	-1.46277
C	1.07531	3.76993	-1.51144
C	-0.17413	3.75062	-0.89704
C	4.03983	0.10442	2.47757
H	1.57875	4.63138	-1.94366
H	3.02708	1.43585	1.10868
H	-2.66287	3.63813	0.43781
H	-4.56188	2.41919	1.52027
N	-2.58521	-1.68465	0.89694
H	-4.43772	-0.08855	1.75781
H	-0.90156	4.53934	-0.72463
H	2.45525	2.00031	-1.85714
H	-0.39944	-2.89588	1.02629
H	0.53916	-1.03834	2.43026
H	3.46183	-0.17696	-0.70373
H	2.43185	-1.93403	-2.14374
H	4.56086	0.91368	3.01717
H	3.81021	-0.69586	3.20271
H	4.73637	-0.30905	1.72859
H	0.86125	1.60118	2.42458
H	1.57070	0.54901	3.68357
H	2.29924	2.13139	3.34373
H	0.08863	-3.15282	-2.53644
H	0.99433	-4.45395	-1.69533
H	-0.63696	-3.96631	-1.12583
O	-2.71701	-2.15089	2.04733
O	-2.51930	-2.36300	-0.13968

G (R = o-NO₂)

SCF = -1160.81558412
H(0 K) = -1160.466290
H(298 K) = -1160.440738
G(298 K) = -1160.522316
BP86 (D3) = -1160.89096028
SCF (MeOH) = -1160.83862032
SCF (DCM) = -1160.83507417
SCF (BS2) = -1606.02121786
Lowest Frequencies = 14.8985cm⁻¹,
31.0935cm⁻¹

46

C	0.99781	-1.25779	1.46319
C	0.45000	-2.31826	0.65604
C	0.94036	-2.56917	-0.65390
C	2.07812	-1.79586	-1.11824
C	2.64338	-0.78953	-0.30918
C	2.09568	-0.46829	0.99638
Ru	0.41825	-0.36028	-0.46769
Cl	-0.57849	-0.38539	-2.67422
C	0.30795	-3.59955	-1.55200
C	2.74209	0.63740	1.82275
C	1.80873	1.26213	2.87473
C	-1.38589	0.39914	0.18904
C	-1.52013	1.81463	0.09886
C	-2.62700	2.54985	0.54869
C	-3.69197	1.86775	1.15341
C	-3.63021	0.47574	1.28339
C	-2.51548	-0.21185	0.77320
N	-0.41416	2.46183	-0.50613
N	0.63539	1.65363	-0.84346

3. meta-substituted species

D (R = m-NMe₂)

SCF = -1319.36118745
H(0 K) = -1318.881707
H(298 K) = -1318.848213
G(298 K) = -1318.948362
BP86 (D3) = -1319.45540939
SCF (MeOH) = -1319.38418118
SCF (DCM) = -1319.38057810
SCF (BS2) = -1764.60670729
Lowest Frequencies = 18.7647cm⁻¹,
23.6451cm⁻¹

60

C	-1.35685	0.00598	2.37133
C	-2.34571	0.90601	1.86525
C	-2.00903	1.98713	0.97893
C	-0.65532	2.19812	0.56057
C	0.35283	1.28665	1.02957
C	-0.01201	0.19714	1.88440
Ru	-1.30675	0.08020	0.13541
O	-3.09685	-0.77180	-0.52370
C	-4.24996	-0.12578	-0.58888
O	-4.50709	0.99948	-0.13428
C	-0.35866	3.35815	-0.38383
C	1.02406	3.29789	-1.05139
C	-1.70908	-1.12838	3.30157
N	-0.63514	-1.93827	-0.29951
N	0.64560	-2.44890	-0.32996
C	0.61166	-3.80453	-0.52956
C	-0.71946	-4.18815	-0.62738
C	-1.45478	-2.99403	-0.48621
C	1.84965	-1.67819	-0.23794
C	2.12626	-0.64907	-1.15538
C	3.35004	0.02298	-1.09890
C	4.34811	-0.32388	-0.14047
C	4.04050	-1.36597	0.78154
C	2.81047	-2.02871	0.72785
Cl	-0.99608	0.50077	-2.23383
C	-0.54732	4.69237	0.37980
C	-5.30705	-0.93283	-1.35215
H	3.53464	0.82044	-1.82176
H	-2.82369	2.56417	0.53816
H	1.37837	1.35592	0.66322
H	0.75391	-0.54265	2.14101
H	-3.40473	0.72210	2.06384
H	-1.12103	3.30014	-1.18346
H	1.14776	2.35550	-1.60733
H	1.12680	4.13245	-1.76565
H	1.83962	3.39553	-0.31131
H	-0.40091	5.54435	-0.30593
H	-1.55586	4.77703	0.81706
H	0.18777	4.78695	1.19908
H	-1.06392	-2.00495	3.12698
H	-1.58005	-0.82033	4.35597
H	-2.75754	-1.43950	3.16787
H	-5.10712	-0.84217	-2.43362
H	-6.30916	-0.53350	-1.13959
H	-5.26185	-2.00348	-1.09591
H	-2.52447	-2.79972	-0.52109
H	-1.10791	-5.18982	-0.79601

H	1.54163	-4.36123	-0.62200
H	1.36433	-0.36559	-1.89125
N	5.57203	0.32458	-0.11044
H	4.76203	-1.66090	1.54623
H	2.59188	-2.82798	1.44429
C	5.81868	1.45301	-1.00060
C	6.53652	0.00813	0.93492
H	6.15112	0.23410	1.95024
H	6.82365	-1.06027	0.90960
H	7.44788	0.60197	0.77669
H	6.83847	1.82749	-0.83300
H	5.73965	1.15532	-2.06312
H	5.11175	2.28930	-0.82730

D^{OAc} (R = m-NMe₂)

SCF = -1532.79579557
H(0 K) = -1532.267175
H(298 K) = -1532.230178
G(298 K) = -1532.338077
BP86 (D3) = -1532.89845715
SCF (MeOH) = -1532.81569431
SCF (DCM) = -1532.81275213
SCF (BS2) = -1532.88253036
Lowest Frequencies = 19.4916cm⁻¹,
20.5170cm⁻¹

66

C	3.45686	1.74370	-0.71923
C	2.40138	1.37805	0.13857
C	2.53223	0.23558	0.94370
C	3.69477	-0.53753	0.88053
C	4.78582	-0.17630	0.03757
C	4.63025	0.98675	-0.77027
N	1.25360	2.23367	0.21062
N	-0.06394	1.85175	0.02200
C	-0.77472	3.00128	-0.01758
C	0.06228	4.12336	0.14726
C	1.33892	3.60002	0.29139
Ru	-1.05724	-0.06746	-0.18648
O	-0.29438	-0.46691	1.72190
C	-0.25722	-1.66087	2.28555
C	0.06404	-1.57102	3.78379
C	-2.28482	-0.05632	-2.02287
C	-2.70020	-1.18600	-1.21780
C	-1.70637	-2.10153	-0.76705
C	-0.31935	-1.91560	-1.12162
C	0.09701	-0.84936	-1.96873
C	-0.91565	0.10292	-2.37266
C	-4.17389	-1.34091	-0.86545
C	-4.88641	-2.04890	-2.04496
C	1.52525	-0.71517	-2.43133
O	-2.47674	0.75156	1.13701
C	-3.48551	1.53028	0.82562
C	-4.33618	1.89321	2.04908
C	-4.43243	-2.07392	0.46246
O	-3.75473	2.00106	-0.30165
O	-0.46020	-2.75905	1.74051
H	-3.00736	0.72880	-2.25557
H	-1.94704	-2.88354	-0.04729
H	0.42196	-2.58174	-0.67354
H	-0.60525	1.00931	-2.90400
H	-4.58219	-0.31730	-0.78638

H	-3.88136	-1.60039	1.29029
H	-5.50971	-2.04629	0.69877
H	-4.13761	-3.13688	0.40921
H	-5.97044	-2.11335	-1.84916
H	-4.74392	-1.50568	-2.99458
H	-4.50252	-3.07593	-2.17814
H	2.23003	-1.13248	-1.69545
H	1.65780	-1.26214	-3.38400
H	1.79869	0.33643	-2.60755
H	-4.46008	1.02811	2.71849
H	-5.31555	2.27498	1.72585
H	-3.82139	2.68279	2.62369
H	-0.83996	-1.23929	4.32278
H	0.36459	-2.55761	4.16535
H	0.85075	-0.82605	3.98485
H	-1.85163	2.94721	-0.18780
H	-0.23142	5.17000	0.17267
H	2.30382	4.07089	0.46514
H	1.70006	-0.04597	1.59512
H	3.75770	-1.42621	1.51218
N	5.95471	-0.92332	0.00937
H	5.42295	1.29751	-1.45401
H	3.35264	2.62219	-1.36471
C	6.99153	-0.60636	-0.96458
C	6.01782	-2.19254	0.72562
H	7.84796	-1.27833	-0.81039
H	6.64606	-0.72208	-2.01300
H	7.35448	0.43047	-0.83798
H	5.26988	-2.92620	0.36105
H	7.01856	-2.62892	0.59584
H	5.85355	-2.04900	1.80935

E (R = m-NMe2)

SCF = -1304.12865360
H(0 K) = -1303.648836
H(298 K) = -1303.617537
G(298 K) = -1303.712786
BP86 (D3) = -1304.21218353
SCF (MeOH) = -1304.18076280
SCF (DCM) = -1304.17618768
SCF (BS2) = -1304.13476271
Lowest Frequencies = 14.8009cm⁻¹,
27.2672cm⁻¹

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C	-2.16301	1.25327	0.21001
C	-1.65094	0.58975	1.34061
C	-2.37941	-0.46443	1.92243
C	-3.60400	-0.86118	1.38142
C	-4.14858	-0.20654	0.23324
C	-3.38396	0.85829	-0.34030
N	-0.42739	1.02003	1.95128
N	0.79322	1.00906	1.31319
C	1.68371	1.52502	2.19526
C	1.04770	1.85942	3.40490
C	-0.29130	1.53304	3.21117
Ru	1.27433	0.16578	-0.57475
O	2.74894	1.71617	-0.58140
C	1.90861	2.56241	-1.07980
C	2.26785	4.00165	-1.29668
C	1.60684	-0.92651	-2.46177
C	2.59217	-1.29539	-1.49782

C	2.24852	-1.82011	-0.19609
C	0.85280	-1.89301	0.10758
C	-0.15866	-1.50567	-0.83384
C	0.20726	-1.00357	-2.12698
C	3.35260	-2.25287	0.76035
C	3.86567	-3.65170	0.33275
C	-0.83854	-0.51806	-3.09484
C	2.94249	-2.24340	2.24309
O	0.73737	2.09666	-1.35539
H	1.49930	2.29382	4.29352
H	2.07807	4.56879	-0.36862
H	3.33637	4.09522	-1.54078
H	1.65057	4.43389	-2.09744
H	4.18437	-1.53358	0.62753
H	-1.98615	-0.97432	2.80827
H	-4.14888	-1.67597	1.86159
H	-3.76685	1.40537	-1.20416
N	-5.36209	-0.58217	-0.29519
H	-1.16668	1.65272	3.84599
H	-1.60288	2.08075	-0.23550
H	1.91400	-0.48059	-3.41187
H	-1.20924	-1.50910	-0.53248
H	3.64707	-1.10197	-1.72172
H	0.54322	-2.16534	1.12028
H	4.71290	-3.95370	0.97008
H	3.07196	-4.41127	0.43881
H	4.20944	-3.66186	-0.71503
H	3.81878	-2.46864	2.87191
H	2.54476	-1.26296	2.55456
H	2.18403	-3.01570	2.46204
H	-0.46803	0.32843	-3.69359
H	-1.09995	-1.33725	-3.78953
H	-1.75305	-0.20767	-2.56688
H	2.72648	1.62512	1.90070
C	-5.91871	0.13650	-1.44013
C	-6.14031	-1.64654	0.33755
H	-6.41433	-1.39331	1.37938
H	-7.06822	-1.79927	-0.22953
H	-5.58728	-2.60454	0.34575
H	-6.88384	-0.31167	-1.71146
H	-6.09023	1.20582	-1.21273
H	-5.25557	0.07114	-2.32348

TS (E-F) (R = m-NMe2)

SCF = -1304.09675320
H(0 K) = -1303.618761
H(298 K) = -1303.587791
G(298 K) = -1303.682161
BP86 (D3) = -1304.18151220
SCF (MeOH) = -1304.15336696
SCF (DCM) = -1304.14811099
SCF (BS2) = -1304.10349427
Lowest Frequencies = -82.1801cm⁻¹,
12.8368cm⁻¹

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C	-1.50766	-0.07551	0.70516
C	-1.31401	-1.45276	0.94619
C	-2.32377	-2.36886	0.60977
C	-3.52447	-1.91567	0.06047
C	-3.75873	-0.52587	-0.18846
C	-2.70627	0.38109	0.13856

N	-0.07705	-1.87367	1.50162
N	1.05207	-1.15360	1.21304
C	2.05092	-1.69053	1.94509
C	1.56894	-2.78420	2.69329
C	0.21087	-2.86936	2.39616
Ru	0.91922	0.52779	-0.04991
O	1.68390	1.43101	1.67638
C	0.86853	2.35451	2.14505
C	1.37015	3.08650	3.37791
C	1.86908	2.11521	-1.25167
C	2.70368	0.94396	-1.16816
C	2.23078	-0.34960	-1.60246
C	0.87325	-0.44356	-2.07406
C	0.03897	0.70669	-2.06521
C	0.52239	2.02350	-1.69550
C	3.18056	-1.53821	-1.57209
C	4.15213	-1.40955	-2.77608
C	-0.38736	3.22421	-1.71303
C	2.49040	-2.91291	-1.56859
O	-0.24727	2.59612	1.63149
H	2.13133	-3.41771	3.37498
H	0.84569	2.68833	4.26328
H	2.45201	2.95856	3.52203
H	1.11705	4.15450	3.29844
H	3.78124	-1.44438	-0.64640
H	-2.17147	-3.44185	0.76206
H	-4.29197	-2.65230	-0.18374
H	-2.83883	1.45865	0.02468
N	-4.95259	-0.08499	-0.71084
H	-0.57137	-3.52691	2.76822
H	-0.86123	0.71703	1.16728
H	2.23742	3.06272	-0.84685
H	-1.02456	0.58845	-2.29386
H	3.70102	1.02818	-0.72567
H	0.44752	-1.41491	-2.33383
H	4.88933	-2.22840	-2.74700
H	3.60573	-1.47810	-3.73218
H	4.70296	-0.45479	-2.76354
H	3.24693	-3.70503	-1.44995
H	1.76643	-3.01115	-0.74383
H	1.96856	-3.10795	-2.52170
H	-0.18393	3.88904	-0.86035
H	-0.23680	3.79165	-2.64933
H	-1.44480	2.92260	-1.66836
H	3.04633	-1.25382	1.90540
C	-5.18012	1.34539	-0.90591
C	-6.03756	-1.03238	-0.96811
H	-6.35500	-1.55458	-0.04563
H	-6.90412	-0.48625	-1.36379
H	-5.74594	-1.79146	-1.71771
H	-6.17877	1.49587	-1.33691
H	-5.12893	1.90644	0.04676
H	-4.44203	1.78106	-1.60608

F (R = m-NMe2)

SCF	=	-1304.12166760
H(0 K)	=	-1303.642584
H(298 K)	=	-1303.611228
G(298 K)	=	-1303.705883
BP86 (D3)	=	-1304.20653862
SCF (MeOH)	=	-1304.17499442
SCF (DCM)	=	-1304.17019374

SCF (BS2) = -1304.12671546
 Lowest Frequencies = 15.7531cm⁻¹,
 31.9903cm⁻¹

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C	-0.97564	-0.22313	0.18455
C	-1.16287	-0.77112	1.48233
C	-2.39281	-1.30084	1.90066
C	-3.48550	-1.28812	1.03340
C	-3.37142	-0.74309	-0.28028
C	-2.09700	-0.21448	-0.67283
N	-0.01654	-0.73297	2.31412
N	1.11778	-0.22544	1.73685
C	2.07481	-0.22773	2.69453
C	1.55264	-0.74955	3.89391
C	0.21985	-1.06129	3.61858
Ru	0.95271	0.41702	-0.22905
O	0.62235	2.35720	0.68717
C	-0.42301	3.01737	0.91508
C	-0.35775	4.39034	1.52470
C	2.87505	1.15912	-1.29760
C	3.07968	-0.14775	-0.81262
C	2.15288	-1.22634	-1.10857
C	1.03172	-0.92073	-1.94492
C	0.81672	0.40972	-2.45106
C	1.70208	1.46791	-2.09043
C	2.44202	-2.62476	-0.57715
C	3.54474	-3.27741	-1.44854
C	1.45499	2.88327	-2.54932
C	1.20257	-3.53107	-0.47973
O	-1.64656	2.58813	0.65524
H	2.07383	-0.88524	4.83849
H	-0.81418	4.36310	2.52861
H	0.68390	4.72544	1.60301
H	-0.94746	5.09841	0.92078
H	2.85078	-2.49314	0.44407
H	-2.51395	-1.72474	2.90293
H	-4.43333	-1.70126	1.38133
H	-1.98564	0.19815	-1.67866
N	-4.44877	-0.72612	-1.14021
H	-0.56258	-1.47890	4.24733
H	-1.60259	1.63868	0.31562
H	3.54708	1.96773	-0.99623
H	-0.06419	0.62794	-3.06106
H	3.92684	-0.34972	-0.14818
H	0.29151	-1.69564	-2.15751
H	3.81958	-4.26197	-1.03573
H	3.18913	-3.42933	-2.48226
H	4.45853	-2.66120	-1.49061
H	1.46928	-4.47194	0.02814
H	0.38851	-3.05250	0.08971
H	0.81662	-3.80374	-1.47770
H	1.70669	3.60959	-1.76045
H	2.09488	3.10590	-3.42231
H	0.40731	3.03548	-2.85146
H	3.06979	0.15075	2.47105
C	-4.31846	-0.14585	-2.47267
C	-5.73596	-1.27421	-0.71374
H	-6.14419	-0.73097	0.15955
H	-6.45678	-1.18169	-1.53717
H	-5.65567	-2.34578	-0.45134
H	-5.28154	-0.22159	-2.99504
H	-4.03957	0.92510	-2.42980

H -3.56139 -0.67808 -3.08103

F1 (R = m-NMe2)

SCF = -1074.99282846
H(0 K)= -1074.575900
H(298 K)= -1074.549941
G(298 K)= -1074.633705
BP86 (D3) = -1075.05606016
SCF (MeOH) = -1075.04807063
SCF (DCM) = -1075.04310344
SCF (BS2) = -1074.92875715
Lowest Frequencies = 7.2258cm⁻¹,
18.7745cm⁻¹

51

C -1.20354 -2.04934 0.21892
C -1.06463 -1.71291 1.59170
C -1.90451 -0.69660 2.18519
C -3.00511 -0.17192 1.41000
C -3.13823 -0.50453 0.04666
C -2.18819 -1.38213 -0.60415
Ru -0.96085 0.11852 0.39070
N -0.87421 2.10206 -0.19769
N 0.38766 2.56322 -0.47982
C 0.34450 3.87406 -0.83622
C -0.99471 4.28831 -0.78510
C -1.71612 3.15670 -0.38497
C 1.44150 1.61738 -0.34098
C 1.03969 0.31157 0.06853
C 2.05356 -0.65587 0.21832
C 3.43315 -0.36730 -0.01803
C 3.76478 0.96094 -0.42658
C 2.78033 1.94077 -0.58540
C -1.69046 -0.26127 3.61212
C -2.33608 -1.67051 -2.09183
C -1.01429 -2.00217 -2.80789
C -3.37590 -2.80746 -2.27302
H -1.38015 5.27934 -1.01134
H -2.75380 -0.75276 -2.54922
H 3.07985 2.94629 -0.89814
H 4.80305 1.23390 -0.62233
H 1.77198 -1.66450 0.52953
N 4.40960 -1.32721 0.13880
H 1.24745 4.42130 -1.09767
H -2.78407 3.03015 -0.21921
H -0.24111 -2.13077 2.17802
H -0.48278 -2.72513 -0.24779
H -3.89164 0.00038 -0.56628
H -3.65219 0.58984 1.85513
H -3.54949 -2.98601 -3.34693
H -3.01239 -3.74882 -1.82627
H -4.34441 -2.55968 -1.80790
H -0.24754 -1.23078 -2.62605
H -0.60987 -2.97936 -2.49090
H -1.18778 -2.06563 -3.89418
H -2.02286 0.77616 3.77283
H -2.27771 -0.91185 4.28722
H -0.63191 -0.34169 3.90404
C 4.04967 -2.67906 0.55525
C 5.81123 -0.99832 -0.11799
H 4.96037 -3.28852 0.62725
H 3.55882 -2.68561 1.54770

H 3.37221 -3.16701 -0.17226
H 6.17251 -0.19549 0.55219
H 6.42806 -1.88922 0.06042
H 5.97178 -0.67810 -1.16490

G (R = m-NMe2)

SCF = -1090.26419311
H(0 K)= -1089.846535
H(298 K)= -1089.819101
G(298 K)= -1089.904808
BP86 (D3) = -1090.34014370
SCF (MeOH) = -1090.28671649
SCF (DCM) = -1090.28308266
SCF (BS2) = -1535.43588969
Lowest Frequencies = 8.2958cm⁻¹,
38.7203cm⁻¹

52

C 1.04084 -1.26483 1.59151
C 0.62704 -2.34028 0.72494
C 1.35498 -2.64520 -0.45944
C 2.58660 -1.91848 -0.71963
C 3.00486 -0.88584 0.14077
C 2.21924 -0.50383 1.30212
Ru 0.82612 -0.44941 -0.42596
Cl 0.16597 -0.56424 -2.75786
C 0.88047 -3.69181 -1.43519
C 2.71110 0.63577 2.18749
C 1.60234 1.30955 3.01515
C -1.07463 0.25157 -0.07516
C -1.24523 1.65129 -0.22681
C -2.47426 2.28984 -0.01716
C -3.58969 1.53280 0.35180
C -3.48342 0.12255 0.51259
C -2.21520 -0.48662 0.28033
N -0.08223 2.34392 -0.64354
N 1.04033 1.57671 -0.78736
C 2.01380 2.39578 -1.24440
C 1.51456 3.70692 -1.38263
C 0.17503 3.63840 -0.99391
C 3.85839 0.13459 3.09766
H 2.05226 4.58796 -1.72492
H 3.13049 1.40120 1.50435
H -2.58161 3.37181 -0.15219
H -4.54308 2.04314 0.49887
H -2.12821 -1.57275 0.35213
N -4.59030 -0.63972 0.89723
H -0.60209 4.39717 -0.95322
H 2.99843 1.99171 -1.46702
H -0.30403 -2.87535 0.93342
H 0.41242 -0.99597 2.44397
H 3.89628 -0.30042 -0.11105
H 3.12894 -2.10891 -1.65007
H 4.27635 0.96751 3.68886
H 3.49022 -0.63183 3.80229
H 4.67942 -0.31306 2.51217
H 0.75632 1.61787 2.37928
H 1.21662 0.63765 3.80243
H 2.00118 2.20487 3.52092
H 0.78002 -3.24657 -2.44015
H 1.60149 -4.52749 -1.48607
H -0.10073 -4.09571 -1.14098

C -4.52129 -2.09206 0.79268
 C -5.91141 -0.02355 0.89113
 H -5.94732 0.83775 1.58224
 H -6.22375 0.33170 -0.11427
 H -6.65160 -0.75774 1.24291
 H -5.47383 -2.52191 1.13696
 H -4.33147 -2.44543 -0.24316
 H -3.72269 -2.49688 1.44070

G^{OAc} (R = m-NMe₂)

SCF = -1303.70231601
 H(0 K) = -1303.235836
 H(298 K) = -1303.204790
 G(298 K) = -1303.298582
 BP86 (D3) = -1303.78518338
 SCF (MeOH) = -1303.71921340
 SCF (DCM) = -1303.71650442
 SCF (BS2) = -1303.71641287
 Lowest Frequencies = 15.5395cm⁻¹,
 35.2177cm⁻¹

58

C -0.01677 0.48315 3.89270
 N 0.13487 0.36285 2.54059
 N -1.06926 0.11124 1.94284
 C -1.98834 0.06362 2.93241
 C -1.37099 0.29717 4.17842
 C 1.25489 0.39721 1.67211
 C 0.95647 0.13359 0.31039
 C 2.04418 0.07902 -0.57560
 C 3.38736 0.31828 -0.15781
 C 3.62191 0.59701 1.21799
 C 2.55906 0.63179 2.12615
 Ru -1.02521 -0.20918 -0.10959
 O -0.56813 -2.14623 0.55253
 C -0.05496 -3.08003 -0.22374
 C 0.35472 -4.32541 0.57413
 C -2.62036 1.24240 -0.49984
 C -3.25841 -0.03042 -0.75038
 C -2.63546 -0.97290 -1.60172
 C -1.40204 -0.59810 -2.26706
 C -0.85472 0.70451 -2.09318
 C -1.45963 1.68003 -1.21902
 C -3.19180 -2.36071 -1.79815
 C -0.85590 3.07322 -1.09292
 C -1.35681 3.96828 -2.25191
 O 0.12381 -3.02450 -1.45406
 C -1.10656 3.74243 0.27007
 H 1.85186 -0.19915 -1.61364
 N 4.44133 0.28744 -1.07353
 H -3.02835 -0.14494 2.69166
 H -0.31904 -4.49753 1.42762
 H 0.37288 -5.20544 -0.08576
 H 1.37125 -4.17130 0.97630
 H 4.63337 0.77063 1.58973
 H 2.76551 0.82718 3.18444
 H -1.84287 0.32584 5.15780
 H 0.83435 0.67978 4.53955
 H 0.09552 0.95153 -2.57886
 H -4.16154 -0.30557 -0.19732
 H -3.05239 1.90054 0.26058
 H -0.85349 -1.35466 -2.82964

H 0.23859 2.94736 -1.20715
 H -1.14291 3.51618 -3.23524
 H -2.44827 4.12352 -2.18293
 H -0.86999 4.95844 -2.21813
 H -2.36812 -3.09008 -1.84540
 H -3.87826 -2.64100 -0.98361
 H -3.74888 -2.41251 -2.75201
 H -2.17474 3.98344 0.41771
 H -0.77806 3.09408 1.09871
 H -0.54954 4.69243 0.33285
 C 5.81204 0.31382 -0.58005
 C 4.20670 -0.24989 -2.40943
 H 3.86024 -1.30419 -2.39885
 H 3.44999 0.34870 -2.94848
 H 5.14216 -0.19608 -2.98609
 H 6.50262 0.30952 -1.43655
 H 6.00651 1.23658 -0.00368
 H 6.05936 -0.55265 0.07021

D (R = m-OMe)

SCF = -1299.91576828
H(0 K) = -1299.475416
H(298 K) = -1299.443961
G(298 K) = -1299.538919
BP86 (D3) = -1300.00504310
SCF (MeOH) = -1299.93783194
SCF (DCM) = -1299.93436059
SCF (BS2) = -1745.16188786
Lowest Frequencies = 19.4019cm⁻¹,
25.8928cm⁻¹

56

C	-1.25616	-0.00238	2.35392
C	-2.23227	0.88526	1.80386
C	-1.86911	1.97149	0.93438
C	-0.50030	2.20237	0.58074
C	0.49685	1.30390	1.09568
C	0.10724	0.20765	1.93025
Ru	-1.10307	0.07665	0.12212
O	-2.84726	-0.79509	-0.62418
C	-4.00547	-0.16443	-0.74037
O	-4.29831	0.95462	-0.29270
C	-0.17513	3.36938	-0.34520
C	1.23330	3.32249	-0.95793
C	-1.63508	-1.14223	3.26674
N	-0.39002	-1.93790	-0.27774
N	0.89349	-2.44000	-0.23663
C	0.87963	-3.79971	-0.41429
C	-0.44224	-4.19418	-0.56981
C	-1.19187	-3.00318	-0.48370
C	2.08677	-1.65594	-0.11662
C	2.36686	-0.62799	-1.02976
C	3.58372	0.06652	-0.94224
C	4.52883	-0.27843	0.04800
C	4.23951	-1.31822	0.96040
C	3.02344	-2.00000	0.88011
Cl	-0.68833	0.50397	-2.23056
C	-0.40424	4.69760	0.41800
C	-5.01374	-0.98159	-1.55651
H	3.78682	0.86437	-1.66024
H	-2.66986	2.53886	0.45703
H	1.53819	1.39164	0.78199
H	0.87020	-0.52141	2.22404
H	-3.29675	0.68739	1.95353
H	-0.90502	3.31088	-1.17448
H	1.38409	2.38363	-1.51343
H	1.35790	4.16122	-1.66368
H	2.01839	3.42282	-0.18596
H	-0.23800	5.55454	-0.25688
H	-1.42992	4.77159	0.81552
H	0.29727	4.79324	1.26598
H	-0.97915	-2.01467	3.11274
H	-1.54521	-0.83683	4.32588
H	-2.67638	-1.45854	3.09513
H	-4.76398	-0.88246	-2.62680
H	-6.03011	-0.59694	-1.38982
H	-4.96606	-2.05288	-1.30353
H	-2.26042	-2.81766	-0.56857
H	-0.81519	-5.20148	-0.73961
H	1.81638	-4.35142	-0.45381
H	1.61995	-0.36095	-1.78737

O	5.74530	0.32526	0.21024
H	4.98159	-1.56965	1.72317
H	2.79369	-2.80295	1.58821
C	6.08653	1.38183	-0.69371
H	7.08666	1.72192	-0.38997
H	6.12261	1.02581	-1.74030
H	5.37463	2.22534	-0.62066

D^{OAc} (R = m-OMe)

SCF = -1513.35061399
H(0 K) = -1512.861123
H(298 K) = -1512.826115
G(298 K) = -1512.929274
BP86 (D3) = -1513.44828385
SCF (MeOH) = -1513.36970820
SCF (DCM) = -1513.36688992
SCF (BS2) = -1513.43785410
Lowest Frequencies = 19.1955cm⁻¹,
21.3696cm⁻¹

62

C	3.70309	1.64579	-0.83874
C	2.65797	1.27921	0.03747
C	2.76314	0.11272	0.80631
C	3.90142	-0.70118	0.69224
C	4.95319	-0.33325	-0.17291
C	4.84576	0.85081	-0.93670
N	1.54009	2.16735	0.16479
N	0.20518	1.82242	0.03957
C	-0.47476	2.99065	0.05686
C	0.39967	4.08754	0.19910
C	1.66734	3.52966	0.26584
Ru	-0.85361	-0.06208	-0.18649
O	-0.02235	-0.55417	1.67313
C	-0.01294	-1.76713	2.19777
C	0.37165	-1.74063	3.68317
C	-2.14665	0.05677	-1.97376
C	-2.57570	-1.08410	-1.19282
C	-1.60105	-2.04938	-0.80837
C	-0.22235	-1.90388	-1.21041
C	0.20350	-0.82620	-2.03803
C	-0.78578	0.17707	-2.36918
C	-4.04145	-1.19978	-0.79595
C	-4.81728	-1.83210	-1.97880
C	1.61682	-0.73104	-2.55359
O	-2.18706	0.75070	1.22401
C	-3.18598	1.56740	0.98448
C	-3.97395	1.90623	2.25557
C	-4.28444	-1.97859	0.50853
O	-3.48843	2.08605	-0.11288
O	-0.28467	-2.83659	1.62692
H	-2.84750	0.87387	-2.15676
H	-1.84486	-2.84599	-0.10591
H	0.50830	-2.61304	-0.81375
H	-0.46077	1.08880	-2.88244
H	-4.40848	-0.16637	-0.66209
H	-3.69025	-1.56169	1.33701
H	-5.35180	-1.92200	0.78160
H	-4.03187	-3.04834	0.40144
H	-5.89586	-1.86640	-1.74862
H	-4.68633	-1.25464	-2.90966
H	-4.47595	-2.86549	-2.16703

H 2.33277 -1.20270 -1.86286
H 1.69012 -1.24847 -3.52870
H 1.92578 0.31451 -2.70656
H -4.10862 1.01572 2.88870
H -4.94814 2.34100 1.98885
H -3.40553 2.64585 2.84578
H -0.49985 -1.40297 4.26993
H 0.65635 -2.74877 4.01763
H 1.18781 -1.02647 3.87831
H -1.55986 2.96842 -0.06196
H 0.13580 5.14065 0.25920
H 2.65144 3.97284 0.40044
H 1.93549 -0.15645 1.46997
H 3.96143 -1.60943 1.29646
O 6.10931 -1.04434 -0.34669
H 5.66555 1.11866 -1.60906
H 3.61106 2.54933 -1.44980
C 6.25964 -2.25445 0.40290
H 7.23818 -2.66400 0.11468
H 6.24958 -2.06238 1.49222
H 5.46842 -2.98719 0.15599

E (R = m-OMe)

SCF = -1284.67892678
H(0 K)= -1284.238440
H(298 K)= -1284.209071
G(298 K)= -1284.300118
BP86 (D3) = -1284.75727733
SCF (MeOH) = -1284.73347098
SCF (DCM) = -1284.72861759
SCF (BS2) = -1284.68548427
Lowest Frequencies = 10.7534cm⁻¹,
29.8980cm⁻¹

55

C -2.47669 0.96119 -0.10080
C -1.90675 0.79148 1.17095
C -2.52629 -0.03696 2.12926
C -3.71324 -0.69737 1.81033
C -4.29758 -0.53599 0.52994
C -3.66673 0.29314 -0.42735
N -0.72216 1.51297 1.53860
N 0.47916 1.40114 0.87619
C 1.32113 2.27629 1.47733
C 0.67257 2.94746 2.53066
C -0.62407 2.44331 2.53635
Ru 1.03395 -0.00515 -0.61673
O 2.29171 1.59725 -1.26542
C 1.34152 2.10442 -1.97965
C 1.50881 3.39791 -2.71823
C 1.46850 -1.65664 -2.01170
C 2.51642 -1.53524 -1.05123
C 2.27698 -1.59427 0.37249
C 0.91148 -1.71605 0.77902
C -0.16426 -1.81696 -0.16570
C 0.10021 -1.77583 -1.57474
C 3.45090 -1.52612 1.34118
C 4.13505 -2.91634 1.39405
C -1.02177 -1.80684 -2.57769
C 3.07778 -1.03986 2.75221
O 0.23548 1.43915 -1.99699
H 1.08789 3.70680 3.18882

H 1.26118 4.23749 -2.04532
H 2.55277 3.51855 -3.04327
H 0.82972 3.43631 -3.58222
H 4.17653 -0.80972 0.90869
H -2.07772 -0.15670 3.12062
H -4.21773 -1.33885 2.53784
H -4.10949 0.44704 -1.41400
O -5.45632 -1.21349 0.32876
H -1.49602 2.69018 3.13849
H -1.99155 1.61277 -0.83328
H 1.69068 -1.55037 -3.07717
H -1.19747 -1.84130 0.18984
H 3.53014 -1.31287 -1.40223
H 0.66587 -1.64271 1.84199
H 5.02893 -2.87179 2.03756
H 3.45175 -3.67549 1.81218
H 4.45368 -3.25741 0.39495
H 3.99081 -0.92282 3.35769
H 2.55929 -0.06663 2.72988
H 2.43565 -1.76788 3.27873
H -0.79137 -1.18489 -3.45660
H -1.16901 -2.84558 -2.92592
H -1.96446 -1.45683 -2.13080
H 2.34177 2.36820 1.11115
C -6.12694 -1.05677 -0.93276
H -7.03385 -1.67180 -0.86171
H -6.40869 -0.00308 -1.10874
H -5.50149 -1.42003 -1.76883

TS (E-F) (R = m-OMe)

SCF = -1284.64657780
H(0 K)= -1284.207891
H(298 K)= -1284.178932
G(298 K)= -1284.268441
BP86 (D3) = -1284.72626600
SCF (MeOH) = -1284.70557552
SCF (DCM) = -1284.70005074
SCF (BS2) = -1284.65378513
Lowest Frequencies = -83.7479cm⁻¹,
12.6912cm⁻¹

55

C 1.73182 0.30268 0.50155
C 1.44686 1.67279 0.66913
C 2.33937 2.65266 0.19682
C 3.52667 2.25766 -0.41973
C 3.83628 0.88323 -0.58813
C 2.92545 -0.09411 -0.13434
N 0.22382 2.03068 1.29639
N -0.85375 1.19615 1.15724
C -1.83439 1.70093 1.93304
C -1.39506 2.88536 2.56195
C -0.08022 3.06413 2.14262
Ru -0.66677 -0.56206 0.01045
O -1.19888 -1.38780 1.85787
C -0.26005 -2.18219 2.33347
C -0.59964 -2.85927 3.64985
C -1.57380 -2.31560 -0.97363
C -2.49684 -1.21182 -0.90919
C -2.17476 0.07270 -1.48503
C -0.87455 0.23246 -2.08248
C 0.05360 -0.84346 -2.05757

C -0.28128 -2.15739 -1.54296
 C -3.21712 1.18090 -1.46380
 C -4.26688 0.87465 -2.56614
 C 0.72183 -3.28139 -1.55226
 C -2.64941 2.60133 -1.62598
 O 0.83915 -2.35127 1.75896
 H -1.95654 3.51825 3.24499
 H -0.02652 -2.37135 4.45647
 H -1.67091 -2.79307 3.88481
 H -0.28019 -3.91191 3.61231
 H -3.73217 1.11745 -0.48539
 H 2.10192 3.71594 0.29644
 H 4.24032 2.99929 -0.78856
 H 3.15123 -1.16062 -0.20034
 O 5.02788 0.62521 -1.18295
 H 0.66500 3.81382 2.39858
 H 1.20252 -0.50581 1.07663
 H -1.82469 -3.25065 -0.46364
 H 1.07899 -0.66224 -2.39419
 H -3.44367 -1.33684 -0.37495
 H -0.55839 1.20758 -2.45861
 H -5.06675 1.63229 -2.53641
 H -3.80637 0.90584 -3.56824
 H -4.73117 -0.11612 -2.43236
 H -3.45902 3.33825 -1.50259
 H -1.87206 2.82542 -0.87779
 H -2.22508 2.75711 -2.63312
 H 0.64086 -3.89568 -0.64318
 H 0.54756 -3.92733 -2.43187
 H 1.75106 -2.89717 -1.61676
 H -2.78700 1.18113 2.00742
 C 5.42594 -0.74695 -1.33874
 H 6.41224 -0.71420 -1.82003
 H 5.50831 -1.25305 -0.36014
 H 4.71957 -1.29847 -1.98652

F (R = m-OMe)

SCF = -1284.67232861
 H(0 K) = -1284.232418
 H(298 K) = -1284.203060
 G(298 K) = -1284.292912
 BP86 (D3) = -1284.75215219
 SCF (MeOH) = -1284.72821110
 SCF (DCM) = -1284.72308364
 SCF (BS2) = -1284.67790756
 Lowest Frequencies = 16.8661cm⁻¹,
 29.5735cm⁻¹

55

C -1.13230 -0.43636 0.02538
 C -1.35537 -1.06854 1.27768
 C -2.50719 -1.82322 1.56018
 C -3.48939 -1.95810 0.57976
 C -3.32078 -1.34075 -0.68177
 C -2.15054 -0.58812 -0.95043
 N -0.31929 -0.87808 2.22711
 N 0.77031 -0.17472 1.78388
 C 1.60997 -0.05809 2.83773
 C 1.05901 -0.69946 3.96557
 C -0.16849 -1.21022 3.54383
 Ru 0.70488 0.50778 -0.17438
 O 0.02859 2.35574 0.74451

C -1.12107 2.82880 0.93389
 C -1.31576 4.18023 1.56178
 C 2.58979 1.55977 -1.02553
 C 2.93659 0.27843 -0.55303
 C 2.21484 -0.91104 -0.97018
 C 1.14739 -0.73750 -1.90798
 C 0.78666 0.56675 -2.39922
 C 1.46796 1.72700 -1.92689
 C 2.65746 -2.27299 -0.45030
 C 3.92560 -2.71804 -1.22214
 C 1.06073 3.10821 -2.37457
 C 1.56535 -3.35518 -0.50624
 O -2.24071 2.20305 0.61072
 H 1.49577 -0.78326 4.95781
 H -1.83362 4.06089 2.52833
 H -0.34822 4.67277 1.71854
 H -1.96504 4.80009 0.92263
 H 2.94119 -2.12634 0.61050
 H -2.64589 -2.30485 2.53320
 H -4.39947 -2.53359 0.76582
 H -2.02861 -0.11574 -1.92885
 O -4.34120 -1.53101 -1.56214
 H -0.93271 -1.76942 4.07799
 H -2.01015 1.28991 0.25313
 H 3.10197 2.44466 -0.63707
 H -0.05309 0.67912 -3.09051
 H 3.73528 0.17561 0.18956
 H 0.55578 -1.60325 -2.21495
 H 4.30356 -3.66838 -0.81085
 H 3.69928 -2.87604 -2.29069
 H 4.73613 -1.97328 -1.15254
 H 1.91979 -4.26724 0.00038
 H 0.63649 -3.02691 -0.01077
 H 1.32440 -3.63927 -1.54563
 H 1.13102 3.83377 -1.54897
 H 1.73917 3.45072 -3.17679
 H 0.03435 3.12062 -2.77264
 H 2.54816 0.48175 2.72954
 C -4.24479 -0.93110 -2.86050
 H -5.16698 -1.21392 -3.38582
 H -4.18568 0.17120 -2.79265
 H -3.37237 -1.31726 -3.42002

F1 (R = m-OMe)

SCF = -1055.54477010
 H(0 K) = -1055.166897
 H(298 K) = -1055.142995
 G(298 K) = -1055.221007
 BP86 (D3) = -1055.60303218
 SCF (MeOH) = -1055.60242832
 SCF (DCM) = -1055.59719173
 SCF (BS2) = -1055.48139920
 Lowest Frequencies = 15.1114cm⁻¹,
 22.9976cm⁻¹

47

C -1.35425 -1.95048 0.10046
 C -1.21353 -1.76884 1.50257
 C -1.90546 -0.69271 2.17066
 C -2.88505 0.06874 1.43030
 C -3.02427 -0.11618 0.03988
 C -2.20394 -1.07257 -0.67561

Ru	-0.79295	0.12576	0.46221
N	-0.39335	2.06039	-0.15641
N	0.92675	2.32462	-0.42977
C	1.08788	3.62944	-0.77501
C	-0.17009	4.24411	-0.72351
C	-1.06038	3.23259	-0.33711
C	1.82401	1.22779	-0.28232
C	1.20959	0.00200	0.11976
C	2.06148	-1.10582	0.27709
C	3.45789	-1.01262	0.05934
C	4.02124	0.22080	-0.33765
C	3.19676	1.34638	-0.50826
C	-1.66552	-0.41810	3.63291
C	-2.35831	-1.21187	-2.18349
C	-1.08670	-1.68406	-2.91134
C	-3.55452	-2.15836	-2.46824
H	-0.39772	5.28444	-0.94234
H	-2.62220	-0.20728	-2.56711
H	3.64912	2.29562	-0.81232
H	5.09411	0.31808	-0.51521
H	1.67216	-2.08258	0.58129
O	4.15870	-2.16090	0.25546
H	2.06552	4.03355	-1.02840
H	-2.13602	3.27150	-0.17741
H	-0.48351	-2.36157	2.06124
H	-0.72874	-2.68459	-0.41362
H	-3.67376	0.55126	-0.53573
H	-3.42175	0.87809	1.93408
H	-3.72858	-2.22073	-3.55498
H	-3.34776	-3.17724	-2.09829
H	-4.48476	-1.80398	-1.99407
H	-0.21612	-1.05551	-2.66075
H	-0.84085	-2.73310	-2.67117
H	-1.24466	-1.63462	-4.00069
H	-1.82857	0.64304	3.87809
H	-2.37296	-1.01557	4.23828
H	-0.64489	-0.69906	3.93529
C	5.58104	-2.13077	0.04722
H	5.93135	-3.14952	0.26009
H	5.82782	-1.86746	-0.99736
H	6.07207	-1.42096	0.73743

G (R = m-OMe)

SCF	=	-1070.82047668
H(0 K)	=	-1070.442005
H(298 K)	=	-1070.416475
G(298 K)	=	-1070.497710
BP86 (D3)	=	-1070.89106317
SCF (MeOH)	=	-1070.84267643
SCF (DCM)	=	-1070.83919006
SCF (BS2)	=	-1515.99285944

Lowest Frequencies = 9.3119cm⁻¹,
44.0964cm⁻¹

48

C	1.11296	-1.08425	1.66533
C	0.83155	-2.26318	0.88482
C	1.55980	-2.54239	-0.30552
C	2.66422	-1.66598	-0.65997
C	2.95660	-0.52892	0.11623
C	2.15874	-0.18416	1.28097
Ru	0.72000	-0.44738	-0.39115

Cl	0.03477	-0.80704	-2.69025
C	1.21152	-3.70994	-1.19310
C	2.50912	1.06956	2.07459
C	1.33631	1.64444	2.88841
C	-1.25406	-0.02405	-0.02101
C	-1.65434	1.31777	-0.27180
C	-2.95634	1.78379	-0.05997
C	-3.93560	0.89799	0.41670
C	-3.58108	-0.44433	0.66318
C	-2.25727	-0.88871	0.44084
N	-0.62105	2.14832	-0.77435
N	0.60752	1.55819	-0.88884
C	1.43026	2.48151	-1.43178
C	0.72631	3.68305	-1.65687
C	-0.57863	3.43513	-1.22976
C	3.73216	0.78957	2.98118
H	1.11214	4.60769	-2.07954
H	2.80768	1.83541	1.33107
H	-3.22699	2.82510	-0.26558
H	-4.95261	1.25975	0.58041
H	-2.05192	-1.94810	0.62259
O	-4.45271	-1.40409	1.12324
H	-1.46588	4.06291	-1.22715
H	2.46394	2.22272	-1.64832
H	-0.00717	-2.90809	1.16259
H	0.47933	-0.85115	2.52440
H	3.74721	0.15756	-0.20672
H	3.19895	-1.83995	-1.59804
H	4.04564	1.70947	3.50405
H	3.48559	0.03103	3.74481
H	4.59374	0.41647	2.40180
H	0.44525	1.79554	2.25734
H	1.05814	0.98137	3.72673
H	1.62155	2.61610	3.32540
H	1.02305	-3.35443	-2.22080
H	2.04170	-4.43874	-1.21497
H	0.30523	-4.22444	-0.83792
C	-5.80790	-1.01242	1.33739
H	-6.33090	-1.91455	1.68721
H	-5.89057	-0.22218	2.10899
H	-6.28364	-0.65465	0.40389

G^{OAc} (R = m-OMe)

SCF	=	-1284.25885574
H(0 K)	=	-1283.831600
H(298 K)	=	-1283.802439
G(298 K)	=	-1283.892278
BP86 (D3)	=	-1284.33691317
SCF (MeOH)	=	-1284.27524097
SCF (DCM)	=	-1284.27273389
SCF (BS2)	=	-1284.27370697

Lowest Frequencies = 13.5912cm⁻¹,
27.9435cm⁻¹

54

C	0.53778	0.82874	3.77549
N	0.55725	0.60872	2.42749
N	-0.67098	0.19507	1.99015
C	-1.47016	0.14590	3.07784
C	-0.75186	0.54182	4.22555
C	1.57375	0.66413	1.43876
C	1.15823	0.25480	0.14793

C	2.15310	0.20973	-0.85078
C	3.48348	0.59347	-0.57400
C	3.84673	1.03519	0.71791
C	2.88833	1.06261	1.73308
Ru	-0.81325	-0.28644	-0.02541
O	-0.11125	-2.12190	0.70558
C	0.44698	-3.03765	-0.06274
C	1.03710	-4.19164	0.75809
C	-2.58502	0.97056	-0.33298
C	-3.10469	-0.37466	-0.42891
C	-2.47393	-1.31153	-1.28181
C	-1.36389	-0.86666	-2.10185
C	-0.94227	0.49279	-2.06984
C	-1.55659	1.46611	-1.20047
C	-2.89284	-2.75945	-1.32462
C	-1.09777	2.91872	-1.23217
C	-1.80864	3.66670	-2.38580
O	0.53848	-3.02487	-1.30350
C	-1.28040	3.66208	0.10294
H	1.88994	-0.17223	-1.83961
O	4.50655	0.57141	-1.49199
H	-2.50281	-0.17910	2.97261
H	0.45369	-4.37715	1.67296
H	1.08866	-5.10202	0.14264
H	2.06306	-3.92148	1.06346
H	4.88220	1.33119	0.90523
H	3.17435	1.38179	2.74118
H	-1.11839	0.60952	5.24716
H	1.42782	1.15719	4.30601
H	-0.07869	0.79612	-2.67168
H	-3.91152	-0.69620	0.23639
H	-3.00546	1.63823	0.42560
H	-0.79920	-1.60356	-2.67425
H	-0.01355	2.89639	-1.45738
H	-1.64789	3.16472	-3.35491
H	-2.89773	3.71529	-2.20811
H	-1.43161	4.70067	-2.47015
H	-2.00480	-3.40370	-1.41918
H	-3.45315	-3.04624	-0.42086
H	-3.53934	-2.93928	-2.20345
H	-2.34801	3.80628	0.34825
H	-0.80336	3.11562	0.93286
H	-0.82480	4.66473	0.04252
C	4.21046	0.06612	-2.79486
H	5.15758	0.10365	-3.35296
H	3.84698	-0.97798	-2.75588
H	3.45755	0.68985	-3.31509

D (R = m-Me)

SCF = -1224.70729383
H(0 K) = -1224.271975
H(298 K) = -1224.241204
G(298 K) = -1224.335302
BP86 (D3) = -1224.79447181
SCF (MeOH) = -1224.72821650
SCF (DCM) = -1224.72488428
SCF (BS2) = -1669.92815007
Lowest Frequencies = 19.8716cm⁻¹,
27.4184cm⁻¹

55

C	-0.98065	-0.02789	2.36092
C	-2.08135	0.71528	1.83247
C	-1.89144	1.81784	0.92884
C	-0.57701	2.21315	0.51894
C	0.54435	1.46083	1.01172
C	0.32861	0.34379	1.88098
Ru	-0.91995	0.01730	0.12385
O	-2.56746	-1.08393	-0.53586
C	-3.79923	-0.60593	-0.62199
O	-4.21434	0.47918	-0.18808
C	-0.43586	3.39058	-0.43936
C	0.94407	3.50786	-1.10526
C	-1.17877	-1.18661	3.30654
N	0.02623	-1.90537	-0.26528
N	1.36011	-2.25276	-0.24051
C	1.50358	-3.60973	-0.38346
C	0.23482	-4.15985	-0.49910
C	-0.64804	-3.06274	-0.42422
C	2.45726	-1.33230	-0.18304
C	2.56512	-0.28223	-1.11132
C	3.70007	0.53974	-1.07254
C	4.73965	0.33126	-0.13970
C	4.60309	-0.72951	0.77847
C	3.47113	-1.55776	0.76548
Cl	-0.64466	0.43448	-2.24946
C	-0.80326	4.69565	0.30986
C	-4.72495	-1.56354	-1.38118
H	3.78356	1.35865	-1.79605
H	-2.77479	2.26738	0.47216
H	1.55376	1.67345	0.65658
H	1.18853	-0.27541	2.15897
H	-3.10573	0.38724	2.02675
H	-1.18259	3.22286	-1.23819
H	1.19288	2.58395	-1.65044
H	0.93587	4.33956	-1.82988
H	1.73806	3.72374	-0.36698
H	-0.77089	5.55182	-0.38531
H	-1.81502	4.64900	0.74548
H	-0.08903	4.89691	1.12821
H	-0.41095	-1.96308	3.15609
H	-1.11149	-0.84641	4.35670
H	-2.16900	-1.64837	3.16498
H	-4.52960	-1.45983	-2.46230
H	-5.77503	-1.30586	-1.18197
H	-4.53277	-2.61382	-1.10931
H	-1.73286	-3.00558	-0.48317
H	-0.02035	-5.20801	-0.63621
H	2.49771	-4.04852	-0.43349
H	1.75513	-0.11061	-1.83092

C	5.97591	1.20419	-0.14641
H	5.39025	-0.90841	1.51943
H	3.36834	-2.37371	1.48849
H	5.72807	2.25498	-0.37090
H	6.49915	1.17435	0.82311
H	6.69299	0.86900	-0.91827

D^{OAc} (R = m-Me)

SCF = -1438.14220049
H(0 K) = -1437.657712
H(298 K) = -1437.623402
G(298 K) = -1437.725720
BP86 (D3) = -1438.23803388
SCF (MeOH) = -1438.16000591
SCF (DCM) = -1438.15734372
SCF (BS2) = -1438.20415815
Lowest Frequencies = 20.6523cm⁻¹,
22.1853cm⁻¹

61

C	4.03613	1.18951	-0.80396
C	2.94482	0.95466	0.05526
C	2.91971	-0.18590	0.87233
C	3.98812	-1.09183	0.81095
C	5.10118	-0.87509	-0.02887
C	5.10400	0.28259	-0.83368
N	1.90856	1.94366	0.11316
N	0.54862	1.71053	0.00083
C	-0.02529	2.93316	-0.04666
C	0.94211	3.95542	0.04496
C	2.15568	3.29340	0.14514
Ru	-0.67787	-0.07909	-0.17813
O	0.07095	-0.57526	1.71278
C	-0.03839	-1.76547	2.27800
C	0.32851	-1.72281	3.76715
C	-1.92476	0.09304	-1.99475
C	-2.47019	-0.97283	-1.18138
C	-1.59644	-2.00993	-0.74422
C	-0.20387	-2.00821	-1.12380
C	0.33354	-1.00581	-1.98055
C	-0.55243	0.07157	-2.36724
C	-3.94546	-0.93737	-0.80516
C	-4.76142	-1.54792	-1.97219
C	1.75742	-1.06214	-2.47242
O	-1.95532	0.90572	1.17588
C	-2.86927	1.80214	0.88774
C	-3.64713	2.25600	2.12874
C	-4.27254	-1.63284	0.52786
O	-3.10061	2.30841	-0.23264
O	-0.40121	-2.82383	1.73837
H	-2.54317	0.96430	-2.22006
H	-1.92589	-2.75367	-0.01907
H	0.45090	-2.76686	-0.68815
H	-0.13532	0.92911	-2.90667
H	-4.21823	0.12990	-0.72101
H	-3.64575	-1.23939	1.34376
H	-5.33132	-1.46234	0.78646
H	-4.12339	-2.72544	0.46850
H	-5.84129	-1.47432	-1.75783
H	-4.56741	-1.02599	-2.92460
H	-4.51357	-2.61523	-2.11087
H	2.41544	-1.57226	-1.75216

H 1.79606 -1.62062 -3.42666
H 2.16508 -0.05644 -2.65805
H -3.87461 1.40459 2.78850
H -4.57220 2.76754 1.82580
H -3.02504 2.96180 2.70611
H -0.51293 -1.28152 4.32844
H 0.51027 -2.74112 4.14008
H 1.20814 -1.08478 3.94962
H -1.10750 3.00011 -0.17622
H 0.77138 5.02924 0.05116
H 3.17439 3.65497 0.26482
H 2.05389 -0.35261 1.52084
H 3.96015 -1.98488 1.44577
C 6.26659 -1.84040 -0.04434
H 5.94818 0.47191 -1.50630
H 4.03794 2.06839 -1.45663
H 6.81721 -1.79678 -0.99831
H 6.98700 -1.60539 0.76091
H 5.93324 -2.87951 0.11291

E (R = m-Me)

SCF = -1209.46992628
H(0 K)= -1209.034292
H(298 K)= -1209.005716
G(298 K)= -1209.095064
BP86 (D3) = -1209.54629340
SCF (MeOH) = -1209.52370071
SCF (DCM) = -1209.51898159
SCF (BS2) = -1209.45150967
Lowest Frequencies = 13.3750cm⁻¹,
33.1441cm⁻¹

54

C 0.12750 -1.51994 -1.86741
C 1.50042 -1.22537 -2.19796
C 2.49207 -1.19804 -1.17435
C 2.19516 -1.51864 0.20401
C 0.82890 -1.80848 0.50578
C -0.19286 -1.82293 -0.50397
Ru 0.87278 0.12282 -0.57071
O 2.04884 1.89210 -0.80871
C 1.12403 2.45771 -1.51290
O 0.07982 1.73703 -1.75004
C 3.31636 -1.52759 1.23532
C 2.84211 -1.33405 2.68589
C -0.94049 -1.46220 -2.92631
N 0.08927 1.19993 1.08793
N -1.15525 1.10181 1.66606
C -1.19510 1.82524 2.82662
C 0.05530 2.40405 3.01620
C 0.82017 1.99280 1.90865
C -2.26217 0.40802 1.07010
C -2.70860 0.75621 -0.21621
C -3.82728 0.09783 -0.74690
C -4.52066 -0.89237 -0.01539
C -4.04752 -1.21787 1.27444
C -2.92649 -0.57723 1.82132
C -5.75601 -1.55637 -0.57952
C 1.24889 3.86985 -1.99900
C 4.12268 -2.84306 1.08372
H 0.36659 3.04767 3.83540
H 0.87815 4.55864 -1.21978

H 2.30351 4.11333 -2.19528
H 0.64434 4.01745 -2.90558
H 3.98996 -0.68734 0.97625
H -2.56594 -0.83959 2.82119
H -4.56480 -1.98397 1.86175
H -4.18451 0.37692 -1.74430
H -2.12121 1.89656 3.39319
H -2.18733 1.53029 -0.78673
H 1.75918 -0.91966 -3.21561
H -1.23529 -1.98444 -0.21826
H 3.49868 -0.84532 -1.42430
H 0.53251 -1.93927 1.55012
H 4.98197 -2.83939 1.77412
H 3.49573 -3.71882 1.32450
H 4.51161 -2.97295 0.06003
H 3.71475 -1.25311 3.35359
H 2.23911 -0.41809 2.80500
H 2.24693 -2.19447 3.03946
H -0.73095 -0.67162 -3.66365
H -0.97102 -2.42745 -3.46419
H -1.93186 -1.28332 -2.48407
H 1.85269 2.21702 1.64816
H -5.74015 -1.57879 -1.68080
H -5.86582 -2.58948 -0.21250
H -6.66512 -1.00526 -0.27732

TS (E-F) (R = m-Me)

SCF = -1209.43823459
H(0 K)= -1209.004324
H(298 K)= -1208.976164
G(298 K)= -1209.064472
BP86 (D3) = -1209.51574759
SCF (MeOH) = -1209.49642208
SCF (DCM) = -1209.49101685
SCF (BS2) = -1209.42054481
Lowest Frequencies = -91.3361cm⁻¹,
12.7797cm⁻¹

54

C 0.60529 1.98840 -1.74903
C 1.84198 2.00902 -1.04868
C 2.56427 0.79249 -0.77956
C 2.10060 -0.48252 -1.27472
C 0.85918 -0.50684 -2.00307
C 0.11827 0.69290 -2.18169
Ru 0.56986 0.52529 -0.02641
O 1.03547 1.46381 1.78660
C 0.16691 2.41258 2.07474
O -0.83329 2.65020 1.36021
C 2.94431 -1.72598 -1.03640
C 2.17431 -3.05402 -1.13402
C -0.19657 3.24270 -1.97876
N 0.37359 -1.10427 1.29945
N -0.81928 -1.77341 1.39122
C -0.75261 -2.73624 2.36391
C 0.52271 -2.68136 2.91616
C 1.18721 -1.64192 2.22948
C -1.90673 -1.33830 0.58749
C -1.96340 0.02723 0.23777
C -3.01393 0.47860 -0.58491
C -4.01078 -0.39917 -1.05298
C -3.91763 -1.76210 -0.68428

C	-2.87561	-2.24021	0.12190
C	-5.16649	0.09555	-1.89238
C	0.45326	3.18287	3.35142
C	4.13238	-1.69963	-2.03576
H	0.91575	-3.29913	3.72007
H	-0.27713	2.87792	4.11988
H	1.46795	2.99572	3.72891
H	0.30549	4.25844	3.16956
H	3.36497	-1.63739	-0.01575
H	-2.80764	-3.30488	0.36487
H	-4.67319	-2.46821	-1.04484
H	-3.07643	1.54779	-0.81378
H	-1.61807	-3.35045	2.60192
H	-1.39152	0.82407	0.78922
H	2.18642	2.94395	-0.59631
H	-0.88228	0.63347	-2.62072
H	3.46000	0.82992	-0.15204
H	0.42989	-1.45739	-2.32635
H	4.79336	-2.56134	-1.84790
H	3.77317	-1.76735	-3.07672
H	4.73443	-0.78133	-1.93937
H	2.83831	-3.88700	-0.85296
H	1.30066	-3.07738	-0.46281
H	1.83195	-3.25078	-2.16489
H	-0.08589	3.94725	-1.14133
H	0.14996	3.73841	-2.90384
H	-1.26706	3.01817	-2.09931
H	2.19105	-1.24498	2.36363
H	-4.98746	1.11307	-2.27288
H	-5.35173	-0.56792	-2.75372
H	-6.09788	0.12185	-1.29911

F (R = m-Me)

SCF = -1209.46457197
H(0 K) = -1209.029619
H(298 K) = -1209.000970
G(298 K) = -1209.090364
BP86 (D3) = -1209.54224668
SCF (MeOH) = -1209.51937395
SCF (DCM) = -1209.51448824
SCF (BS2) = -1209.44516066
Lowest Frequencies = 17.8820cm⁻¹,
23.1582cm⁻¹

54

C	1.57380	2.08451	-1.37380
C	2.45852	1.87113	-0.24591
C	2.82928	0.56522	0.13018
C	2.36989	-0.59994	-0.60602
C	1.54799	-0.37113	-1.75537
C	1.16648	0.95986	-2.14968
Ru	0.55880	0.55393	-0.04677
O	-0.51531	2.17807	0.91814
C	-1.71887	2.53794	0.85800
O	-2.64737	1.89795	0.16689
C	2.82964	-1.98582	-0.17118
C	1.91410	-3.13058	-0.63860
C	1.12781	3.48066	-1.72864
N	0.21363	-0.42863	1.74907
N	-0.87047	-1.26739	1.79520
C	-1.01273	-1.79470	3.04834
C	0.01136	-1.27557	3.83802

C	0.75091	-0.42565	2.98863
C	-1.61506	-1.37615	0.59281
C	-1.15716	-0.53587	-0.46013
C	-1.88596	-0.61922	-1.67238
C	-2.99815	-1.47604	-1.84443
C	-3.39310	-2.28685	-0.75880
C	-2.70863	-2.24420	0.46226
C	-3.75023	-1.52450	-3.15579
C	-2.20745	3.75674	1.58889
C	4.28711	-2.20478	-0.65081
H	0.19817	-1.48592	4.88837
H	-2.94776	3.45400	2.34833
H	-1.37010	4.27462	2.07256
H	-2.72358	4.43143	0.88680
H	2.83525	-1.98138	0.93668
H	-3.02879	-2.88289	1.29166
H	-4.24936	-2.96028	-0.86781
H	-1.58889	0.00949	-2.52069
H	-1.82033	-2.48324	3.28459
H	-2.23605	1.07113	-0.23605
H	2.75574	2.72426	0.37071
H	0.50917	1.10812	-3.01082
H	3.43437	0.41434	1.03076
H	1.15328	-1.22367	-2.31309
H	4.66363	-3.17361	-0.28373
H	4.33988	-2.21490	-1.75310
H	4.96681	-1.41705	-0.28489
H	2.24162	-4.07828	-0.18168
H	0.86281	-2.95818	-0.35385
H	1.95998	-3.26980	-1.73288
H	0.91708	4.07554	-0.82601
H	1.93262	3.99452	-2.28488
H	0.23041	3.47083	-2.36628
H	1.62406	0.18707	3.20223
H	-3.29509	-0.86455	-3.91103
H	-3.76896	-2.54845	-3.56747
H	-4.80116	-1.21223	-3.02439

F1 (R = m-Me)

SCF = -980.335688524
H(0 K) = -979.962773
H(298 K) = -979.939586
G(298 K) = -980.016945
BP86 (D3) = -980.392178654
SCF (MeOH) = -980.393068437
SCF (DCM) = -980.387902247
SCF (BS2) = -980.247282231
Lowest Frequencies = 12.9500cm⁻¹,
22.3455cm⁻¹

46

C	-1.61483	-1.67375	0.12414
C	-1.41896	-1.51511	1.52245
C	-1.80835	-0.28959	2.17903
C	-2.56624	0.68677	1.43172
C	-2.76140	0.52475	0.04487
C	-2.22014	-0.61870	-0.66023
Ru	-0.53680	0.19349	0.45387
N	0.33999	1.96611	-0.17530
N	1.68304	1.88199	-0.44572
C	2.17572	3.10063	-0.79694
C	1.11874	4.01617	-0.75275

C	-0.00283	3.26710	-0.36269
C	2.27025	0.59219	-0.28879
C	1.36708	-0.43280	0.11738
C	1.92403	-1.72451	0.27641
C	3.28913	-2.00195	0.06164
C	4.12784	-0.93691	-0.33949
C	3.63106	0.36330	-0.51724
C	-1.49680	-0.06822	3.63677
C	-2.41915	-0.73358	-2.16502
C	-1.31994	-1.52872	-2.89243
C	-3.82219	-1.34143	-2.42935
H	1.16456	5.07883	-0.97786
H	-2.41723	0.29987	-2.56247
H	4.30694	1.16671	-0.82653
H	5.19172	-1.12581	-0.51760
H	1.27404	-2.55168	0.58546
C	3.85258	-3.39197	0.25330
H	3.22491	3.23854	-1.04903
H	-1.03258	3.58261	-0.20663
H	-0.86087	-2.26784	2.08665
H	-1.20424	-2.55058	-0.38273
H	-3.22372	1.32848	-0.53723
H	-2.87356	1.61326	1.92575
H	-4.01609	-1.37098	-3.51411
H	-3.88330	-2.37407	-2.04509
H	-4.62456	-0.75174	-1.95586
H	-0.31390	-1.14421	-2.65594
H	-1.35270	-2.60250	-2.63822
H	-1.46914	-1.45416	-3.98156
H	-1.38382	1.00223	3.86916
H	-2.32849	-0.45988	4.25224
H	-0.57871	-0.59519	3.93925
H	3.06332	-4.11882	0.50124
H	4.36529	-3.74492	-0.65802
H	4.59636	-3.41057	1.06919

G (R = m-Me)

SCF	=	-995.612779146
H(0 K)	=	-995.239217
H(298 K)	=	-995.214433
G(298 K)	=	-995.294186
BP86 (D3)	=	-995.681745816
SCF (MeOH)	=	-995.633209630
SCF (DCM)	=	-995.629929920
SCF (BS2)	=	-1440.75989622
Lowest Frequencies	=	15.9976cm ⁻¹ , 37.2755cm ⁻¹

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C	1.23958	-0.85342	1.65335
C	0.99247	-2.11978	1.01051
C	1.58449	-2.43027	-0.24586
C	2.52834	-1.48283	-0.81587
C	2.79197	-0.25754	-0.17597
C	2.11748	0.10928	1.05804
Ru	0.51131	-0.44758	-0.37137
Cl	-0.41041	-1.06887	-2.52784
C	1.25604	-3.70187	-0.98576
C	2.42487	1.45870	1.69754
C	1.31230	1.98119	2.62344
C	-1.43775	-0.20585	0.22715
C	-2.01662	1.05819	-0.05256

C	-3.32707	1.40687	0.30487
C	-4.11789	0.45511	0.96069
C	-3.60918	-0.82977	1.24472
C	-2.28081	-1.13224	0.87303
N	-1.15706	1.95216	-0.74044
N	0.10590	1.48665	-0.98423
C	0.73861	2.44338	-1.69590
C	-0.12247	3.54279	-1.90085
C	-1.32285	3.19527	-1.28194
C	3.78091	1.38814	2.44074
H	0.09662	4.46534	-2.43318
H	2.53333	2.18103	0.86389
H	-3.73275	2.39895	0.07864
H	-5.14365	0.71124	1.24769
H	-1.90563	-2.14097	1.08345
C	-4.48462	-1.87746	1.90115
H	-2.26879	3.72400	-1.19866
H	1.75831	2.27823	-2.03555
H	0.27627	-2.81930	1.45122
H	0.70343	-0.60926	2.57356
H	3.45251	0.47267	-0.65662
H	2.95177	-1.68587	-1.80364
H	4.05365	2.37855	2.84388
H	3.72550	0.67994	3.28614
H	4.59536	1.05508	1.77523
H	0.33381	1.98049	2.11590
H	1.22647	1.37246	3.54098
H	1.53895	3.01307	2.93995
H	0.90197	-3.46130	-2.00301
H	2.15076	-4.34553	-1.06322
H	0.46300	-4.26801	-0.47302
H	-3.88488	-2.61135	2.46515
H	-5.21014	-1.42300	2.59695
H	-5.06512	-2.44135	1.14738

G^{OAc} (R = m-Me)

SCF	=	-1209.05055716
H(0 K)	=	-1208.628155
H(298 K)	=	-1208.599788
G(298 K)	=	-1208.687989
BP86 (D3)	=	-1209.12618132
SCF (MeOH)	=	-1209.06615633
SCF (DCM)	=	-1209.06370592
SCF (BS2)	=	-1209.03998578
Lowest Frequencies	=	19.4371cm ⁻¹ , 31.1829cm ⁻¹

53

C	1.93507	0.26788	3.30220
N	1.48555	0.24372	2.01206
N	0.14571	-0.03051	1.97409
C	-0.24952	-0.18948	3.25436
C	0.84467	-0.00527	4.12737
C	2.11866	0.39202	0.75015
C	1.25812	0.20104	-0.36205
C	1.87095	0.27344	-1.62841
C	3.24483	0.55944	-1.79882
C	4.04113	0.76630	-0.65400
C	3.48567	0.67827	0.62994
Ru	-0.69668	-0.23301	0.08632
O	0.06085	-2.17134	0.35034
C	0.20147	-3.04221	-0.63064

C	0.95645	-4.29841	-0.17629
C	-2.34048	1.15207	0.51557
C	-2.98953	-0.13990	0.48983
C	-2.77851	-1.01130	-0.60361
C	-1.96653	-0.54646	-1.71280
C	-1.43525	0.77362	-1.71722
C	-1.62338	1.67811	-0.60899
C	-3.32974	-2.41458	-0.62491
C	-1.06587	3.09449	-0.67474
C	-2.04730	4.00717	-1.44887
O	-0.18605	-2.92190	-1.80643
C	-0.71935	3.69527	0.69895
H	1.27150	0.06766	-2.52292
C	3.84273	0.65540	-3.18738
H	-1.28652	-0.43597	3.47112
H	0.74971	-4.53524	0.87870
H	0.69138	-5.14911	-0.82142
H	2.04082	-4.11517	-0.27299
H	5.10893	0.98486	-0.76516
H	4.11797	0.81812	1.51363
H	0.84411	-0.06433	5.21325
H	2.97891	0.46567	3.53194
H	-0.80320	1.08939	-2.55412
H	-3.55404	-0.48333	1.36201
H	-2.41607	1.75495	1.42595
H	-1.69799	-1.24884	-2.50281
H	-0.12690	3.03070	-1.25862
H	-2.26804	3.60646	-2.45268
H	-3.00452	4.10207	-0.90594
H	-1.62394	5.01923	-1.57082
H	-2.58921	-3.10000	-1.06586
H	-3.59039	-2.76333	0.38685
H	-4.24223	-2.45175	-1.24841
H	-1.62413	3.87603	1.30678
H	-0.04568	3.03215	1.26594
H	-0.21738	4.66889	0.56988
H	4.92952	0.46904	-3.17441
H	3.37996	-0.07296	-3.87452
H	3.68848	1.65944	-3.62559

D (R = m-F)

SCF = -1284.62266372
H(0 K) = -1284.222014
H(298 K) = -1284.192320
G(298 K) = -1284.283461
BP86 (D3) = -1284.70712081
SCF (MeOH) = -1284.64335644
SCF (DCM) = -1284.64004950
SCF (BS2) = -1729.87307904
Lowest Frequencies = 20.0631cm-1,
27.4155cm-1

52

C -0.98556 -0.03078 2.36337
C -2.09540 0.68971 1.82297
C -1.91855 1.79155 0.91603
C -0.60857 2.21067 0.51592
C 0.52237 1.48112 1.02063
C 0.32033 0.36329 1.89219
Ru -0.90747 0.00564 0.12624
O -2.52874 -1.12906 -0.53893
C -3.76881 -0.67389 -0.63636
O -4.20582 0.40598 -0.21159
C -0.48159 3.38884 -0.44328
C 0.90005 3.52979 -1.10097
C -1.16992 -1.18795 3.31358
N 0.07437 -1.90093 -0.24897
N 1.41552 -2.22097 -0.23592
C 1.58604 -3.57518 -0.37923
C 0.32797 -4.15109 -0.48227
C -0.57673 -3.07219 -0.40095
C 2.49127 -1.27705 -0.18269
C 2.57226 -0.22992 -1.11910
C 3.68429 0.62347 -1.09560
C 4.69686 0.40595 -0.15138
C 4.63043 -0.63575 0.78227
C 3.51137 -1.48058 0.76645
Cl -0.62514 0.41869 -2.24738
C -0.87600 4.68804 0.30272
C -4.67161 -1.65238 -1.39605
H 3.77858 1.44492 -1.81070
H -2.80629 2.22302 0.45056
H 1.53061 1.71542 0.67586
H 1.18900 -0.23827 2.18176
H -3.11508 0.34385 2.01082
H -1.22076 3.20764 -1.24619
H 1.16756 2.61043 -1.64495
H 0.88175 4.36088 -1.82594
H 1.68636 3.75982 -0.35888
H -0.85422 5.54379 -0.39326
H -1.88939 4.62434 0.73231
H -0.17010 4.90240 1.12486
H -0.38410 -1.94883 3.17709
H -1.12212 -0.83993 4.36219
H -2.14842 -1.67150 3.16364
H -4.47285 -1.54915 -2.47659
H -5.72741 -1.41406 -1.20325
H -4.46070 -2.69764 -1.11892
H -1.66285 -3.03763 -0.45339
H 0.09315 -5.20442 -0.61589
H 2.58825 -3.99415 -0.43805
H 1.75588 -0.08169 -1.83745

F 5.77306 1.22753 -0.13895
H 5.43863 -0.77099 1.50537
H 3.42702 -2.29807 1.48944

D^{OAc} (R = m-F)

SCF = -1498.05771239
H(0 K) = -1497.607838
H(298 K) = -1497.574621
G(298 K) = -1497.673991
BP86 (D3) = -1498.15090136
SCF (MeOH) = -1498.07531820
SCF (DCM) = -1498.07268211
SCF (BS2) = -1498.14906926
Lowest Frequencies = 19.5047cm-1,
22.1464cm-1

58

C 4.05740 1.12251 -0.81791
C 2.96454 0.90628 0.04642
C 2.92255 -0.22540 0.87778
C 3.97327 -1.15267 0.83351
C 5.05866 -0.91937 -0.02052
C 5.11998 0.20958 -0.84693
N 1.94348 1.90991 0.09972
N 0.58138 1.69469 -0.02666
C 0.02530 2.92468 -0.08660
C 1.00591 3.93416 0.00954
C 2.20908 3.25663 0.12680
Ru -0.66373 -0.08233 -0.17853
O 0.08734 -0.55477 1.71951
C -0.06541 -1.72568 2.31643
C 0.30607 -1.65921 3.80322
C -1.90109 0.07818 -2.00321
C -2.47059 -0.96209 -1.17398
C -1.61840 -2.00635 -0.71201
C -0.22454 -2.03789 -1.08458
C 0.33576 -1.06378 -1.95944
C -0.52748 0.02334 -2.36871
C -3.94703 -0.89296 -0.80766
C -4.76667 -1.50562 -1.97117
C 1.75868 -1.15909 -2.44800
O -1.92974 0.93488 1.16047
C -2.82954 1.84123 0.85797
C -3.60561 2.32137 2.08983
C -4.29599 -1.56236 0.53310
O -3.04818 2.33695 -0.26957
O -0.46966 -2.78194 1.80402
H -2.50230 0.95573 -2.24967
H -1.96522 -2.72965 0.02553
H 0.41373 -2.80134 -0.63282
H -0.09206 0.86214 -2.92299
H -4.19999 0.18040 -0.74143
H -3.66688 -1.16990 1.34767
H -5.35277 -1.36720 0.78211
H -4.16832 -2.65844 0.49043
H -5.84619 -1.40880 -1.76465
H -4.55729 -1.00148 -2.92987
H -4.53797 -2.57926 -2.09251
H 2.40323 -1.67638 -1.72066
H 1.78662 -1.73090 -3.39455
H 2.18929 -0.16542 -2.64650
H -3.84082 1.48319 2.76357

H -4.52600 2.83516 1.77665
H -2.97908 3.03239 2.65592
H -0.52423 -1.18647 4.35545
H 0.46366 -2.67321 4.19817
H 1.20065 -1.03841 3.97180
H -1.05509 3.00522 -0.22486
H 0.84982 5.01020 0.00808
H 3.23118 3.60564 0.25526
H 2.05276 -0.37082 1.52751
H 3.96535 -2.04364 1.46711
F 6.07913 -1.80946 -0.05090
H 5.97896 0.35505 -1.50684
H 4.06961 1.99782 -1.47454

E (R = m-F)

SCF = -1269.38199036
H(0 K)= -1268.981059
H(298 K)= -1268.953520
G(298 K)= -1269.040320
BP86 (D3) = -1269.45552382
SCF (MeOH) = -1269.43831733
SCF (DCM) = -1269.43334600
SCF (BS2) = -1269.39235105
Lowest Frequencies = 13.1584cm⁻¹,
32.6996cm⁻¹

51

C -2.73313 0.70429 -0.23055
C -2.29439 0.33214 1.05384
C -2.94611 -0.68189 1.78015
C -4.04868 -1.33975 1.21750
C -4.47156 -0.96863 -0.06699
C -3.82884 0.04161 -0.79949
N -1.21014 1.03595 1.67619
N 0.04147 1.16182 1.11786
C 0.74720 1.95261 1.96161
C -0.03978 2.33420 3.06464
C -1.27820 1.74038 2.84779
Ru 0.86105 0.14581 -0.56269
O 1.98567 1.95280 -0.75563
C 1.04745 2.50866 -1.44937
C 1.13403 3.93373 -1.90429
C 1.54418 -1.14263 -2.21617
C 2.52426 -1.11253 -1.18138
C 2.22353 -1.47712 0.18483
C 0.86304 -1.81334 0.46449
C -0.14748 -1.83190 -0.55620
C 0.17769 -1.48674 -1.90865
C 3.33443 -1.48252 1.22723
C 4.17763 -2.77150 1.04991
C -0.87917 -1.43763 -2.97902
C 2.84108 -1.33996 2.67734
O 0.02374 1.76429 -1.70495
H 0.25004 2.96883 3.89862
H 0.73647 4.59471 -1.11424
H 2.18247 4.21241 -2.08617
H 0.53282 4.08265 -2.81291
H 3.98758 -0.61810 0.99696
H -2.59229 -0.95401 2.77934
H -4.57984 -2.12756 1.75729
H -4.20697 0.31492 -1.78805
F -5.52727 -1.59896 -0.61394

H -2.21300 1.78861 3.40253
H -2.22099 1.50291 -0.77445
H 1.80436 -0.80466 -3.22318
H -1.18708 -2.03425 -0.28691
H 3.52257 -0.72463 -1.41170
H 0.56087 -1.98027 1.50203
H 5.02958 -2.76255 1.74925
H 3.57253 -3.66988 1.26130
H 4.58015 -2.86389 0.02744
H 3.70471 -1.25202 3.35574
H 2.21152 -0.44451 2.81388
H 2.26717 -2.22554 3.00280
H -0.68774 -0.62271 -3.69442
H -0.87065 -2.38966 -3.54071
H -1.88223 -1.30435 -2.54725
H 1.77932 2.19836 1.71954

TS(E-F) (R = m-F)

SCF = -1269.34915562
H(0 K)= -1268.950134
H(298 K)= -1268.922989
G(298 K)= -1269.009081
BP86 (D3) = -1269.42380590
SCF (MeOH) = -1269.40989795
SCF (DCM) = -1269.40426731
SCF (BS2) = -1269.36006558
Lowest Frequencies = -94.9590cm⁻¹,
9.5176cm⁻¹

51

C -1.96566 0.08199 0.14644
C -1.96635 -1.27489 0.54100
C -2.94440 -2.16775 0.07321
C -3.94778 -1.69986 -0.78616
C -3.94251 -0.35132 -1.17863
C -2.96684 0.54530 -0.72712
N -0.92092 -1.71338 1.39593
N 0.29501 -1.08380 1.32143
C 1.06206 -1.61708 2.29272
C 0.34469 -2.61436 2.98860
C -0.91430 -2.64729 2.39892
Ru 0.57059 0.51563 -0.02564
O 0.98159 1.48433 1.78227
C 0.11033 2.44044 2.03861
C 0.38010 3.23557 3.30335
C 1.92680 1.94956 -1.01119
C 2.60091 0.71506 -0.70211
C 2.12078 -0.55092 -1.20546
C 0.90970 -0.54610 -1.98207
C 0.21229 0.67376 -2.19977
C 0.71934 1.95917 -1.76135
C 2.91599 -1.81601 -0.92045
C 4.14375 -1.83582 -1.87108
C -0.03371 3.23405 -2.03843
C 2.11071 -3.12151 -1.03558
O -0.87736 2.66907 1.30413
H 0.69349 -3.21896 3.82238
H -0.40068 2.99668 4.04481
H 1.36620 3.01100 3.73221
H 0.29797 4.31083 3.08078
H 3.29769 -1.72836 0.11552
H -2.91695 -3.22354 0.35770

H -4.72502 -2.36847 -1.16447
H -3.02149 1.60152 -1.00290
F -4.90723 0.09092 -2.00536
H -1.80496 -3.22786 2.62846
H -1.39972 0.88560 0.70195
H 2.28142 2.87820 -0.55370
H -0.77005 0.63970 -2.68097
H 3.47179 0.73288 -0.03975
H 0.46690 -1.48650 -2.31661
H 4.77056 -2.71416 -1.64688
H 3.82505 -1.90565 -2.92496
H 4.76851 -0.93451 -1.76001
H 2.73720 -3.97042 -0.71851
H 1.21018 -3.11083 -0.40043
H 1.80486 -3.32053 -2.07741
H 0.06549 3.94753 -1.20707
H 0.36478 3.70602 -2.95494
H -1.10498 3.04160 -2.20052
H 2.07283 -1.24644 2.44828

F (R = m-F)

SCF = -1269.37739944
H(0 K) = -1268.976950
H(298 K) = -1268.949420
G(298 K) = -1269.035226
BP86 (D3) = -1269.45221677
SCF (MeOH) = -1269.43465622
SCF (DCM) = -1269.42951103
SCF (BS2) = -1269.38686474
Lowest Frequencies = 18.5008cm⁻¹,
32.0575cm⁻¹

51

C -1.13982 -0.53955 -0.52731
C -1.63216 -1.40908 0.48969
C -2.70799 -2.28982 0.30306
C -3.35259 -2.32769 -0.94103
C -2.89276 -1.48120 -1.95737
C -1.81227 -0.60129 -1.77100
N -0.93575 -1.31568 1.72197
N 0.14144 -0.46673 1.73366
C 0.63199 -0.48479 2.99249
C -0.13050 -1.35854 3.79573
C -1.11947 -1.87016 2.95788
Ru 0.54258 0.55927 -0.02561
O -0.57717 2.15041 0.94051
C -1.77615 2.51428 0.83252
C -2.30175 3.70934 1.57562
C 2.43056 1.90255 -0.12793
C 2.80541 0.59485 0.23672
C 2.39011 -0.56129 -0.53892
C 1.60949 -0.31961 -1.71400
C 1.22489 1.01384 -2.09686
C 1.58790 2.12834 -1.28569
C 2.85253 -1.94945 -0.11472
C 4.33242 -2.13528 -0.53684
C 1.14085 3.52608 -1.63205
C 1.97669 -3.09738 -0.64602
O -2.66838 1.89697 0.07504
H 0.01880 -1.58903 4.84784
H -3.08455 3.38461 2.28147
H -1.49150 4.20728 2.12222

H -2.77618 4.40918 0.86865
H 2.81123 -1.96937 0.99224
H -3.05102 -2.94671 1.10824
H -4.19624 -2.99620 -1.12621
H -1.51494 0.02895 -2.61485
F -3.50462 -1.50602 -3.15937
H -1.92839 -2.57061 3.15073
H -2.23627 1.08628 -0.33273
H 2.69217 2.74690 0.51634
H 0.59990 1.17066 -2.98037
H 3.37874 0.43439 1.15615
H 1.24846 -1.16584 -2.30338
H 4.70821 -3.10633 -0.17505
H 4.43163 -2.12025 -1.63582
H 4.98367 -1.34604 -0.12534
H 2.30067 -4.04988 -0.19679
H 0.91148 -2.94929 -0.40200
H 2.07087 -3.21100 -1.74013
H 0.88596 4.10135 -0.72810
H 1.96306 4.05886 -2.14328
H 0.27202 3.51994 -2.30807
H 1.49041 0.13115 3.25160

F1 (R = m-F)

SCF = -1040.24782564
H(0 K) = -1039.909547
H(298 K) = -1039.887437
G(298 K) = -1039.961919
BP86 (D3) = -1040.30172927
SCF (MeOH) = -1040.30806995
SCF (DCM) = -1040.30259341
SCF (BS2) = -1040.18842352
Lowest Frequencies = 12.2286cm⁻¹,
22.4296cm⁻¹

43

C -1.66397 -1.63049 0.11318
C -1.48529 -1.48223 1.51491
C -1.84272 -0.24624 2.16835
C -2.55402 0.75833 1.41173
C -2.73267 0.60637 0.02177
C -2.22093 -0.55448 -0.67835
Ru -0.53024 0.20105 0.46203
N 0.41297 1.93100 -0.17594
N 1.75448 1.80003 -0.43869
C 2.28944 2.99962 -0.79183
C 1.26360 3.95122 -0.75692
C 0.11556 3.24318 -0.37095
C 2.29805 0.49213 -0.27351
C 1.35477 -0.49725 0.13584
C 1.85539 -1.80709 0.30792
C 3.21151 -2.08306 0.08867
C 4.11801 -1.09045 -0.31273
C 3.65336 0.22076 -0.49691
C -1.54400 -0.03755 3.63035
C -2.40085 -0.65983 -2.18588
C -1.32222 -1.49542 -2.89857
C -3.82227 -1.21433 -2.47052
H 1.34750 5.01077 -0.98573
H -2.35465 0.37329 -2.58149
H 4.35480 1.00110 -0.80701
H 5.16733 -1.34774 -0.47546

H	1.20647	-2.63076	0.61938
F	3.66077	-3.34165	0.26506
H	3.34393	3.10229	-1.03873
H	-0.90379	3.59396	-0.22232
H	-0.96243	-2.25499	2.08581
H	-1.27517	-2.51963	-0.38960
H	-3.15880	1.42651	-0.56512
H	-2.83746	1.69346	1.90377
H	-4.00099	-1.23510	-3.55804
H	-3.92745	-2.24442	-2.08916
H	-4.60881	-0.59539	-2.00796
H	-0.30560	-1.14912	-2.64863
H	-1.39865	-2.56745	-2.64664
H	-1.45350	-1.41433	-3.98947
H	-1.39649	1.02783	3.86657
H	-2.39867	-0.39973	4.23235
H	-0.65071	-0.59831	3.94597

G (R = m-F)

SCF	=	-1055.53030880
H(0 K)	=	-1055.191212
H(298 K)	=	-1055.167544
G(298 K)	=	-1055.244133
BP86 (D3)	=	-1055.59654963
SCF (MeOH)	=	-1055.55050181
SCF (DCM)	=	-1055.54732253
SCF (BS2)	=	-1500.70734017
Lowest Frequencies	=	16.9541cm-1, 46.0040cm-1

44

C	-1.50809	3.07997	-1.34001
N	-1.27330	1.86253	-0.76665
N	0.00719	1.45224	-1.01824
C	0.58113	2.41771	-1.76714
C	-0.33578	3.46732	-1.98835
C	-2.07664	0.94966	-0.03693
C	-1.42717	-0.27658	0.26934
C	-2.20461	-1.22836	0.95849
C	-3.52618	-0.93748	1.32208
C	-4.14240	0.28456	1.02415
C	-3.39906	1.24563	0.32549
Ru	0.51576	-0.44269	-0.36244
Cl	-0.42280	-1.16441	-2.47816
F	-4.24231	-1.88072	1.99221
C	1.30684	-0.76397	1.65548
C	1.10527	-2.05579	1.04859
C	1.68436	-2.37017	-0.21273
C	2.56782	-1.39281	-0.82721
C	2.78714	-0.14102	-0.22273
C	2.12537	0.22382	1.01863
C	1.40317	-3.67534	-0.91217
C	2.38455	1.60060	1.61992
C	3.75724	1.60730	2.33552
C	1.26904	2.09606	2.55704
H	-0.17057	4.38373	-2.54987
H	2.44398	2.30655	0.76755
H	-3.85837	2.20544	0.06716
H	-5.17618	0.46645	1.32648
H	-1.80877	-2.21800	1.20352
H	-2.47686	3.56546	-1.25594
H	1.60227	2.29256	-2.11920

H	0.43355	-2.77733	1.52277
H	0.78062	-0.52298	2.58227
H	3.40120	0.60722	-0.73608
H	2.97793	-1.59959	-1.81978
H	3.99388	2.61827	2.70916
H	3.75024	0.91841	3.19843
H	4.57200	1.29402	1.66087
H	0.28166	2.04412	2.06975
H	1.22676	1.50494	3.48896
H	1.45822	3.14318	2.84685
H	1.02922	-3.48114	-1.93202
H	2.32435	-4.28162	-0.98064
H	0.64071	-4.25992	-0.37449

G^{OAc} (R = m-F)

SCF	=	-1268.96788741
H(0 K)	=	-1268.580050
H(298 K)	=	-1268.552738
G(298 K)	=	-1268.638018
BP86 (D3)	=	-1269.04076851
SCF (MeOH)	=	-1268.98360009
SCF (DCM)	=	-1268.98120240
SCF (BS2)	=	-1268.98709555
Lowest Frequencies	=	17.7583cm-1, 38.6555cm-1

50

C	2.10742	0.16254	3.19363
N	1.59367	0.17637	1.92753
N	0.24827	-0.07032	1.95127
C	-0.08580	-0.25053	3.24618
C	1.05400	-0.10760	4.06649
C	2.16585	0.34224	0.63906
C	1.24393	0.18963	-0.43225
C	1.78456	0.29039	-1.72975
C	3.14762	0.56314	-1.91134
C	4.03433	0.73525	-0.84111
C	3.53017	0.61547	0.46170
Ru	-0.68980	-0.22306	0.10537
O	0.04853	-2.17711	0.29851
C	0.12083	-3.03070	-0.70583
C	0.87029	-4.31117	-0.31600
C	-2.28226	1.19043	0.63352
C	-2.95211	-0.09142	0.63671
C	-2.82131	-0.95800	-0.47275
C	-2.06524	-0.49911	-1.62325
C	-1.51120	0.81088	-1.64899
C	-1.61955	1.71053	-0.52577
C	-3.39881	-2.35065	-0.47211
C	-1.03968	3.11670	-0.61364
C	-2.05073	4.05569	-1.31477
O	-0.32287	-2.87643	-1.85704
C	-0.59399	3.69545	0.74080
H	1.16666	0.12517	-2.61666
F	3.63227	0.66225	-3.17866
H	-1.11550	-0.48172	3.50933
H	0.72342	-4.55931	0.74630
H	0.54447	-5.14480	-0.95551
H	1.95073	-4.15332	-0.47875
H	5.08925	0.94620	-1.03093
H	4.20428	0.72964	1.31713
H	1.10659	-0.19101	5.14946

H	3.16513	0.33433	3.37589
H	-0.92405	1.12239	-2.51948
H	-3.47194	-0.43126	1.53763
H	-2.29694	1.78843	1.55003
H	-1.85393	-1.20021	-2.43165
H	-0.14168	3.04180	-1.25754
H	-2.34296	3.66992	-2.30604
H	-2.96900	4.16352	-0.71051
H	-1.61565	5.06034	-1.45442
H	-2.69832	-3.04640	-0.95974
H	-3.60821	-2.70300	0.55019
H	-4.34566	-2.36578	-1.04299
H	-1.45394	3.88716	1.40743
H	0.10116	3.01292	1.25664
H	-0.08179	4.66036	0.58912

D (R = m-CF3)

SCF = -1522.42378221
H(0 K) = -1522.010678
H(298 K) = -1521.978124
G(298 K) = -1522.077064
BP86 (D3) = -1522.51306142
SCF (MeOH) = -1522.44454586
SCF (DCM) = -1522.44120646
SCF (BS2) = -1967.75403993
Lowest Frequencies = 15.1766cm-1,
19.1954cm-1

55

C	-1.57100	0.03892	2.35825
C	-2.54824	0.93114	1.81874
C	-2.19172	1.99964	0.92479
C	-0.82808	2.21287	0.54067
C	0.16864	1.30927	1.04585
C	-0.21520	0.22708	1.90098
Ru	-1.46784	0.08736	0.12070
O	-3.24010	-0.76767	-0.57417
C	-4.39294	-0.12197	-0.67233
O	-4.65841	1.00595	-0.23150
C	-0.50769	3.36709	-0.40225
C	0.88595	3.29761	-1.04604
C	-1.94253	-1.08231	3.29672
N	-0.79788	-1.95249	-0.27169
N	0.46952	-2.49342	-0.21165
C	0.41530	-3.86061	-0.33660
C	-0.91719	-4.21758	-0.47565
C	-1.63042	-3.00062	-0.43160
C	1.68416	-1.73995	-0.16556
C	1.91292	-0.69506	-1.07882
C	3.14832	-0.03502	-1.05316
C	4.14626	-0.41714	-0.13714
C	3.90971	-1.46781	0.76541
C	2.67494	-2.12970	0.75573
Cl	-1.10553	0.47991	-2.24449
C	-0.70119	4.70327	0.35773
C	-5.43022	-0.93419	-1.45545
H	3.34438	0.77143	-1.76516
H	-2.99615	2.57070	0.45824
H	1.20501	1.38842	0.71461
H	0.54569	-0.50557	2.19240
H	-3.61131	0.74914	1.99592
H	-1.25798	3.31359	-1.21347
H	1.01193	2.35563	-1.60252
H	1.00604	4.13085	-1.75864
H	1.69087	3.39158	-0.29441
H	-0.53834	5.55278	-0.32699
H	-1.71641	4.79450	0.77794
H	0.02134	4.79459	1.18817
H	-1.29563	-1.96237	3.14786
H	-1.83218	-0.75878	4.34842
H	-2.98895	-1.39347	3.14879
H	-5.20500	-0.84889	-2.53234
H	-6.43707	-0.53429	-1.26862
H	-5.39087	-2.00343	-1.19260
H	-2.69429	-2.78609	-0.51052
H	-1.32154	-5.21830	-0.60819
H	1.33378	-4.44283	-0.36478
H	1.12167	-0.40455	-1.78208

C	5.44676	0.35097	-0.08201
H	4.68783	-1.76510	1.47303
H	2.47479	-2.94274	1.46052
F	5.83734	0.77134	-1.31661
F	5.32793	1.46538	0.69967
F	6.45792	-0.39779	0.44128

D^{OAc} (R = m-CF3)

SCF = -1735.85881162
H(0 K) = -1735.396683
H(298 K) = -1735.360522
G(298 K) = -1735.468220
BP86 (D3) = -1735.95671238
SCF (MeOH) = -1735.87687365
SCF (DCM) = -1735.87417396
SCF (BS2) = -1736.03029264
Lowest Frequencies = 13.3708cm-1,
17.0154cm-1

61

C	3.29403	1.88929	-0.73672
C	2.21767	1.48655	0.08031
C	2.31673	0.33797	0.88217
C	3.49709	-0.41602	0.84881
C	4.57875	-0.01877	0.04199
C	4.47602	1.13957	-0.74731
N	1.05345	2.31619	0.11145
N	-0.25895	1.88132	0.01684
C	-1.00537	3.00519	-0.04472
C	-0.19869	4.16146	0.02428
C	1.09943	3.68977	0.12146
Ru	-1.21826	-0.07035	-0.17416
O	-0.41680	-0.46679	1.72031
C	-0.37831	-1.66219	2.28767
C	-0.02483	-1.57351	3.77730
C	-2.46422	-0.06324	-1.99968
C	-2.86319	-1.19821	-1.19512
C	-1.85678	-2.10563	-0.75406
C	-0.47535	-1.91109	-1.12398
C	-0.07568	-0.84027	-1.97315
C	-1.09933	0.10664	-2.36160
C	-4.33232	-1.37005	-0.83311
C	-5.04432	-2.07520	-2.01509
C	1.34470	-0.69684	-2.45791
O	-2.62666	0.71646	1.17688
C	-3.65651	1.47735	0.88836
C	-4.50312	1.80050	2.12464
C	-4.57468	-2.11837	0.48929
O	-3.94481	1.95914	-0.22961
O	-0.60462	-2.75589	1.74591
H	-3.19574	0.71481	-2.22791
H	-2.08496	-2.89105	-0.03404
H	0.27486	-2.57599	-0.68879
H	-0.80137	1.01550	-2.89605
H	-4.75077	-0.35157	-0.74292
H	-4.02100	-1.65019	1.31844
H	-5.65018	-2.10091	0.73388
H	-4.27306	-3.17858	0.42276
H	-6.12592	-2.15339	-1.81180
H	-4.91509	-1.52156	-2.96053
H	-4.65020	-3.09657	-2.16039
H	2.06154	-1.14891	-1.75539

H 1.45535 -1.20936 -3.43187
H 1.62161 0.35881 -2.60522
H -4.61918 0.91541 2.76886
H -5.48600 2.18502 1.81625
H -3.99053 2.57536 2.72071
H -0.91848 -1.24596 4.33576
H 0.28620 -2.55998 4.15009
H 0.76385 -0.82698 3.96372
H -2.08642 2.91069 -0.17147
H -0.52700 5.19798 0.01806
H 2.05223 4.20196 0.23364
H 1.46117 0.04843 1.50267
H 3.58546 -1.30930 1.47351
C 5.82153 -0.87518 -0.02790
H 5.31608 1.44869 -1.37463
H 3.19836 2.77506 -1.37175
F 6.91921 -0.14913 -0.38340
F 6.08974 -1.47488 1.16490
F 5.68492 -1.87115 -0.95306

E (R = m-CF3)

SCF = -1507.18095180
H(0 K)= -1506.767651
H(298 K)= -1506.737222
G(298 K)= -1506.832170
BP86 (D3) = -1507.25964850
SCF (MeOH) = -1507.23879945
SCF (DCM) = -1507.23357080
SCF (BS2) = -1507.27060684
Lowest Frequencies = 11.9460cm⁻¹,
14.9914cm⁻¹

54

C 1.96151 1.20408 0.41712
C 1.51232 1.27925 -0.91366
C 2.29074 0.78962 -1.97694
C 3.52907 0.19157 -1.70114
C 3.97574 0.08766 -0.37329
C 3.19764 0.60226 0.68066
N 0.26168 1.91473 -1.20950
N -0.92144 1.58001 -0.59147
C -1.84091 2.46173 -1.05125
C -1.25861 3.36313 -1.96319
C 0.07865 2.99097 -2.03632
Ru -1.38304 -0.15259 0.56448
O -2.76924 1.18397 1.48841
C -1.87730 1.59134 2.33075
C -2.15930 2.67804 3.32288
C -1.57870 -2.09297 1.58792
C -2.71326 -1.86356 0.75878
C -2.59605 -1.59282 -0.65817
C -1.26996 -1.50909 -1.17958
C -0.10971 -1.72612 -0.35754
C -0.24584 -2.01668 1.03621
C -3.85437 -1.41033 -1.49671
C -4.47030 -2.80550 -1.77760
C 0.95416 -2.20452 1.92534
C -3.63518 -0.62999 -2.80404
O -0.72415 1.01657 2.24562
H -1.74338 4.18416 -2.48587
H -1.95116 3.65895 2.86065
H -3.21867 2.65843 3.61835

H -1.51155 2.56848 4.20473
H -4.57217 -0.84497 -0.87070
H 1.92621 0.86642 -3.00588
H 4.14596 -0.19735 -2.51507
H 3.56966 0.54757 1.70756
C 5.26161 -0.64742 -0.04923
H 0.92388 3.42335 -2.56799
H 1.34850 1.60811 1.22723
H -1.71089 -2.23498 2.66434
H 0.88833 -1.59715 -0.78386
H -3.70435 -1.80978 1.22219
H -1.12601 -1.19277 -2.21625
H -5.42085 -2.69278 -2.32407
H -3.79186 -3.41798 -2.39597
H -4.67876 -3.36009 -0.84756
H -4.60414 -0.45469 -3.29808
H -3.16422 0.35165 -2.62641
H -3.00923 -1.19496 -3.51707
H 0.81928 -1.69367 2.89218
H 1.08210 -3.28268 2.13299
H 1.87618 -1.83775 1.45127
H -2.86710 2.39052 -0.69596
F 5.94314 -0.03545 0.95265
F 4.97891 -1.91763 0.36834
F 6.07813 -0.74064 -1.12756

TS(E-F) (R = m-CF3)

SCF = -1507.14878524
H(0 K)= -1506.737309
H(298 K)= -1506.707268
G(298 K)= -1506.801271
BP86 (D3) = -1507.22847640
SCF (MeOH) = -1507.21090845
SCF (DCM) = -1507.20505607
SCF (BS2) = -1507.23899471
Lowest Frequencies = -97.8299cm⁻¹,
9.3253cm⁻¹

54

C -1.27619 0.00017 0.81824
C -1.11991 -1.35590 1.18464
C -2.16142 -2.28086 1.01778
C -3.37818 -1.84469 0.47334
C -3.54670 -0.50109 0.09183
C -2.50148 0.41880 0.27231
N 0.14430 -1.75427 1.68919
N 1.25852 -1.06728 1.27637
C 2.29659 -1.57483 1.96768
C 1.85606 -2.60992 2.82284
C 0.48325 -2.69706 2.62586
Ru 1.07223 0.53333 -0.09050
O 1.99653 1.51863 1.50693
C 1.20486 2.43110 2.03468
C 1.81409 3.24084 3.16433
C 2.05506 1.98170 -1.43248
C 2.80008 0.75259 -1.34982
C 2.19879 -0.51569 -1.69258
C 0.81041 -0.51763 -2.06810
C 0.07055 0.69662 -2.05568
C 0.67652 1.98431 -1.78116
C 3.05194 -1.77459 -1.67159
C 3.92422 -1.78343 -2.95648

C -0.13448 3.25324 -1.81187
 C 2.26036 -3.08647 -1.53563
 O 0.02861 2.60841 1.64345
 H 2.45883 -3.20371 3.50589
 H 1.32281 2.95512 4.10964
 H 2.89621 3.07522 3.25611
 H 1.60492 4.30922 2.99977
 H 3.73526 -1.68460 -0.80469
 H -2.02170 -3.33295 1.28206
 H -4.19844 -2.55366 0.33577
 H -2.65150 1.47627 0.03726
 C -4.83049 -0.04350 -0.57375
 H -0.27602 -3.31970 3.09375
 H -0.60105 0.82137 1.19742
 H 2.52488 2.91125 -1.09677
 H -1.01060 0.65548 -2.22079
 H 3.83087 0.77573 -0.98319
 H 0.29405 -1.45992 -2.26269
 H 4.59633 -2.65672 -2.94083
 H 3.29469 -1.85494 -3.85961
 H 4.54568 -0.87706 -3.04174
 H 2.96063 -3.93049 -1.43130
 H 1.60099 -3.08386 -0.65244
 H 1.64781 -3.28745 -2.43163
 H 0.22903 3.98110 -1.07164
 H -0.06365 3.71084 -2.81551
 H -1.19813 3.05768 -1.60852
 H 3.29339 -1.16269 1.82642
 F -5.17140 1.20934 -0.17667
 F -4.66869 -0.01017 -1.92935
 F -5.86413 -0.87647 -0.30162

F (R = m-CF3)

SCF = -1507.17749953
 H(0 K) = -1506.764710
 H(298 K) = -1506.734222
 G(298 K) = -1506.828341
 BP86 (D3) = -1507.25730022
 SCF (MeOH) = -1507.23694107
 SCF (DCM) = -1507.23158498
 SCF (BS2) = -1507.26642895
 Lowest Frequencies = 15.4600cm⁻¹,
 16.5746cm⁻¹

54

C -0.83726 -0.02125 0.31576
 C -0.98968 -0.27500 1.71146
 C -2.21245 -0.60471 2.31195
 C -3.35678 -0.69700 1.50678
 C -3.25828 -0.45637 0.12773
 C -2.01713 -0.12445 -0.45443
 N 0.21225 -0.16825 2.45349
 N 1.34519 0.08484 1.71978
 C 2.35823 0.19191 2.60479
 C 1.87756 -0.00127 3.91869
 C 0.51050 -0.22779 3.78766
 Ru 1.10279 0.30767 -0.32954
 O 1.09423 2.42667 0.14994
 C 0.14899 3.24181 0.30597
 C 0.40473 4.69896 0.56506
 C 2.99088 0.57812 -1.65012
 C 3.10637 -0.61070 -0.90351

C 2.05807 -1.61638 -0.90313
 C 0.90760 -1.36712 -1.71711
 C 0.78125 -0.15662 -2.48573
 C 1.79431 0.84444 -2.42320
 C 2.25554 -2.89981 -0.10655
 C 3.21602 -3.83129 -0.88950
 C 1.65139 2.14735 -3.16823
 C 0.94924 -3.62832 0.25397
 O -1.12911 2.90309 0.25803
 H 2.45159 0.02039 4.84198
 H -0.00050 4.97086 1.55408
 H 1.48038 4.91120 0.53157
 H -0.13095 5.30895 -0.18050
 H 2.75979 -2.60995 0.83641
 H -2.28633 -0.79259 3.38736
 H -4.32265 -0.94782 1.95113
 H -1.98688 0.07104 -1.53107
 C -4.46786 -0.61423 -0.77072
 H -0.25829 -0.41747 4.53278
 H -1.18879 1.90775 0.13342
 H 3.76157 1.35045 -1.57317
 H -0.12172 0.02555 -3.07515
 H 3.98328 -0.76363 -0.26507
 H 0.08157 -2.08241 -1.71448
 H 3.42980 -4.73567 -0.29673
 H 2.76247 -4.14942 -1.84387
 H 4.17726 -3.34036 -1.11609
 H 1.16862 -4.47139 0.92858
 H 0.23237 -2.96197 0.76214
 H 0.45722 -4.05232 -0.63871
 H 2.05033 2.99052 -2.58267
 H 2.22647 2.09630 -4.11053
 H 0.60155 2.35584 -3.42548
 H 3.36558 0.40877 2.25584
 F -4.48094 0.33656 -1.74784
 F -4.45202 -1.82712 -1.39300
 F -5.63003 -0.52125 -0.07740

F1 (R = m-CF3)

SCF = -1278.04756859
 H(0 K) = -1277.696923
 H(298 K) = -1277.671907
 G(298 K) = -1277.754133
 BP86 (D3) = -1278.10643227
 SCF (MeOH) = -1278.11010659
 SCF (DCM) = -1278.10434951
 SCF (BS2) = -1278.06756038
 Lowest Frequencies = 12.9746cm⁻¹,
 14.7150cm⁻¹

46

C -1.18376 -2.07770 -0.01518
 C -1.04547 -1.96273 1.39437
 C -1.95180 -1.13256 2.14988
 C -3.10399 -0.57424 1.48116
 C -3.23844 -0.69160 0.08277
 C -2.24200 -1.37980 -0.71356
 Ru -1.11866 0.04457 0.48407
 N -1.20880 2.04499 -0.05060
 N 0.00079 2.62581 -0.34864
 C -0.16069 3.94972 -0.62253
 C -1.52079 4.24695 -0.49719

C -2.13426 3.03404 -0.14213
 C 1.13561 1.76723 -0.28659
 C 0.83851 0.41831 0.06979
 C 1.94116 -0.46009 0.13954
 C 3.25139 -0.02144 -0.11993
 C 3.49380 1.31843 -0.46973
 C 2.42867 2.22845 -0.55694
 C -1.73680 -0.90806 3.62414
 C -2.41089 -1.45619 -2.22396
 C -1.09140 -1.58078 -3.00682
 C -3.37060 -2.63256 -2.54748
 H -1.99521 5.21354 -0.64815
 H -2.90962 -0.51735 -2.53357
 H 2.62505 3.26909 -0.83158
 H 4.51324 1.64982 -0.68198
 H 1.78767 -1.51198 0.39783
 C 4.40610 -0.99145 0.03681
 H 0.68389 4.58469 -0.88136
 H -3.18216 2.81363 0.05194
 H -0.18059 -2.40394 1.89817
 H -0.42074 -2.60805 -0.59065
 H -4.04509 -0.16051 -0.43295
 H -3.80085 0.04774 2.05068
 H -3.56253 -2.66601 -3.63241
 H -2.92525 -3.59772 -2.25135
 H -4.34046 -2.52996 -2.03315
 H -0.37697 -0.78662 -2.73334
 H -0.60645 -2.55885 -2.84355
 H -1.29430 -1.50215 -4.08686
 H -2.13760 0.06449 3.94991
 H -2.26536 -1.69619 4.19297
 H -0.67021 -0.96094 3.89182
 F 4.04764 -2.24675 -0.35379
 F 5.48276 -0.61256 -0.69722
 F 4.79789 -1.06988 1.33817

G (R = m-CF3)

SCF = -1293.33352249
 H(0 K) = -1292.982130
 H(298 K) = -1292.955496
 G(298 K) = -1293.040731
 BP86 (D3) = -1293.40457980
 SCF (MeOH) = -1293.35387347
 SCF (DCM) = -1293.35071819
 SCF (BS2) = -1738.59044562
 Lowest Frequencies = 9.6231cm⁻¹,
 16.9512cm⁻¹

47

C 1.09091 -1.38859 1.50809
 C 0.65134 -2.37256 0.55118
 C 1.40157 -2.63221 -0.62983
 C 2.67511 -1.95172 -0.79867
 C 3.12010 -1.01108 0.14843
 C 2.31418 -0.67101 1.30892
 Ru 0.98403 -0.41855 -0.45652
 Cl 0.45150 -0.32238 -2.81890
 C 0.90791 -3.58166 -1.69120
 C 2.83635 0.36815 2.29475
 C 1.73754 1.05273 3.12663
 C -0.90418 0.31723 -0.16251
 C -1.04316 1.72849 -0.24137

C -2.25737 2.40827 -0.06209
 C -3.41036 1.66235 0.20866
 C -3.32380 0.26050 0.27865
 C -2.09158 -0.39546 0.08891
 N 0.16250 2.40996 -0.53665
 N 1.27530 1.61976 -0.65243
 C 2.29122 2.43728 -0.99538
 C 1.83213 3.77013 -1.08869
 C 0.47200 3.71677 -0.79373
 C 3.90810 -0.27408 3.20891
 H 2.41279 4.65371 -1.34268
 H 3.33481 1.15074 1.68845
 H -2.31535 3.49886 -0.13832
 H -4.37177 2.16155 0.34950
 H -2.07623 -1.48869 0.11328
 C -4.54324 -0.55382 0.62955
 H -0.28727 4.49369 -0.75899
 H 3.28052 2.02344 -1.17545
 H -0.31148 -2.87210 0.69301
 H 0.45165 -1.15297 2.36229
 H 4.05065 -0.46132 -0.03097
 H 3.23684 -2.10219 -1.72495
 H 4.35158 0.48442 3.87643
 H 3.46091 -1.06265 3.83920
 H 4.72377 -0.73205 2.62410
 H 0.94410 1.46681 2.48318
 H 1.27187 0.35263 3.84257
 H 2.17092 1.87748 3.71664
 H 0.88437 -3.07111 -2.66918
 H 1.57618 -4.45849 -1.76408
 H -0.10962 -3.93708 -1.46666
 F -4.56320 -1.75365 -0.02099
 F -4.58865 -0.83856 1.96946
 F -5.70432 0.09507 0.32698

G^{OAc} (R = m-CF3)

SCF = -1506.77090362
 H(0 K) = -1506.370662
 H(298 K) = -1506.340458
 G(298 K) = -1506.433707
 BP86 (D3) = -1506.84868715
 SCF (MeOH) = -1506.78699772
 SCF (DCM) = -1506.78454884
 SCF (BS2) = -1506.86996631
 Lowest Frequencies = 14.7612cm⁻¹,
 16.2618cm⁻¹

53

C -0.37839 -0.85033 3.85771
 N -0.14752 -0.53252 2.54758
 N -1.32834 -0.42282 1.86217
 C -2.30922 -0.68366 2.74890
 C -1.75759 -0.95338 4.02175
 C 1.02862 -0.34934 1.77796
 C 0.78933 -0.11363 0.39738
 C 1.93854 0.01670 -0.40535
 C 3.23543 -0.03805 0.14436
 C 3.42353 -0.24586 1.52207
 C 2.30765 -0.41390 2.35099
 Ru -1.17401 -0.08574 -0.18065
 O -0.95250 -2.17029 -0.13047
 C -0.50425 -2.88146 -1.14923

C	-0.27235	-4.34827	-0.76592
C	-2.58218	1.59705	-0.16280
C	-3.32927	0.53834	-0.80455
C	-2.75838	-0.17132	-1.88611
C	-1.45106	0.23509	-2.36655
C	-0.78567	1.35470	-1.79342
C	-1.34111	2.08963	-0.68326
C	-3.44503	-1.35709	-2.51480
C	-0.61000	3.30521	-0.12698
C	-0.94595	4.55142	-0.98129
O	-0.25905	-2.47518	-2.29808
C	-0.87972	3.56862	1.36506
H	1.83436	0.12836	-1.48821
C	4.42523	0.19933	-0.75137
H	-3.34688	-0.67358	2.42292
H	-0.97688	-4.68116	0.01148
H	-0.35406	-4.98516	-1.65906
H	0.74985	-4.45159	-0.36197
H	4.43272	-0.29250	1.93783
H	2.44371	-0.59852	3.42161
H	-2.29162	-1.19296	4.93824
H	0.44081	-0.98428	4.55945
H	0.20965	1.62643	-2.16098
H	-4.29029	0.22086	-0.38876
H	-2.99283	2.04842	0.74572
H	-0.94927	-0.37628	-3.11752
H	0.47168	3.09665	-0.24073
H	-0.71454	4.38721	-2.04720
H	-2.01884	4.80204	-0.90330
H	-0.36647	5.42541	-0.63739
H	-2.70311	-2.13354	-2.75787
H	-4.21211	-1.78234	-1.84858
H	-3.93759	-1.04999	-3.45592
H	-1.92444	3.88064	1.54370
H	-0.67607	2.67150	1.97255
H	-0.23260	4.38480	1.72740
F	5.57606	-0.31822	-0.23092
F	4.25318	-0.34705	-1.98847
F	4.64807	1.53800	-0.94418

D (R = m-NO₂)

SCF = -1389.91043676
H(0 K) = -1389.499618
H(298 K) = -1389.468197
G(298 K) = -1389.563793
BP86 (D3) = -1389.99816049
SCF (MeOH) = -1389.93420427
SCF (DCM) = -1389.93048023
SCF (BS2) = -1835.19079988
Lowest Frequencies = 19.2037cm⁻¹,
24.2949cm⁻¹

54

C	-1.36383	-0.03159	2.35930
C	-2.38897	0.81204	1.83148
C	-2.09160	1.91435	0.95689
C	-0.74123	2.21511	0.58466
C	0.30394	1.36167	1.07876
C	-0.01943	0.24303	1.91151
Ru	-1.25489	0.06353	0.12260
O	-2.97230	-0.87384	-0.60056
C	-4.16064	-0.29336	-0.69136
O	-4.49145	0.80757	-0.22789
C	-0.48436	3.40360	-0.33455
C	0.91168	3.42478	-0.97660
C	-1.67283	-1.18838	3.27699
N	-0.47197	-1.93431	-0.30153
N	0.81910	-2.41741	-0.22688
C	0.82895	-3.78703	-0.35873
C	-0.48291	-4.20245	-0.51761
C	-1.25195	-3.01880	-0.47613
C	1.99669	-1.61311	-0.17522
C	2.15659	-0.51753	-1.04592
C	3.36328	0.19308	-1.02456
C	4.38170	-0.20607	-0.14672
C	4.23299	-1.29574	0.72188
C	3.02501	-2.00094	0.71001
Cl	-0.89735	0.51538	-2.23193
C	-0.75358	4.71126	0.45182
C	-5.14580	-1.14677	-1.49706
H	3.53360	1.04276	-1.68932
H	-2.92605	2.44581	0.49632
H	1.33533	1.50975	0.75561
H	0.78141	-0.44902	2.19562
H	-3.44031	0.56604	2.00105
H	-1.22996	3.32495	-1.14802
H	1.09040	2.50313	-1.55250
H	0.98625	4.27744	-1.67202
H	1.70991	3.54880	-0.22227
H	-0.63821	5.58177	-0.21582
H	-1.77278	4.73681	0.87160
H	-0.03800	4.82683	1.28516
H	-0.97489	-2.02656	3.11734
H	-1.58556	-0.87628	4.33424
H	-2.69872	-1.55751	3.11916
H	-4.92019	-1.02713	-2.57058
H	-6.17455	-0.80826	-1.30860
H	-5.04753	-2.21720	-1.25534
H	-2.32401	-2.85269	-0.56315
H	-0.83945	-5.21960	-0.66174
H	1.77267	-4.32753	-0.38220
H	1.33721	-0.23237	-1.71977

N	5.65836	0.54630	-0.13284
H	5.05291	-1.56272	1.39165
H	2.87111	-2.84494	1.38909
O	5.75553	1.52261	-0.89582
O	6.54686	0.15067	0.64285

D^{OAc} (R = m-NO₂)

SCF = -1603.34593261
H(0 K) = -1602.885980
H(298 K) = -1602.850990
G(298 K) = -1602.955123
BP86 (D3) = -1603.44220574
SCF (MeOH) = -1603.36657303
SCF (DCM) = -1603.36381055
SCF (BS2) = -1603.46722518
Lowest Frequencies = 18.7453cm⁻¹,
19.5324cm⁻¹

60

C	3.62554	1.72609	-0.67387
C	2.51824	1.31577	0.10293
C	2.55078	0.10976	0.82596
C	3.69884	-0.68995	0.76813
C	4.79662	-0.26504	0.00668
C	4.77775	0.93623	-0.71532
N	1.39491	2.19211	0.17350
N	0.06075	1.81844	0.10171
C	-0.63411	2.97558	0.10172
C	0.22552	4.09284	0.19169
C	1.50248	3.56296	0.23392
Ru	-1.00331	-0.07185	-0.17824
O	-0.18594	-0.61628	1.67145
C	-0.24169	-1.83585	2.18726
C	0.16105	-1.84728	3.66619
C	-2.25440	0.11602	-1.99263
C	-2.72604	-1.03160	-1.24905
C	-1.78048	-2.02521	-0.86100
C	-0.39087	-1.90417	-1.23012
C	0.07755	-0.81919	-2.02490
C	-0.88155	0.21388	-2.35266
C	-4.20350	-1.12927	-0.89409
C	-4.95648	-1.71182	-2.11714
C	1.50195	-0.74698	-2.51412
O	-2.34349	0.70685	1.24123
C	-3.33918	1.53276	1.01669
C	-4.15185	1.81869	2.28403
C	-4.49733	-1.94289	0.37836
O	-3.61842	2.09390	-0.06603
O	-0.58501	-2.87675	1.60612
H	-2.93413	0.94992	-2.17929
H	-2.05848	-2.83027	-0.18142
H	0.31439	-2.64075	-0.83677
H	-0.52519	1.12825	-2.84005
H	-4.55521	-0.09355	-0.73967
H	-3.91675	-1.56724	1.23572
H	-5.56998	-1.87045	0.62505
H	-4.26595	-3.01421	0.24360
H	-6.04106	-1.73380	-1.91619
H	-4.79125	-1.10879	-3.02601
H	-4.62803	-2.74494	-2.32775
H	2.18690	-1.29383	-1.84810
H	1.57094	-1.20385	-3.51901

H 1.85425 0.29321 -2.59866
H -4.33174 0.89481 2.85523
H -5.10455 2.29890 2.01853
H -3.57863 2.49994 2.93634
H -0.68470 -1.47153 4.26726
H 0.39586 -2.87310 3.98431
H 1.01669 -1.18069 3.85977
H -1.72130 2.93495 -0.00265
H -0.05666 5.14198 0.23467
H 2.47827 4.02994 0.34473
H 1.67069 -0.18527 1.41115
H 3.76408 -1.63114 1.31867
N 6.01293 -1.10751 -0.04256
H 5.65171 1.22038 -1.30494
H 3.57423 2.64961 -1.25762
O 6.97103 -0.69084 -0.71871
O 5.99661 -2.17519 0.59410

E (R = m-NO₂)

SCF = -1374.66390907
H(0 K) = -1374.253111
H(298 K) = -1374.223750
G(298 K) = -1374.315416
BP86 (D3) = -1374.74044104
SCF (MeOH) = -1374.72757441
SCF (DCM) = -1374.72163435
SCF (BS2) = -1374.70459759
Lowest Frequencies = 12.4110cm⁻¹,
27.6522cm⁻¹

53

C 2.24388 0.89212 0.51979
C 1.84343 1.13848 -0.80761
C 2.64151 0.74949 -1.90127
C 3.86180 0.10270 -1.66721
C 4.24497 -0.14815 -0.34402
C 3.45902 0.23509 0.75119
N 0.63593 1.86199 -1.07035
N -0.57172 1.58379 -0.46993
C -1.41871 2.55832 -0.87791
C -0.76684 3.46486 -1.73659
C 0.53731 2.99718 -1.83332
Ru -1.20378 -0.17911 0.55677
O -2.48431 1.20670 1.55941
C -1.57458 1.47340 2.43806
C -1.77615 2.50639 3.50390
C -1.61385 -2.15439 1.43940
C -2.69058 -1.76817 0.59096
C -2.49686 -1.42132 -0.80022
C -1.14959 -1.42709 -1.27211
C -0.04500 -1.79783 -0.42938
C -0.25958 -2.16048 0.93864
C -3.70173 -1.07477 -1.66493
C -4.42746 -2.38892 -2.05386
C 0.88585 -2.50144 1.85317
C -3.36572 -0.23959 -2.91212
O -0.47457 0.80611 2.32241
H -1.18569 4.35040 -2.20851
H -1.46700 3.49431 3.11963
H -2.83897 2.56541 3.78105
H -1.16077 2.27228 4.38470
H -4.38946 -0.48602 -1.02680

H 2.30612 0.94567 -2.92404
H 4.51404 -0.21579 -2.48350
H 3.82036 0.03344 1.76232
N 5.53496 -0.84963 -0.09144
H 1.41513 3.39836 -2.33576
H 1.61649 1.21897 1.35365
H -1.79940 -2.35188 2.49900
H 0.97554 -1.73585 -0.81515
H -3.68952 -1.65239 1.02532
H -0.93915 -1.06185 -2.28100
H -5.34296 -2.15744 -2.62226
H -3.78300 -3.02160 -2.68801
H -4.71916 -2.97771 -1.16832
H -4.29623 0.05199 -3.42473
H -2.81736 0.68320 -2.65747
H -2.76582 -0.81451 -3.63945
H 0.71804 -2.11045 2.86903
H 0.97477 -3.60080 1.92673
H 1.84008 -2.10817 1.47297
H -2.44915 2.54460 -0.52797
O 5.81872 -1.09439 1.09140
O 6.22122 -1.13990 -1.08254

TS(E-F) (R = m-NO₂)

SCF = -1374.63163532
H(0 K) = -1374.222600
H(298 K) = -1374.193713
G(298 K) = -1374.284185
BP86 (D3) = -1374.70974312
SCF (MeOH) = -1374.69953580
SCF (DCM) = -1374.69298702
SCF (BS2) = -1374.67283267
Lowest Frequencies = -104.5261cm⁻¹,
10.5842cm⁻¹

53

C -1.52772 0.04321 0.65151
C -1.44148 -1.31292 1.04627
C -2.50469 -2.20895 0.83909
C -3.67787 -1.74605 0.22939
C -3.75179 -0.40596 -0.17717
C -2.70338 0.49600 0.02955
N -0.22388 -1.74662 1.62469
N 0.93592 -1.09371 1.28391
C 1.91207 -1.63879 2.03320
C 1.38743 -2.66312 2.85439
C 0.02811 -2.70553 2.57430
Ru 0.89648 0.52500 -0.07481
O 1.73853 1.46522 1.59246
C 0.92628 2.37369 2.09541
C 1.47819 3.15766 3.27112
C 2.05964 1.92992 -1.31416
C 2.71771 0.65426 -1.20981
C 2.06278 -0.56602 -1.62401
C 0.70689 -0.47091 -2.09047
C 0.04592 0.78939 -2.09670
C 0.71069 2.03022 -1.75453
C 2.83140 -1.87712 -1.57468
C 3.78292 -1.92048 -2.80147
C -0.01485 3.34865 -1.81446
C 1.95122 -3.13716 -1.51551
O -0.22481 2.56997 1.64258

H	1.92851	-3.27866	3.56914
H	0.89796	2.89976	4.17277
H	2.54101	2.94497	3.44937
H	1.33222	4.23404	3.08959
H	3.46173	-1.84542	-0.66459
H	-2.41223	-3.26095	1.12308
H	-4.52876	-2.40621	0.04601
H	-2.83096	1.54410	-0.25121
N	-4.98978	0.07609	-0.84910
H	-0.77695	-3.30585	2.99211
H	-0.85498	0.85071	1.07173
H	2.56364	2.81987	-0.92489
H	-1.02202	0.82232	-2.33451
H	3.72136	0.60430	-0.77663
H	0.14680	-1.37386	-2.34208
H	4.39733	-2.83443	-2.75980
H	3.21016	-1.93817	-3.74411
H	4.46355	-1.05389	-2.82896
H	2.58818	-4.02620	-1.38354
H	1.23759	-3.10562	-0.67597
H	1.38603	-3.28432	-2.45213
H	0.37567	4.05811	-1.07023
H	0.11349	3.79284	-2.81846
H	-1.09422	3.22521	-1.63927
H	2.92886	-1.25975	1.95555
O	-4.98096	1.24475	-1.26735
O	-5.92673	-0.72911	-0.94708

F (R = m-NO2)

SCF = -1374.66203199
H(0 K) = -1374.251529
H(298 K) = -1374.222179
G(298 K) = -1374.312807
BP86 (D3) = -1374.74038743
SCF (MeOH) = -1374.72721887
SCF (DCM) = -1374.72109377
SCF (BS2) = -1374.70165802
Lowest Frequencies = 17.1869cm⁻¹,
31.5662cm⁻¹

53

C	-1.04855	-0.17503	0.14238
C	-1.31269	-0.66462	1.45882
C	-2.55363	-1.17754	1.86971
C	-3.60805	-1.21742	0.94850
C	-3.37745	-0.74474	-0.34846
C	-2.13470	-0.23416	-0.75843
N	-0.20191	-0.59830	2.33149
N	0.97162	-0.15054	1.77276
C	1.88097	-0.12199	2.76805
C	1.29452	-0.56136	3.97665
C	-0.02846	-0.85638	3.66543
Ru	0.90689	0.39266	-0.23011
O	0.67730	2.39614	0.57930
C	-0.34185	3.11616	0.73833
C	-0.23736	4.52423	1.24910
C	2.86249	1.03290	-1.30064
C	3.03934	-0.24356	-0.73372
C	2.10201	-1.32466	-0.98624
C	1.00565	-1.05377	-1.86526
C	0.81996	0.24728	-2.45273
C	1.71464	1.31199	-2.14172

C	2.36191	-2.69504	-0.37405
C	3.47641	-3.40223	-1.18732
C	1.50485	2.69775	-2.69712
C	1.11171	-3.58410	-0.25866
O	-1.57407	2.71052	0.47561
H	1.77398	-0.65232	4.94843
H	-0.79069	4.61132	2.19903
H	0.81337	4.79971	1.40141
H	-0.71539	5.21449	0.53477
H	2.75167	-2.51438	0.64719
H	-2.70816	-1.54756	2.88758
H	-4.59383	-1.60415	1.21427
H	-2.05215	0.11752	-1.79026
N	-4.48846	-0.78383	-1.33615
H	-0.84583	-1.21816	4.28453
H	-1.53443	1.74885	0.19183
H	3.53941	1.84918	-1.03218
H	-0.04427	0.43854	-3.09504
H	3.87247	-0.41751	-0.04426
H	0.26199	-1.83168	-2.05418
H	3.73000	-4.36657	-0.71759
H	3.14121	-3.60408	-2.21907
H	4.39818	-2.79908	-1.24020
H	1.35785	-4.49988	0.30227
H	0.28948	-3.07185	0.26840
H	0.74407	-3.90445	-1.24902
H	1.76058	3.47088	-1.95551
H	2.16517	2.84604	-3.57079
H	0.46697	2.85046	-3.03058
H	2.89551	0.21713	2.56963
O	-4.24646	-0.35581	-2.47797
O	-5.57420	-1.24120	-0.94927

F1 (R = m-NO2)

SCF = -1145.53176730
H(0 K) = -1145.183406
H(298 K) = -1145.159547
G(298 K) = -1145.238271
BP86 (D3) = -1145.58938546
SCF (MeOH) = -1145.60056413
SCF (DCM) = -1145.59394671
SCF (BS2) = -1145.50263884
Lowest Frequencies = 13.9501cm⁻¹,
25.4609cm⁻¹

45

C	-1.19970	-2.00380	-0.08985
C	-1.06212	-1.96771	1.32435
C	-1.87362	-1.07287	2.11098
C	-2.94848	-0.35646	1.46292
C	-3.08632	-0.40022	0.06103
C	-2.16826	-1.16337	-0.76137
Ru	-0.89881	0.07296	0.49796
N	-0.74737	2.07683	-0.00709
N	0.52695	2.51931	-0.27870
C	0.52363	3.85902	-0.52746
C	-0.79369	4.30900	-0.41205
C	-1.54916	3.16838	-0.08944
C	1.55343	1.53644	-0.21958
C	1.09486	0.22430	0.10701
C	2.08425	-0.77867	0.17461
C	3.42807	-0.46467	-0.06305

C	3.85243	0.83250	-0.38136
C	2.89712	1.85562	-0.46139
C	-1.64606	-0.93441	3.59371
C	-2.33448	-1.15914	-2.27375
C	-1.03122	-1.39223	-3.05899
C	-3.41237	-2.21258	-2.64613
H	-1.15111	5.32675	-0.54868
H	-2.72883	-0.16088	-2.54571
H	3.21412	2.87361	-0.70581
H	4.91339	1.02060	-0.55962
H	1.84250	-1.81646	0.41687
N	4.44252	-1.55048	0.02072
H	1.43940	4.39690	-0.76327
H	-2.61846	3.06871	0.08694
H	-0.25699	-2.52592	1.81082
H	-0.49611	-2.59186	-0.68475
H	-3.82532	0.23869	-0.43340
H	-3.57443	0.31605	2.05688
H	-3.60048	-2.18064	-3.73175
H	-3.07400	-3.23100	-2.38973
H	-4.36870	-2.02807	-2.12937
H	-0.23869	-0.68879	-2.75403
H	-0.65268	-2.42145	-2.93377
H	-1.21894	-1.25067	-4.13531
H	-1.92665	0.06678	3.95655
H	-2.27445	-1.67222	4.12750
H	-0.59730	-1.13096	3.86447
O	4.03030	-2.68673	0.30747
O	5.62179	-1.23998	-0.20255

G (R = m-NO₂)

SCF	=	-1160.82280700
H(0 K)	=	-1160.473512
H(298 K)	=	-1160.448059
G(298 K)	=	-1160.529672
BP86 (D3)	=	-1160.89250889
SCF (MeOH)	=	-1160.84613605
SCF (DCM)	=	-1160.84272817
SCF (BS2)	=	-1606.02978955

Lowest Frequencies = 10.9770cm⁻¹,
41.2682cm⁻¹

46

C	1.07586	-1.32251	1.52920
C	0.64903	-2.35498	0.61904
C	1.34235	-2.58876	-0.60135
C	2.55124	-1.82372	-0.86112
C	2.98670	-0.83458	0.03952
C	2.23025	-0.52543	1.24119
Ru	0.78022	-0.40571	-0.44371
Cl	0.11967	-0.39548	-2.77470
C	0.85544	-3.59561	-1.61147
C	2.73754	0.56786	2.17485
C	1.64576	1.19659	3.05844
C	-1.14042	0.18893	-0.06167
C	-1.39798	1.58335	-0.17846
C	-2.65341	2.17706	0.04265
C	-3.73047	1.36087	0.39723
C	-3.50570	-0.01999	0.51067
C	-2.24997	-0.60553	0.28108
N	-0.26810	2.34609	-0.54970
N	0.90079	1.64343	-0.69408

C	1.82891	2.52871	-1.10605
C	1.25871	3.81797	-1.21555
C	-0.07720	3.66615	-0.85748
C	3.90166	0.01784	3.03468
H	1.75439	4.73642	-1.52066
H	3.14626	1.36800	1.52579
H	-2.79816	3.25689	-0.06198
H	-4.72795	1.76226	0.58239
H	-2.17470	-1.69163	0.36233
N	-4.63977	-0.89006	0.88600
H	-0.89444	4.38102	-0.80960
H	2.84031	2.19133	-1.31984
H	-0.26557	-2.91692	0.82977
H	0.47605	-1.11444	2.41841
H	3.86458	-0.22720	-0.20659
H	3.06479	-1.95511	-1.81780
H	4.33097	0.81849	3.66084
H	3.54610	-0.78465	3.70439
H	4.71087	-0.39757	2.41051
H	0.79091	1.54489	2.45589
H	1.26973	0.48302	3.81263
H	2.05694	2.06000	3.60750
H	0.74430	-3.11434	-2.59811
H	1.57658	-4.42777	-1.70199
H	-0.12156	-4.01182	-1.32150
O	-4.42062	-2.11041	1.00844
O	-5.74873	-0.35057	1.06316

G^oAc (R = m-NO₂)

SCF	=	-1374.25994833
H(0 K)	=	-1373.861954
H(298 K)	=	-1373.832855
G(298 K)	=	-1373.923306
BP86 (D3)	=	-1374.33620261
SCF (MeOH)	=	-1374.27921673
SCF (DCM)	=	-1374.27639153
SCF (BS2)	=	-1374.30890479

Lowest Frequencies = 10.2540cm⁻¹,
35.1938cm⁻¹

52

C	0.28549	-1.28427	3.68121
N	0.35484	-0.80280	2.40132
N	-0.90184	-0.63781	1.87827
C	-1.76519	-1.02907	2.83482
C	-1.06197	-1.43941	3.99131
C	1.42692	-0.49297	1.53275
C	1.02239	-0.09158	0.22806
C	2.06808	0.19205	-0.67074
C	3.40857	0.10891	-0.25744
C	3.77907	-0.27597	1.04018
C	2.76607	-0.58639	1.95138
Ru	-0.99417	-0.07431	-0.11630
O	-0.71839	-2.14493	-0.30785
C	-0.41076	-2.74344	-1.44530
C	-0.09484	-4.23034	-1.24256
C	-2.40670	1.56712	0.24078
C	-3.21928	0.55212	-0.39329
C	-2.79261	-0.04124	-1.60270
C	-1.56284	0.43635	-2.20829
C	-0.84166	1.51658	-1.62915
C	-1.25275	2.13372	-0.39128

C	-3.54560	-1.17759	-2.24604
C	-0.46983	3.31323	0.17200
C	-0.92434	4.61837	-0.52520
O	-0.34648	-2.22461	-2.57250
C	-0.55274	3.44672	1.70277
H	1.87127	0.45826	-1.71117
N	4.47670	0.44010	-1.22418
H	-2.83476	-1.00483	2.63861
H	-0.66625	-4.65672	-0.40407
H	-0.29914	-4.78478	-2.17032
H	0.97887	-4.33615	-1.00868
H	4.83603	-0.32725	1.30611
H	3.02433	-0.89694	2.96875
H	-1.48073	-1.80176	4.92718
H	1.18357	-1.48300	4.26028
H	0.09022	1.84603	-2.10075
H	-4.11346	0.17663	0.11356
H	-2.69934	1.92594	1.23232
H	-1.15755	-0.09241	-3.07174
H	0.59097	3.13840	-0.09377
H	-0.82617	4.54855	-1.62156
H	-1.98162	4.83837	-0.29360
H	-0.31583	5.47272	-0.18246
H	-2.83585	-1.91427	-2.65333
H	-4.21826	-1.67619	-1.53051
H	-4.15661	-0.79512	-3.08445
H	-1.56986	3.72147	2.03533
H	-0.26514	2.50751	2.20353
H	0.12619	4.24360	2.04928
O	5.65761	0.31287	-0.84661
O	4.13502	0.83263	-2.35540