Electronic Supplementary Material (ESI) for RSC Advances.
This journal is © The Royal Society of Chemistry 2020

Electronic Supplementary Information

Ru-Catalysed Oxidative Cyclisation of 1,5-Dienes: Unprecedented Role for Co-Oxidant

Aqeel A. Hussein

School of Chemistry, University of Southampton, Southampton, Hampshire, SO17 1BJ, United Kingdom.

College of Dentistry, University of Al-Ameed, Karbala PO Box 198, Iraq.

Email: aahh1f19@soton.ac.uk

TABLE OF CONTENTS

1- Additional computational results

1.1 High spin oxidative cyclisations of 1,5-diene

High spin multiplicities for the oxidative cyclisation have been calculated to account for further investigations. These calculations were performed for the second reaction step, the cyclisation steps. The Ru(VI) glycolate intermediates have two electrons in *d* orbitals and ,so, only singlet and triplet spin multiplicities were computationally done as indicated. Also, the singlet, triplet and quintet spins were suggested for the transition states of cyclisations and the cycloadduct Ru(IV) THF-diolate intermediates. All the calculations for high spin multiplicities triplet and quintet are done to confirm that singlet spin is the favored one during Ru(VI) glycolate cyclisation. Calculations show that high spin cyclisations are not favoured either without additive (Fig. ESI1) or with additive either H_2O (Fig. ESI2) or $NaIO_4$ (Fig. ESI3) because the singlet Ru(VI) glycolate intermediates **7**, $\mathbf{7_{H2O}}$, and $\mathbf{7_{NaIO}}$ are energetically more stable than for those triplet Ru(VI) glycolate intermediates **7t**, $\mathbf{7t_{H2O}}$, and $\mathbf{7t_{NaIO}}$. The disfavourability of high spin, triplet, is increased when Ru(VI) glycolate is complexed with H_2O and $NaIO_4$ (see Fig. ESI2 and $NaIO_4$ Fig. ESI3). Therefore, all cyclisations would more likely occur via singlet spin multiplicity.

It is important to mention that the calculations with triplet and quintet spin multiplicities have shown no problem with spin contamination by which the calculated value of total spin operator $\langle S^2 \rangle$ is compared to $s(s+1)$, where s is 1/2 the number of unpaired electrons. The results have indicated that $\langle S^2 \rangle = 2.0$ for optimized triplet structures and $\langle S^2 \rangle = 6.0$ for optimized quintets structures.

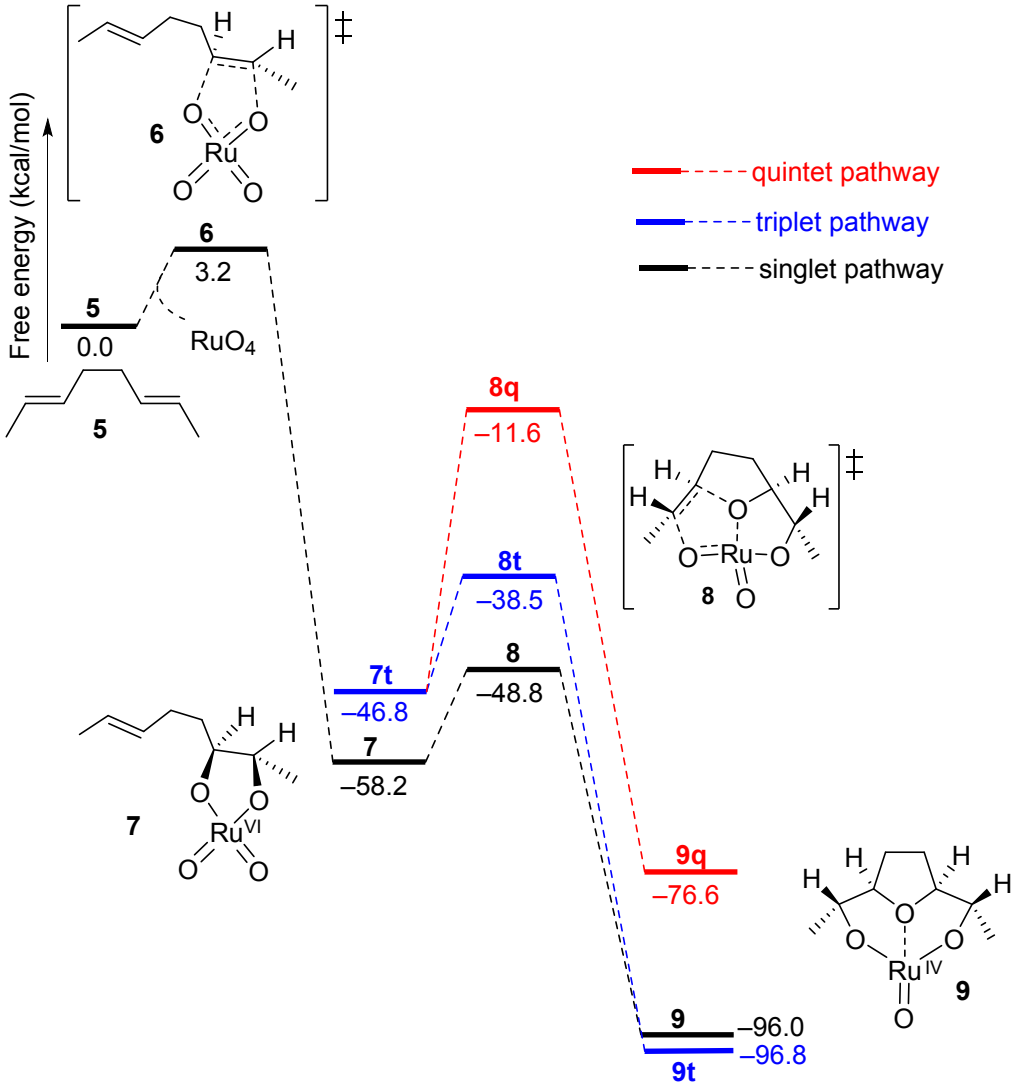

Fig. ESI1 Oxidative cyclisation of 1,5-diene **5** by RuO_4 without any additives, showing high spin cyclisation. t for triplet and q for quintet.

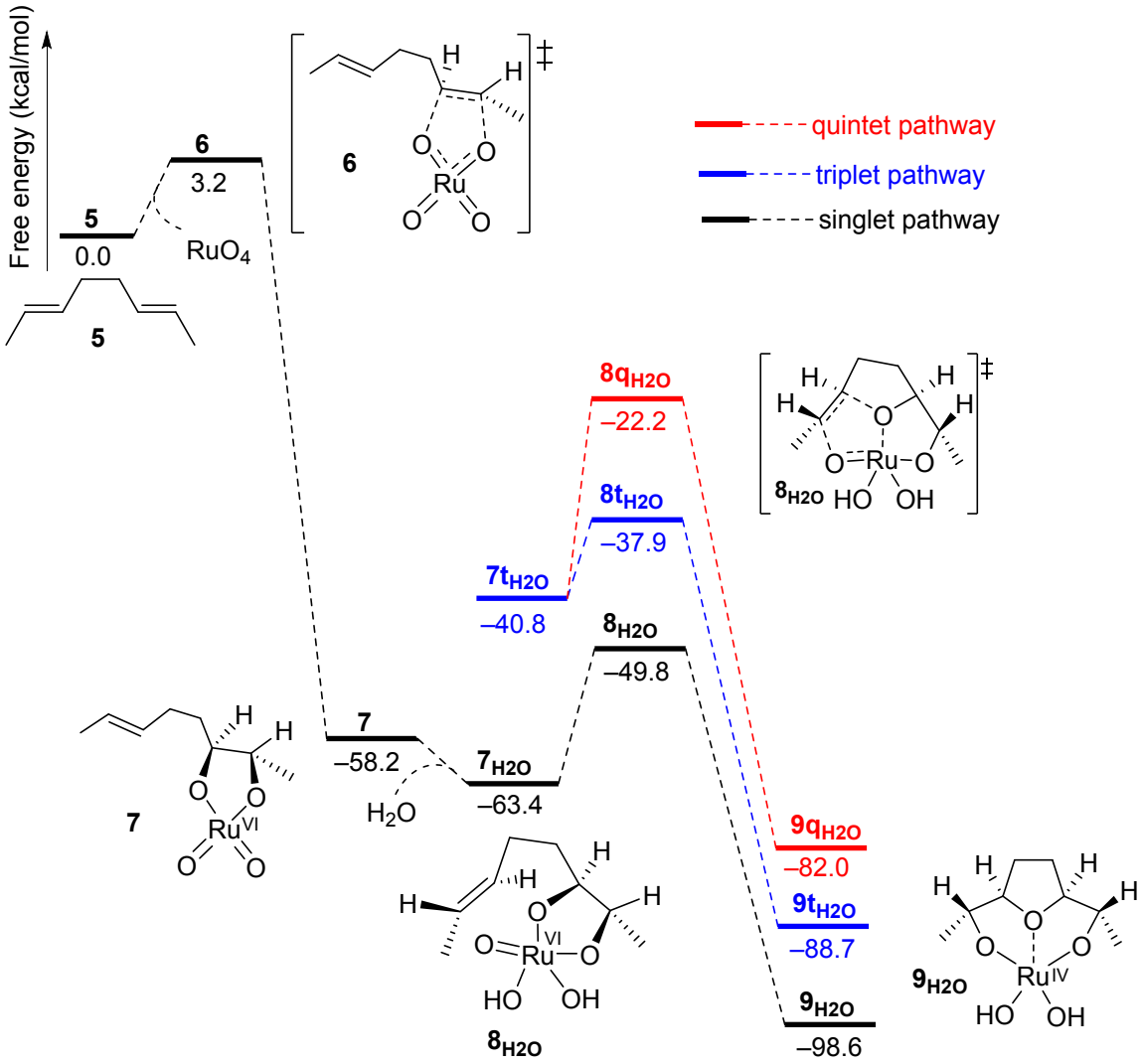

Fig. ESI2 Oxidative cyclisation of 1,5-diene **5** by RuO_4 with water added to Ru(VI) glcycolate **7**, showing high spin cyclisation. t for triplet and q for quintet.

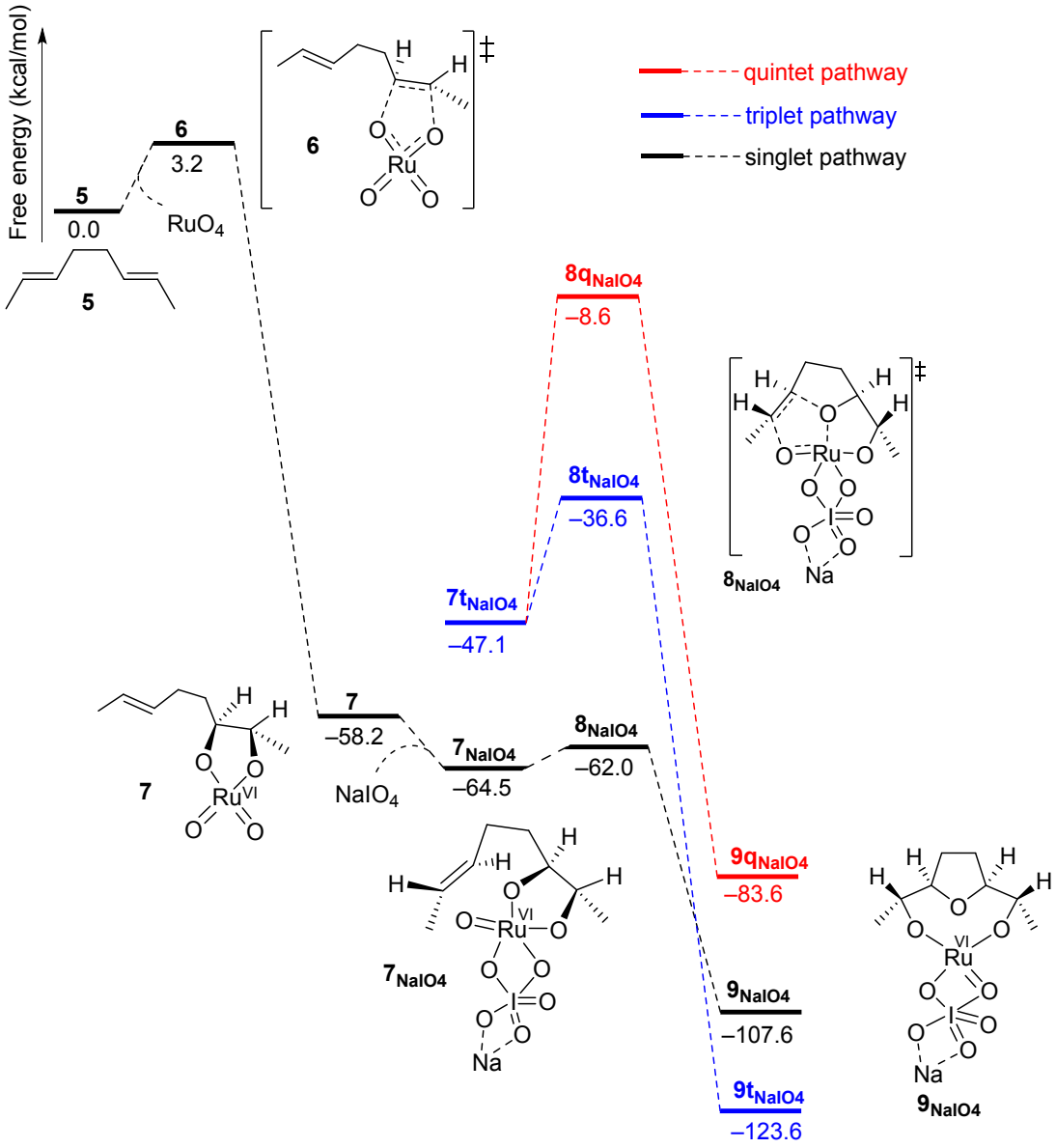

Fig. ESI3 Oxidative cyclisation of 1,5-diene **5** by RuO_4 with $NaIO_4$ added to Ru(VI) glcycolate **7**, showing high spin cyclisation. t for triplet and q for quintet.

2.1. Hydrolysis pathways considered for $9_{[ox]}$

Fig. ESI4 shows hydrolysis via Ru(VI) and Ru(VIII) competed with entering second cycle pathway. The results indicate a favourability of hydrolysis through Ru(VI) and outpace other pathways.

More importantly, the calculated barrier for proton transfer from OH ligand to glycolate bond of intermediate **18** to release THF-diol **15** was found to be very high of 21.7 kcal/mol via TS **22**. However, proton transfer process involving electronegative atoms are obviously fast and diffusion controlled, and therefore proton transfer is more likely to proceed through intermediate **19** as a slightly endergonic step (ΔG_r = 6.3 kcal/mol).

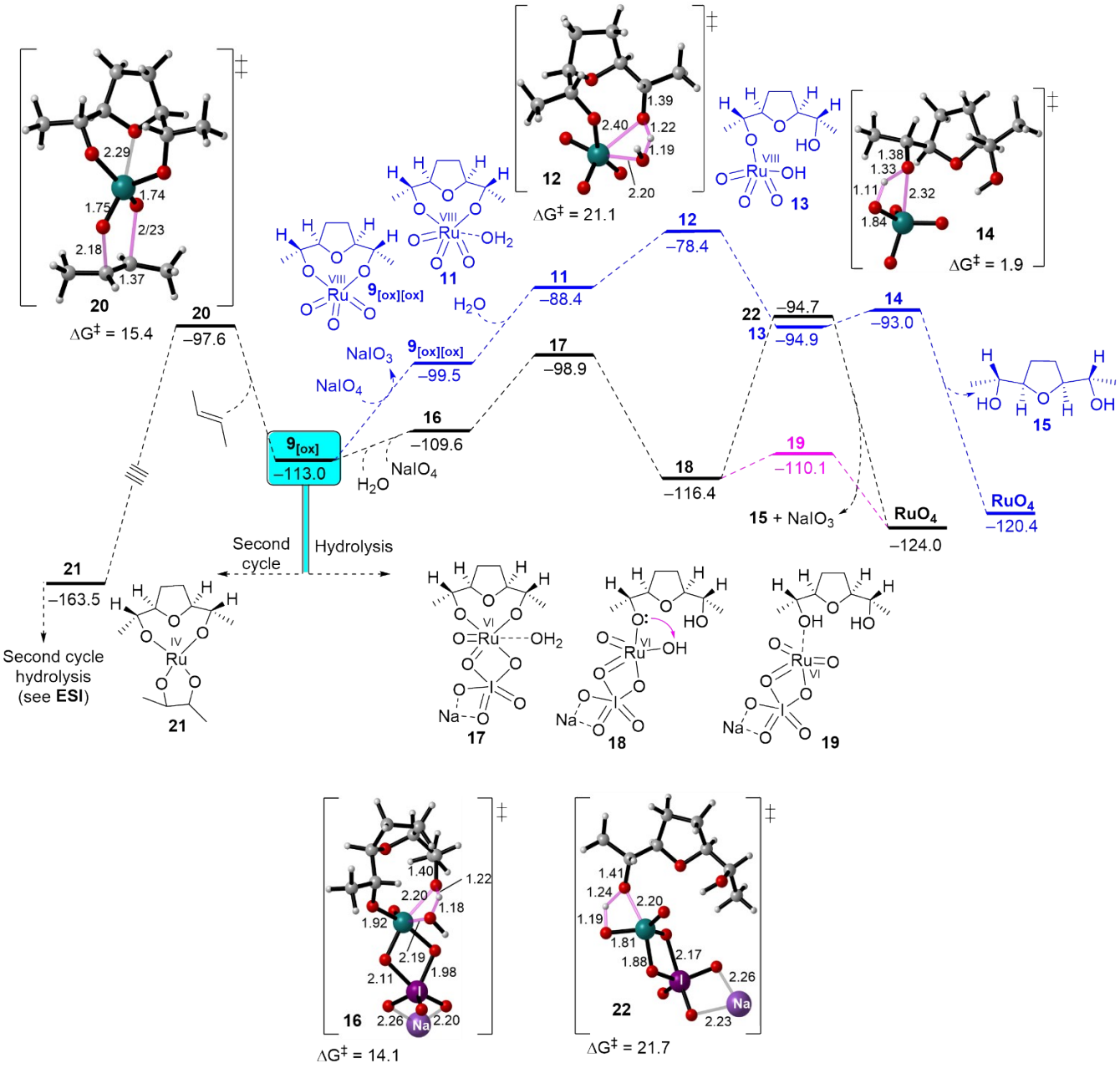

Fig. ESI4 Free energy evaluations for divergent reactions of $\mathbf{9_{[ox]}}$, showing hydrolysis via Ru(VI) or Ru(VIII) or entering second cycle through another ruthenylation. *E*-but-2-ene was used as a model for **5** to reduce computational cost.

2.4 Reoxidation of Ru(IV)→Ru(VI) bisglycolate intermediate and hydrolysis to release either THF-diol or vicinal diol

Fig. ESI5 show DFT simulations on intermolecular ruthenylation of $\mathbf{9}_{[ox]}$ and their mechanism of THF-diol **15** and vicinal diol **22** release. The results indicated that even the Ru(IV) tetraester **21** was formed, which is unlikely as shown in Fig. ESI4, reoxidation to Ru(VI) tetraester $\mathbf{21}_{[ox]}$ and the latter prefer hydrolysis to release THF-diol **15** rather than to vicinal diol **32**.

Here, we have also considered a stepwise THF-diol or vicinal diol release for the second glycolate bond (see intermediates **25** and **30**) rather than proceeding through TSs **26** and **31**, likely to intermediate **18**.

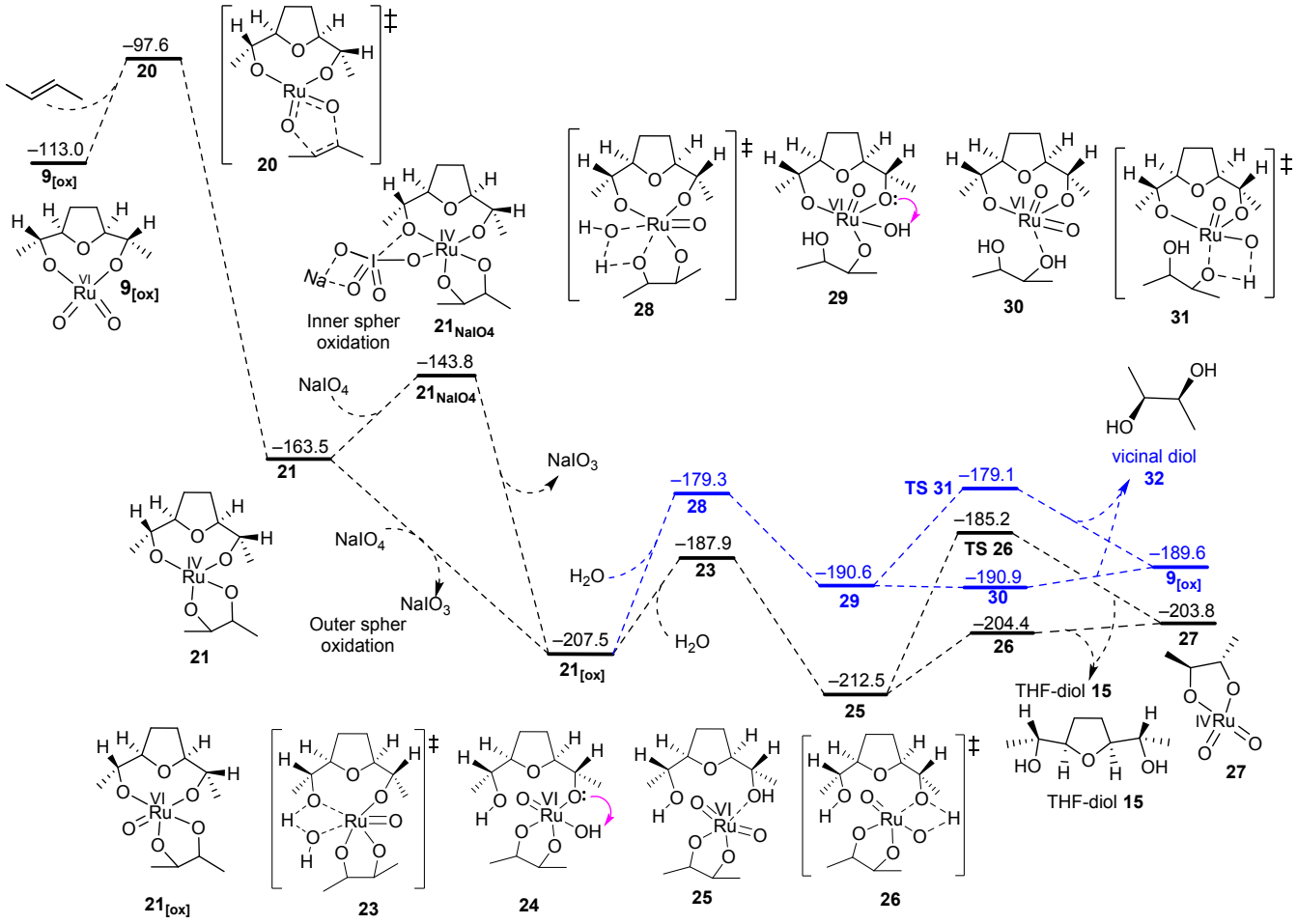

Fig. ESI5 Free energy evaluations for intermolecular ruthenylation of $\mathbf{9}_{[ox]}$ with *E*-but-2-ene (was used as a model for **5** to reduce computational cost), showing reoxidation Ru(IV)→Ru(VI) and hydrolysis to either release THF-diol (**15**, favourable) or vicinal diol (**32**, disfavourable, blue pathway). *E*-but-2-ene was used as a model for **5** to reduce computational cost.

3 Absolute energies and cartesian coordinates

(a) The cartesian coordinates, electronic energies and free energies for the Ru-catalysed oxidative cyclisation of symmetric 1,5-diene (**5**). All energies are in Hartree. Here, t and q refer to triplet and quintet spin multiplicity, respectively.

5

C	1.4931369	0.0609484	0.3782998
C	2.7700589	0.1360594	-0.0052802
H	3.1880929	1.1293954	-0.2266392
H	1.0765419	-0.9312656	0.6076148
C	3.6900959	-1.0265906	-0.1535162
C	0.5739619	1.2317904	0.5103848
H	0.1320679	1.2492614	1.5249678
H	1.1564419	2.1636414	0.3996958
C	-0.5739791	1.2317814	-0.5104282
H	4.5659549	-0.9388396	0.5122578
H	3.1795839	-1.9740206	0.0808628
H	4.0890939	-1.1002596	-1.1798702
H	-1.1564661	2.1636284	-0.3997442
H	-0.1320871	1.2492484	-1.5250122
C	-1.4931451	0.0609334	-0.3783312
C	-2.7700531	0.1360344	0.0052978
H	-1.0765551	-0.9312766	-0.6076732
C	-3.6900811	-1.0266206	0.1535528
H	-3.1880831	1.1293654	0.2266858
H	-4.5659541	-0.9388746	-0.5122032
H	-3.1795691	-1.9740486	-0.0808372
H	-4.0890581	-1.1002916	1.1799148

E_{THF} = -313.007243192

G_{THF} = -312.847811

RuO_4

O	0.9837000	0.9837000	0.9837000
O	-0.9837000	-0.9837000	0.9837000
O	-0.9837000	0.9837000	-0.9837000
O	0.9837000	-0.9837000	-0.9837000
Ru	0.0000000	0.0000000	0.0000000

E_{THF} = -394.515807243

G_{THF} = -394.530558

6

C	1.3487797	1.1568639	0.3261875
H	1.1857607	1.1233209	1.4089425
O	0.1648647	-0.8494801	0.8687285
O	0.9584467	-3.5473911	0.4330375
O	-1.0647213	-2.1915901	-1.1571975
C	0.4073607	1.9805589	-0.4999735

H	0.0766967	2.8454799	0.1039405
H	0.9587287	2.3921069	-1.3633225
C	-0.8316133	1.2540069	-1.0289225
H	-1.4243663	1.9779169	-1.6201165
H	-0.5247833	0.4725559	-1.7502125
C	-1.6934603	0.6418469	0.0317475
H	-1.5545303	0.9893479	1.0649995
O	1.6390767	-1.3258421	-1.2759395
C	2.4891777	0.5904709	-0.1613455
H	2.7634157	0.7902309	-1.2038795
C	-2.6466973	-0.2799581	-0.2135915
H	-2.8388293	-0.5684731	-1.2544495
Ru	0.4284217	-2.0994511	-0.3083085
C	-3.4707183	-0.9316871	0.8370865
H	-3.1879753	-0.5856601	1.8435655
H	-4.5476613	-0.7400901	0.6910725
H	-3.3431023	-2.0271451	0.8022505
C	3.4750687	-0.1262091	0.6896035
H	3.0453237	-0.3697691	1.6742085
H	3.8096027	-1.0610351	0.2127015
H	4.3777347	0.4890739	0.8491865

E_{THF} = -707.540125386

G_{THF} = -707.373114

7

C	-2.0122386	0.0241647	-0.5396084
C	-2.8951396	-0.6266943	0.2225866
H	-3.2747786	-0.1235943	1.1251666
H	-1.6249566	-0.4700643	-1.4402374
O	0.8346774	-0.2878273	-0.9747544
O	2.4793234	-2.7331573	-0.7812054
O	2.2228274	-0.5262153	1.1383976
C	-3.4064056	-1.9995333	-0.0434424
C	-1.4686846	1.3814427	-0.2066034
H	-1.3507236	1.9875007	-1.1245764
H	-2.2022146	1.9133807	0.4241946
C	-0.1369636	1.3547207	0.5452136
H	-3.1608766	-2.6829293	0.7872496
H	-4.5048366	-2.0134923	-0.1479834
H	-2.9676156	-2.4173433	-0.9635214
H	0.0769384	2.3580567	0.9581806
H	-0.2122296	0.6672477	1.4092916
C	1.0632614	0.9584547	-0.2968924
C	2.3241984	0.7720127	0.5247936
H	1.2146374	1.6984707	-1.1090444
C	3.5960764	0.8561877	-0.2878344
H	2.3541794	1.4852437	1.3712146
H	4.4634504	0.5763267	0.3273216
H	3.5487064	0.1729757	-1.1522554
H	3.7489274	1.8802157	-0.6638734
O	-0.0418106	-2.4024743	0.8443976
Ru	1.3322704	-1.8030773	0.0538256

E_{THF} = -707.644755923
G_{THF} = -707.470910

7_{H2O}

C	2.2430355	0.2082816	0.4607478
H	1.7883075	-0.2727334	1.3371548
O	-0.6375325	-0.0120874	0.9557008
O	-2.2037085	-0.1270404	-1.0025642
C	1.7514725	1.5753536	0.0965618
H	1.6977825	2.2183276	0.9960828
H	2.4820315	2.0489306	-0.5827272
C	0.3845515	1.5855506	-0.5929812
H	0.1903275	2.5927816	-1.0070422
H	0.3931865	0.8911886	-1.4558532
C	-0.7864805	1.2484006	0.3123458
H	-0.8498825	1.9930826	1.1327428
C	3.1419785	-0.4751964	-0.2521122
H	3.5897495	0.0089836	-1.1335352
C	-2.1167315	1.1766346	-0.4329222
H	-2.1095155	1.8840006	-1.2865412
Ru	-1.0999615	-1.4699724	-0.1920992
O	0.1948035	-1.8917504	-1.1532882
O	-2.6057475	-2.5967774	-0.5637002
H	-3.1535585	-2.1212564	-1.2143282
O	-1.0738885	-2.4686804	1.4167978
H	-1.6821085	-3.2186544	1.2651808
C	-3.3153105	1.4165876	0.4560878
H	-3.3370135	2.4575986	0.8155348
H	-4.2478415	1.2174686	-0.0918092
H	-3.2732475	0.7471566	1.3315318
C	3.5727645	-1.8702074	0.0424568
H	4.6609855	-1.9394714	0.2119838
H	3.0581535	-2.2643424	0.9331828
H	3.3433985	-2.5421584	-0.8025882

E_{THF} = -784.084545408
G_{THF} = -783.888283

7_{NaIO4}

C	1.7401698	1.9669497	0.1138855
H	1.7689968	2.0111377	-0.9817905
O	0.6524898	-0.2424173	-0.7167065
O	-0.2173642	-2.1014403	0.7383375
C	2.7586468	1.1064137	0.7973285
H	3.6635658	1.0304567	0.1687715
H	3.0731558	1.5775007	1.7454065
C	2.2489088	-0.3034433	1.1063095
H	3.0637368	-0.9214713	1.5247105
H	1.4613758	-0.2547663	1.8811095
C	1.6922668	-0.9976713	-0.1255795
H	2.4863488	-1.1093283	-0.8928205
C	0.7939358	2.6835367	0.7515275

H	0.7914318	2.6875637	1.8511505
C	1.0678608	-2.3602733	0.1845925
H	1.6466868	-2.8705583	0.9802885
Ru	-1.0299962	-0.4624963	0.2101165
O	-0.9793002	0.8232027	1.2982015
O	-2.7390412	-1.3287143	0.5476625
C	0.9299958	-3.2414683	-1.0356455
H	1.9180108	-3.5340103	-1.4252435
H	0.3675228	-4.1522393	-0.7851095
H	0.3850318	-2.7038273	-1.8293955
C	-0.2201892	3.5257067	0.0615585
H	-0.0736542	4.5972087	0.2843555
H	-0.1740592	3.3901287	-1.0302915
H	-1.2415782	3.2724597	0.3906885
I	-3.8921842	-0.7653533	-0.9601795
O	-3.9164752	-1.7940373	-2.4242805
O	-5.3791892	-1.2204613	0.0026505
O	-4.4203252	0.9806087	-1.1380805
O	-1.9006132	-0.0557403	-1.3498475
Na	-6.3261692	0.7668447	0.0563185

E_{THF} = -1181.96155653

G_{THF} = -1181.785427

$7t_{NaIO4}$

C	1.9084075	1.7379575	-0.4882315
H	1.2430735	1.4761325	-1.3209215
O	0.4730745	-0.8091685	-0.9920215
O	-0.5007335	-1.8871505	1.0487045
C	2.8733825	0.6889225	-0.0352815
H	3.4360185	0.2840675	-0.8989285
H	3.6182765	1.1526315	0.6353525
C	2.2127565	-0.4770525	0.7052565
H	2.9890045	-1.0695325	1.2249655
H	1.5400825	-0.0834735	1.4906055
C	1.4494555	-1.4353615	-0.1937525
H	2.1617375	-1.9179915	-0.8983355
C	1.7756745	2.9336975	0.0919645
H	2.4419255	3.1883385	0.9302525
C	0.6980545	-2.5165715	0.5931835
H	1.2643125	-2.7959015	1.5041315
Ru	-1.2140455	-0.5264885	-0.0480205
O	-0.9678345	1.1149745	0.4438785
O	-3.0412275	-0.6395915	1.0700235
C	0.3589855	-3.7358005	-0.2300425
H	1.2703665	-4.2938915	-0.4978175
H	-0.3080455	-4.4056385	0.3318745
H	-0.1504565	-3.4319795	-1.1599315
C	0.7618315	3.9523185	-0.2985565
H	1.2274905	4.9112545	-0.5854245
H	0.1486555	3.5961995	-1.1412905
H	0.0785445	4.1713155	0.5407525
I	-4.4727015	-0.3752625	-0.0827115

O	-5.0708365	-1.8004965	-0.9771885
O	-5.7261475	0.1609835	1.1180735
O	-4.3939625	1.2142655	-0.9698275
O	-2.3194525	-0.7096035	-1.3929885
Na	-5.7656655	2.3278955	0.4822545

E_{THF} = -1181.93078492

G_{THF} = -1181.757686

$7_{[ox]}$

C	2.0320542	0.2328694	0.3511352
C	2.5423352	-0.8362596	-0.2949138
H	2.6901052	-0.7679666	-1.3796648
H	1.9144502	0.1797634	1.4372172
O	-0.5382978	-0.1005006	0.8231942
O	-1.2510688	-2.4884706	1.3848212
O	-2.2503808	-0.3301336	-0.9260468
C	2.9954432	-2.0949556	0.3709902
C	1.6195752	1.5053474	-0.3369858
H	1.7186642	2.3510404	0.3614462
H	2.2970392	1.7032254	-1.1818928
C	0.1799002	1.4630084	-0.8705918
H	2.5262332	-2.9700026	-0.1040348
H	4.0861222	-2.2163746	0.2738192
H	2.7367482	-2.0941356	1.4389012
H	-0.0862948	2.4331204	-1.3213468
H	0.0995232	0.6992294	-1.6623138
C	-0.8245378	1.1302384	0.2263812
C	-2.2503588	0.9378744	-0.3096258
H	-0.8146618	1.8996114	1.0213392
C	-3.3092848	1.0148814	0.7746792
H	-2.4558618	1.6562154	-1.1233298
H	-4.2830208	0.7122544	0.3681552
H	-3.0437488	0.3400074	1.6033042
H	-3.3895548	2.0383124	1.1686572
O	0.3736822	-1.9653576	-0.8551818
Ru	-1.1422348	-1.7423376	-0.1257548
O	-2.1725708	-2.6905046	-1.1123568

E_{THF} = -782.744546776

G_{THF} = -782.566809

7t

C	1.9632103	0.2940514	0.5227880
C	2.8340103	-0.3965256	-0.2190520
H	3.1223563	0.0117754	-1.2000020
H	1.6670073	-0.1088416	1.5000460
O	-0.8222827	-0.3737426	0.9240800
O	-1.3896437	-2.9931286	0.9918540
O	-2.2083767	-0.7038226	-1.1266730
C	3.4432193	-1.6971086	0.1718250
C	1.3132993	1.5677324	0.0724380
H	1.1656133	2.2508274	0.9293630

H	1.9867753	2.0904684	-0.6291430
C	-0.0287937	1.3626804	-0.6338310
H	3.2072943	-2.4816336	-0.5668710
H	4.5436283	-1.6332696	0.2260840
H	3.0688373	-2.0332576	1.1519700
H	-0.3768697	2.3223184	-1.0582860
H	0.1054623	0.6737634	-1.4897290
C	-1.1335347	0.8459674	0.2704150
C	-2.4392627	0.5509364	-0.4886200
H	-1.3069077	1.5744494	1.0907050
C	-3.6482587	0.4735694	0.4122080
H	-2.5924387	1.2897464	-1.2994810
H	-4.5271277	0.1357404	-0.1556470
H	-3.4646327	-0.2385756	1.2333460
H	-3.8735857	1.4593044	0.8487810
O	0.3693803	-2.3705566	-1.1946870
Ru	-0.9783787	-1.8728676	-0.2838820

E_{THF} = -707.622806270

G_{THF} = -707.452549

$7t_{H2O}$

C	2.2940895	-0.1742678	0.4489075
H	1.6308715	-0.7460078	1.1101745
O	-0.6176675	0.1135712	0.9833025
O	-2.0788475	0.1217482	-1.0761065
C	1.9656735	1.2715152	0.2462165
H	1.9058665	1.7942032	1.2211475
H	2.7897875	1.7495062	-0.3120235
C	0.6601025	1.5087672	-0.5144945
H	0.6447175	2.5353772	-0.9252165
H	0.5993355	0.8180442	-1.3776015
C	-0.6030715	1.3468312	0.3244645
H	-0.6247785	2.1392062	1.1057615
C	3.2993415	-0.8085178	-0.1595185
H	3.9567365	-0.2323078	-0.8283615
C	-1.8821225	1.4234882	-0.5080915
H	-1.7421085	2.1065232	-1.3684135
Ru	-1.5921505	-1.3329248	0.0346815
O	-0.1548285	-2.2400178	-0.1847065
O	-2.6682585	-2.4530368	-1.1481205
H	-3.2359505	-1.8667768	-1.6764795
O	-2.6325725	-1.8491898	1.5053045
H	-3.2308005	-2.5562648	1.1953195
C	-3.0991485	1.8128952	0.2984985
H	-3.0208815	2.8568342	0.6410975
H	-4.0136315	1.7138052	-0.3045185
H	-3.1900455	1.1647452	1.1870575
C	3.5978395	-2.2601468	-0.0058475
H	4.6138285	-2.4292158	0.3912405
H	2.8771065	-2.7435658	0.6719915
H	3.5515675	-2.7848198	-0.9756645

E_{THF} = -784.045922537

G_{THF} = -783.852250

8

C	-1.7299792	0.4569954	-0.4210914
H	-1.7725282	0.3810264	-1.5120514
O	0.3646678	-0.2176656	-0.7691854
O	-0.9091292	-1.6535106	1.0911996
O	1.9932598	-0.8225796	1.1200906
C	-1.2352522	1.7368364	0.1741426
H	-1.1792342	2.5114264	-0.6092164
H	-1.9456372	2.0982894	0.9388656
C	0.1467008	1.5616884	0.8079696
H	0.5590468	2.5310134	1.1374616
H	0.0809198	0.9128134	1.6998136
C	1.0635858	0.9011524	-0.2082334
H	1.2762448	1.5965364	-1.0459754
O	1.1367038	-3.2701646	-0.5275364
Ru	0.6311538	-1.8487526	0.2477096
C	2.3490568	0.3530414	0.3962696
H	2.7471108	1.0647074	1.1493346
C	-2.3364442	-0.5567316	0.3181596
H	-2.6200002	-0.3051626	1.3470806
C	3.4074678	0.0556684	-0.6435074
H	3.7644328	0.9802624	-1.1251674
H	4.2650728	-0.4484786	-0.1746284
H	3.0031648	-0.6091386	-1.4256894
C	-3.1128422	-1.6394066	-0.3565804
H	-3.2108052	-2.5181766	0.2960236
H	-4.1286652	-1.2975216	-0.6199954
H	-2.6080722	-1.9541686	-1.2852624

E_{THF} = -707.630654506

G_{THF} = -707.455962

8_{H2O}

C	-1.9756412	0.3040198	-0.3334826
H	-2.0628772	0.2967328	-1.4238606
O	0.1365838	0.2370618	-0.7529526
O	-0.5293632	-1.6693982	1.0234664
O	2.0631778	0.0396678	0.9763184
C	-1.8714062	1.6237638	0.3645204
H	-2.0691022	2.4407638	-0.3492626
H	-2.6312832	1.6949178	1.1619374
C	-0.4721002	1.7947028	0.9522584
H	-0.3149252	2.8161458	1.3388144
H	-0.3190752	1.0966248	1.7956094
C	0.5136658	1.4673668	-0.1548726
H	0.4724518	2.2585768	-0.9335336
Ru	0.9557158	-1.3010832	0.2381994
C	1.9507868	1.3075108	0.3413894
H	2.1561428	2.0656128	1.1247834

C	-2.2764642	-0.8763482	0.3399964
H	-2.5655392	-0.7883712	1.3938874
O	2.2045228	-2.6143892	1.0086094
H	1.9984068	-3.5062192	0.6880544
O	1.2342218	-2.1439602	-1.4276326
H	1.8626198	-2.8712932	-1.2629736
C	2.9687068	1.4115338	-0.7733546
H	2.9672158	2.4192648	-1.2188166
H	3.9760488	1.1989388	-0.3870916
H	2.7371928	0.6790368	-1.5651656
C	-2.6933632	-2.1037982	-0.3945656
H	-2.5229602	-3.0061752	0.2104334
H	-3.7679862	-2.0685152	-0.6459776
H	-2.1253722	-2.2026922	-1.3347346

E_{THF} = -784.065460975

G_{THF} = -783.866579

$8_{[ox]}$

C	1.9887446	0.2611839	0.3342100
H	1.9091896	0.2438659	1.4243450
O	-0.4796404	-0.0865591	0.7915990
O	0.4366026	-1.9446941	-0.8783540
O	-2.2252474	-0.3454261	-0.9297080
C	1.6021826	1.5266589	-0.3790840
H	1.7188546	2.3823209	0.3037450
H	2.2807086	1.6933409	-1.2298140
C	0.1577906	1.4954599	-0.9019440
H	-0.1142154	2.4705739	-1.3370760
H	0.0659816	0.7388619	-1.6989260
C	-0.8174684	1.1396729	0.2140070
H	-0.8099244	1.9080869	1.0098090
O	-1.1772954	-2.4937541	1.3644290
Ru	-1.0878074	-1.7414961	-0.1453900
C	-2.2482614	0.9122789	-0.2953080
H	-2.4933724	1.6377319	-1.0916810
C	2.4717766	-0.8397891	-0.2939070
H	2.6197996	-0.7962321	-1.3790170
O	-2.0939274	-2.7126041	-1.1393450
C	-3.2827824	0.9441379	0.8150740
H	-3.3800714	1.9579979	1.2294670
H	-4.2576274	0.6231279	0.4257970
H	-2.9806744	0.2617989	1.6249600
C	2.9517196	-2.0675401	0.4092260
H	2.5339596	-2.9692351	-0.0625900
H	4.0492076	-2.1432331	0.3464460
H	2.6617966	-2.0565361	1.4690300

E_{THF} = -782.745269680

G_{THF} = -782.565999

8_{NaIO4}

C	-1.7692302	1.6246225	0.5061152

H	-1.7204272	1.5420315	1.5963482
O	-0.6633112	-0.3297355	0.7189832
O	0.1735918	-1.8600055	-1.1569258
C	-2.9083622	0.9623655	-0.2009868
H	-3.7193572	0.7548245	0.5172572
H	-3.3198602	1.6373405	-0.9715238
C	-2.4659682	-0.3501115	-0.8555968
H	-3.3338982	-0.9273215	-1.2177938
H	-1.8254752	-0.1402155	-1.7314188
C	-1.6728762	-1.1508835	0.1618802
H	-2.3380132	-1.4809035	0.9872932
C	-0.8865512	2.4887445	-0.1083478
H	-1.1172442	2.8075555	-1.1314508
C	-0.9479092	-2.3588275	-0.4394818
H	-1.6002492	-2.8518325	-1.1885838
Ru	0.9396918	-0.2828675	-0.4296128
O	0.5616528	1.2491355	-1.1068878
O	2.6477678	-0.7009565	-1.3309178
C	-0.4951182	-3.3495645	0.6095392
H	-1.3568192	-3.8095995	1.1191482
H	0.1031678	-4.1458805	0.1440422
H	0.1301628	-2.8428905	1.3636992
C	0.1309168	3.2587055	0.6577042
H	-0.2938692	4.2049115	1.0377452
H	0.4937148	2.6754125	1.5199592
H	0.9961238	3.5144545	0.0288802
I	4.0043348	-0.4684665	0.0604682
O	4.4029668	-1.8311785	1.1534052
O	5.3517088	-0.4427485	-1.1772268
O	4.3725668	1.2309335	0.6501752
O	2.0534418	-0.2154145	1.0030662
Na	6.0727298	1.5883665	-0.7889538

E_{THF} = -1181.95971009

G_{THF} = -1181.781490

$8t_{NaIO4}$

C	-1.5612435	1.6422128	0.5408423
H	-1.5141035	1.5983598	1.6330853
O	-0.7331705	-0.5848482	0.8800853
O	0.1762835	-2.0815872	-0.9785197
C	-2.7201055	1.0254748	-0.1597967
H	-3.5398345	0.8754028	0.5626713
H	-3.0868405	1.7224538	-0.9366557
C	-2.3943065	-0.3234242	-0.8287097
H	-3.3219905	-0.7658422	-1.2315397
H	-1.7153035	-0.1634802	-1.6845637
C	-1.7412255	-1.2581342	0.1857613
H	-2.5113875	-1.5883772	0.9183503
C	-0.5474645	2.3807788	-0.1150827
H	-0.7913025	2.7712048	-1.1108647
C	-1.0826495	-2.4874002	-0.4433287
H	-1.6770605	-2.8483102	-1.3088057

Ru	0.9046055	-0.4524342	-0.3283667
O	0.4905715	1.0333058	-1.1954747
O	2.6191865	-0.7939982	-1.1819797
C	-0.8643055	-3.6003342	0.5565613
H	-1.8240235	-4.0272102	0.8899353
H	-0.2584935	-4.4026312	0.1110123
H	-0.3308215	-3.2045612	1.4364423
C	0.5330395	3.0463198	0.6550023
H	0.7854395	4.0266938	0.2261773
H	0.2375305	3.1699488	1.7085373
H	1.4661635	2.4484348	0.6618413
I	3.9357695	-0.0668862	0.1351613
O	4.6949425	-0.9961422	1.4693033
O	5.2241845	0.0209988	-1.1622517
O	3.8482125	1.7644898	0.3237483
O	1.9641675	-0.0802102	1.0936263
Na	5.3355365	2.1997338	-1.3222047

E_{THF} = -1181.91582028

G_{THF} = -1181.740922

8t

C	-1.8697202	0.4315714	-0.4668074
H	-1.9150992	0.2643484	-1.5488964
O	0.5977638	-0.2479676	-0.9396944
O	-0.9289182	-1.8035776	0.8406336
O	2.0450568	-0.8516886	1.0783526
C	-1.2300822	1.6832294	0.0364076
H	-1.1008262	2.3941804	-0.7974354
H	-1.9021242	2.1719094	0.7665266
C	0.1244858	1.4543914	0.7146746
H	0.5085188	2.4089274	1.1170766
H	0.0020738	0.7719054	1.5758566
C	1.1415238	0.8686604	-0.2507104
H	1.3829718	1.6174504	-1.0352854
O	1.0699128	-3.1654816	-0.8926804
Ru	0.7236948	-1.8615016	0.1520816
C	2.4049838	0.3798584	0.4459026
H	2.6908328	1.0744104	1.2613296
C	-2.4092472	-0.5447596	0.3593706
H	-2.5093952	-0.2967996	1.4243796
C	3.5630818	0.1662284	-0.5009974
H	3.9218298	1.1244974	-0.9103314
H	4.3975268	-0.3254976	0.0199336
H	3.2495828	-0.4746786	-1.3419584
C	-3.3087422	-1.6059126	-0.1715934
H	-3.3217942	-2.4846706	0.4878476
H	-4.3423132	-1.2247576	-0.2489084
H	-2.9855782	-1.9242756	-1.1750734

E_{THF} = -707.610606792

G_{THF} = -707.439343

$8t_{H2O}$

C	2.2016932	-0.3161098	0.1789267
H	2.3316562	-0.1114618	1.2480297
O	-0.0184178	0.1824652	0.6748877
O	-0.5836888	-1.5852358	-1.5463423
O	-2.1433568	0.8462202	-0.6975763
C	2.3144442	0.8223442	-0.7791233
H	2.9012532	1.6378712	-0.3245963
H	2.8523142	0.4978422	-1.6870623
C	0.9274212	1.3557922	-1.1809513
H	1.0153422	2.3450282	-1.6614423
H	0.4534212	0.6705432	-1.9041563
C	0.0804262	1.4332072	0.0779867
H	0.5582612	2.1455142	0.7891247
Ru	-1.5564228	-0.9140298	-0.3013013
C	-1.3786578	1.9067792	-0.1646123
H	-1.3663188	2.7083632	-0.9316103
C	2.0174712	-1.6124718	-0.2008813
H	1.9584912	-1.8368668	-1.2739563
O	-3.2988348	-1.6249698	-0.8697513
H	-3.1767898	-2.5398518	-1.1694033
O	-1.7472788	-1.8930758	1.2965437
H	-2.6313738	-2.3038578	1.2420907
C	-2.0150828	2.3992432	1.1175857
H	-1.5122878	3.3038912	1.4948637
H	-3.0759128	2.6322052	0.9455127
H	-1.9482238	1.6128862	1.8880397
C	1.7766822	-2.7156998	0.7501327
H	0.7139142	-3.0221988	0.6970157
H	2.3707582	-3.6110708	0.5035947
H	1.9790962	-2.4132958	1.7884327

E_{THF} = -784.040177843

G_{THF} = -783.847598

8q

C	2.0590580	0.4185126	0.6612087
H	2.8146430	0.2695986	1.4461297
O	-1.0913360	-0.3321514	1.3037307
O	1.2703260	-2.1231324	0.2736027
O	-1.5071210	-0.8582294	-1.1368313
C	1.0203720	1.4422876	0.9781717
H	0.6633810	1.2646016	2.0095817
H	1.5570580	2.4102336	1.0358467
C	-0.1708670	1.5591206	0.0325627
H	-0.4496390	2.6187296	-0.0927383
H	0.1029450	1.2073566	-0.9767763
C	-1.4173060	0.8044796	0.5136107
H	-2.0216010	1.4672216	1.1674477
O	-0.7661720	-3.5209494	0.7583437
Ru	-0.5987760	-1.8636554	0.2287507
C	-2.2367420	0.2774576	-0.6620283
H	-2.2533470	1.0223436	-1.4845363

C	2.2319240	-0.3117884	-0.4820473
H	1.5363790	-0.1690044	-1.3192953
C	-3.6479140	-0.1148184	-0.2901133
H	-4.2445310	0.7727916	-0.0236983
H	-4.1383260	-0.6249064	-1.1319933
H	-3.6399540	-0.7980504	0.5755607
C	3.4835380	-1.0612344	-0.7822703
H	4.0286810	-1.3096404	0.1408187
H	3.2692190	-1.9950204	-1.3210863
H	4.1461070	-0.4521524	-1.4219513

E_{THF} = -707.564976753

G_{THF} = -707.396510

$8q_{H2O}$

C	1.6401197	1.1171877	0.4451387
H	1.7564697	0.9339147	1.5185557
O	-0.4981893	0.1186037	0.9950397
O	0.8907827	-1.0462593	-1.3049413
O	-1.8280963	-0.9297063	-0.9281113
C	0.8230937	2.2612177	-0.0297193
H	0.5755497	2.9263337	0.8134897
H	1.4159897	2.8476357	-0.7573033
C	-0.4715623	1.7958447	-0.7146473
H	-1.0265463	2.6687157	-1.0985873
H	-0.2373613	1.1428297	-1.5737503
C	-1.3047583	1.0220257	0.3001447
H	-1.7401763	1.7395447	1.0319687
Ru	-0.2202933	-1.6204763	-0.0125413
C	-2.4300983	0.1982517	-0.3593163
H	-2.8840493	0.7996147	-1.1778713
C	2.3928757	0.3194547	-0.4331323
H	2.4261247	0.6259307	-1.4851093
O	-0.3997323	-3.4657103	-0.5591693
H	-0.3084713	-3.5631593	-1.5200903
O	0.9869897	-2.1513513	1.4387347
H	1.1445177	-3.1059773	1.3494817
C	-3.4965403	-0.1952233	0.6441317
H	-4.0400173	0.6858207	1.0236067
H	-4.2210503	-0.8803333	0.1797247
H	-3.0306493	-0.7103673	1.5014027
C	3.3412927	-0.6932473	0.0617457
H	3.7932867	-1.2726563	-0.7524753
H	4.1444857	-0.2014683	0.6416777
H	2.8060137	-1.3669893	0.7619217

E_{THF} = -784.014172522

G_{THF} = -783.822596

$8q_{NaIO4}$

C	-1.7525814	1.5870458	0.4888344
H	-1.8166104	1.6030778	1.5820804
O	-0.7382224	-0.2672302	0.6894694

O	0.1480536	-1.8910192	-1.1067186
C	-2.8794904	0.9526408	-0.2657106
H	-3.7227664	0.7908658	0.4259454
H	-3.2305184	1.6433418	-1.0522796
C	-2.4734694	-0.3834082	-0.8866726
H	-3.3566034	-0.9362762	-1.2469156
H	-1.8057014	-0.2231412	-1.7538816
C	-1.7000024	-1.1626142	0.1632584
H	-2.3786174	-1.4716862	0.9875614
C	-0.8741634	2.5153918	-0.0854876
H	-0.8791744	2.6182748	-1.1781826
C	-0.9694744	-2.3759022	-0.4148066
H	-1.6438254	-2.8819672	-1.1410396
Ru	1.0666506	-0.3582602	-0.2582976
O	1.2196366	1.4675648	-0.1316636
O	2.7091946	-0.4839022	-1.4632166
C	-0.5535604	-3.3622682	0.6593824
H	-1.4308614	-3.8038002	1.1608764
H	0.0410536	-4.1720682	0.2124044
H	0.0722566	-2.8620842	1.4179344
C	-0.1899134	3.5471078	0.7269974
H	-0.8879154	4.3818168	0.9332094
H	0.1322356	3.1309428	1.6941934
H	0.6878696	3.9564348	0.2120654
I	4.1747626	-0.6639622	-0.2592016
O	4.6353636	-2.2986332	0.3085824
O	5.4033856	-0.2183832	-1.5356496
O	4.5990816	0.7647218	0.8047164
O	2.3305766	-0.8206702	0.9714204
Na	6.0633516	1.6780508	-0.6592076

E_{THF} = -1181.86799996

G_{THF} = -1181.696370

9

C	1.2081653	0.7548328	0.2253810
H	1.5130933	1.2169108	1.1827140
O	-0.0244587	0.0284908	0.4763500
O	1.5773913	-1.1102832	-1.1852860
O	-1.7297887	-1.0465712	-1.1541020
C	0.8646463	1.8078858	-0.8337100
H	1.1628173	2.8088978	-0.4879740
H	1.4110853	1.6001108	-1.7658410
C	-0.6482107	1.6992708	-1.0502180
H	-1.1491877	2.6774218	-1.0902520
H	-0.8681327	1.1634058	-1.9872480
C	-1.1546017	0.8625108	0.1124750
H	-1.4128327	1.4773518	0.9967240
O	-0.1187197	-3.5516552	-0.3323980
C	-2.2657157	-0.1154452	-0.2408880
H	-3.0492917	0.4533198	-0.7860230
C	2.2107173	-0.3048032	-0.2158870
H	3.0461733	0.2170738	-0.7292690

C	-2.8790467	-0.7796562	0.9750650
H	-3.3919347	-0.0453562	1.6175970
H	-3.6101687	-1.5375542	0.6579960
H	-2.1006377	-1.2829222	1.5736850
C	2.7673613	-1.1121292	0.9401500
H	3.4059763	-1.9213722	0.5561910
H	3.3694033	-0.4818012	1.6152260
H	1.9519923	-1.5693662	1.5273190
Ru	-0.0860937	-1.9085682	-0.5977770

E_{THF} = -707.710409087

G_{THF} = -707.531105

9_{H2O}

C	1.2343791	-1.1244826	0.1608449
H	1.8973621	-1.4014856	1.0025899
O	0.4578061	0.0229234	0.5715329
O	-0.7683039	-1.7266256	-0.9941991
O	-0.9201719	1.6411564	-1.0093071
C	2.0266941	-0.6804756	-1.0679561
H	3.0587511	-1.0576556	-1.0225381
H	1.5619931	-1.0950576	-1.9761521
C	1.9578831	0.8508554	-1.0742861
H	2.9519061	1.3194414	-1.0318551
H	1.4586771	1.2145474	-1.9859591
C	1.1278781	1.2321694	0.1506989
H	1.7626051	1.5752004	0.9899109
C	0.0216111	2.2402264	-0.1342001
H	0.4761001	3.0821214	-0.6968241
C	0.2235601	-2.2306686	-0.1144961
H	0.7520791	-3.0331326	-0.6700191
O	-3.3124509	-0.1545506	-1.2648361
H	-3.2487869	-0.1550506	-2.2300401
O	-2.5236749	-0.1083346	1.1294219
H	-3.4501219	-0.1512196	0.8151349
C	-0.6507609	2.7654424	1.1172949
H	0.0741181	3.2918564	1.7588319
H	-1.4489949	3.4701274	0.8422329
H	-1.1063049	1.9439574	1.6936059
C	-0.3989199	-2.8032406	1.1420379
H	-1.1298329	-3.5799336	0.8738549
H	0.3704521	-3.2557506	1.7881349
H	-0.9273009	-2.0211336	1.7109169
Ru	-1.5282319	-0.0712266	-0.4743761

E_{THF} = -784.147828776

G_{THF} = -783.944377

9_{NaIO4}

C	-1.5153033	-1.0603548	-0.6356011
H	-1.4823133	-1.4985428	-1.6425111
O	-0.7774283	0.1929372	-0.7263441
O	0.4540247	-1.6394078	0.7908849

O	0.3462137	1.5522712	1.2638259
C	-2.9180883	-0.6375888	-0.1952501
H	-3.5340233	-0.3643678	-1.0638431
H	-3.4297033	-1.4381018	0.3550649
C	-2.6179633	0.6037982	0.6516759
H	-3.4986433	1.2331722	0.8303809
H	-2.1734443	0.3274272	1.6220249
C	-1.5733733	1.2986452	-0.2040421
H	-2.0476173	1.7942682	-1.0671291
C	-0.6004813	2.2683562	0.4785049
H	-1.1777123	2.8886472	1.1861129
C	-0.8544083	-2.0159118	0.3914149
H	-1.4669513	-2.0007948	1.3128329
O	2.8023347	0.0135572	1.3788139
C	0.1251607	3.1548132	-0.5248391
H	-0.5858143	3.7776372	-1.0870061
H	0.8295327	3.8067452	0.0078899
H	0.7022987	2.5390422	-1.2333161
C	-0.8098923	-3.4342848	-0.1513941
H	-0.3941813	-4.1100398	0.6063779
H	-1.8187283	-3.7825858	-0.4218581
H	-0.1682403	-3.4664368	-1.0442581
Ru	1.0769917	0.0759452	0.3696049
I	4.1174307	0.3420462	0.0456449
O	4.3994917	2.0303362	-0.4646281
O	2.2326487	0.3359052	-0.9855441
O	5.4889817	-0.0504578	1.1770679
O	4.5870527	-0.9919918	-1.1047141
Na	6.2821477	-1.7446818	0.0841549

E_{THF} = -1182.04195156

G_{THF} = -1181.854119

$9t_{NaIO4}$

C	-1.3058792	-0.4396516	-1.1841592
H	-1.1414302	-1.0317226	-2.1009452
O	-0.0044182	0.0521804	-0.7988552
O	-0.8980902	-2.2575396	0.3637868
O	0.4209498	-0.1049026	1.6922638
C	-2.1104022	0.8299844	-1.3932982
H	-1.8824252	1.2631744	-2.3802032
H	-3.1963232	0.6605744	-1.3388482
C	-1.5872132	1.7239314	-0.2730072
H	-1.7169772	2.7968674	-0.4772582
H	-2.1069642	1.5039344	0.6753038
C	-0.1147012	1.3370674	-0.1731952
H	0.5234468	2.0208164	-0.7633172
C	0.4498458	1.2184744	1.2676148
H	-0.2409872	1.7655264	1.9465248
C	-1.8556312	-1.3486726	-0.0845512
H	-2.1691532	-0.7051556	0.7715338
O	1.2943658	-2.8959536	1.6946108
C	1.8209688	1.8759614	1.3803378

H	1.7246188	2.9689154	1.2683878
H	2.2375818	1.6762574	2.3842128
H	2.4966538	1.5125184	0.5886938
C	-3.0488062	-2.1468776	-0.5750252
H	-3.3987282	-2.8161766	0.2235678
H	-3.8863122	-1.4963526	-0.8749152
H	-2.7541332	-2.7694406	-1.4356382
Ru	0.9493318	-1.6348956	0.5579948
I	3.8455728	-0.9268726	-0.9110082
O	2.9453188	-0.9300176	0.7840528
O	1.5755538	-2.0817126	-1.0274422
O	5.3964518	-0.4000966	-0.0602272
O	3.2131058	0.6040604	-1.6264822
Na	4.5248088	0.1757964	1.8794888

E_{THF} = -1182.06177322

G_{THF} = -1181.879657

$9q_{NaIO4}$

C	-1.2767970	-1.1890150	-0.6761689
H	-0.9272860	-1.8636920	-1.4775159
O	-0.5919140	0.0591790	-0.8754639
O	0.4805720	-1.6828960	0.8547391
O	-0.0530280	1.2025500	1.3787341
C	-2.7496540	-0.8304660	-0.7673509
H	-3.0598870	-0.7616410	-1.8226609
H	-3.3977820	-1.5681770	-0.2703979
C	-2.7756780	0.5397730	-0.1046969
H	-3.6411040	1.1517870	-0.3979669
H	-2.7905000	0.4478380	0.9949581
C	-1.4610340	1.1626070	-0.5507029
H	-1.5952890	1.7517050	-1.4782049
C	-0.7724500	2.0428720	0.5097181
H	-1.5694960	2.5204460	1.1180521
C	-0.8940710	-1.8147430	0.6789341
H	-1.4353680	-1.2672620	1.4830471
O	3.1624510	-0.8691670	0.9348211
C	0.0941340	3.1204080	-0.1098339
H	-0.5402330	3.8413480	-0.6512279
H	0.6549310	3.6578020	0.6688781
H	0.8265310	2.6897440	-0.8094979
C	-1.2609520	-3.2839310	0.7250201
H	-0.9806720	-3.7093110	1.6991901
H	-2.3406340	-3.4448720	0.5749551
H	-0.7076260	-3.8304330	-0.0559079
Ru	1.3775740	0.0514390	0.7647531
I	4.4118650	0.3646870	0.1226311
O	5.0588870	1.6954600	1.1291681
O	2.5418800	1.3199010	-0.0196149
O	5.7247710	-0.9118060	0.1433831
O	4.4612670	0.5001970	-1.7033909
Na	6.0265920	-1.0923310	-2.0103799

E = -1181.99187483

G = -1181.815803

$9_{[ox]}$

C	1.0417263	-1.1663308	0.3412305
H	1.5356673	-1.6466878	1.2070525
O	0.5026713	0.0844402	0.7635995
O	-0.8838337	-1.2710048	-1.0111495
O	-1.3425237	1.5581402	-0.9572445
C	2.0268123	-0.8498828	-0.7811225
H	3.0373523	-0.7119758	-0.3619095
H	2.0811773	-1.6588808	-1.5249975
C	1.5033423	0.4628502	-1.3468175
H	2.2861583	1.0727192	-1.8220195
H	0.6986403	0.2898572	-2.0766135
C	0.9459413	1.1341342	-0.1047955
H	1.7503873	1.6961362	0.4170525
O	-2.5629867	0.3353832	1.2831565
C	-0.1966657	2.1100762	-0.3349215
H	0.1715993	2.8464592	-1.0813045
C	-0.1420797	-2.0364088	-0.1057675
H	0.2489743	-2.8906658	-0.6978275
O	-3.4888067	-0.5071348	-1.3752895
C	-0.5891757	2.8333412	0.9390355
H	0.2642573	3.4171512	1.3199885
H	-1.4259657	3.5200782	0.7468135
H	-0.8881617	2.1175512	1.7203555
C	-0.9401927	-2.5693818	1.0694395
H	-1.8684537	-3.0512938	0.7234265
H	-0.3482197	-3.3193648	1.6172045
H	-1.1981447	-1.7600998	1.7728735
Ru	-2.2194977	-0.0392058	-0.3394495

E_{THF} = -782.850685761

G_{THF} = -782.669620

$9_{[ox][NaIO4]}$

C	-1.9179640	-0.8428380	-0.4872800
H	-2.0576080	-1.6086960	-1.2701500
O	-0.9869510	0.1147460	-1.0340810
O	-0.0274200	-1.9374710	0.5611970
O	0.5692290	0.6276940	0.8712230
C	-3.1529640	-0.0062450	-0.2054190
H	-3.7016000	0.1789990	-1.1425070
H	-3.8451970	-0.4841380	0.5035550
C	-2.5360650	1.2812360	0.3303820
H	-3.1845740	2.1592580	0.1982290
H	-2.3203450	1.1932080	1.4086490
C	-1.2372280	1.4091920	-0.4608300
H	-1.3513910	2.1081810	-1.3088730
O	1.1552030	-1.3392240	-1.9007740
C	0.0089300	1.8046360	0.3672450
H	-0.3351640	2.3654930	1.2623130

C	-1.3386000	-1.5076100	0.7659720
H	-1.3229060	-0.7575930	1.5889940
O	2.6065010	-1.6062640	0.5339030
C	0.9556850	2.6879970	-0.4218420
H	0.4528340	3.6462720	-0.6350760
H	1.8743880	2.8856020	0.1455000
H	1.2440730	2.2244960	-1.3780620
C	-2.1473230	-2.7172700	1.1958250
H	-1.6673120	-3.1894160	2.0641830
H	-3.1770550	-2.4435280	1.4741110
H	-2.1849610	-3.4590610	0.3817160
Ru	1.2290980	-0.7681610	-0.3209560
I	4.3090990	-0.3994660	-0.0045860
O	4.7707540	-0.1850550	1.7100200
O	2.7305970	0.5136710	-0.6676590
O	4.9103910	-1.8891350	-0.8828720
O	5.3928520	0.7280850	-0.9557980
Na	6.2829930	-0.7875940	-2.2862510

E_{THF} = -1257.17637437

G_{THF} = -1256.990454

$9_{[ox][ox]}$

C	0.9983878	-1.4794843	0.2194079
H	1.3185798	-2.3170383	0.8678959
O	1.0539688	-0.2979593	0.9940139
O	-0.7250412	-0.5998813	-0.9724241
O	-0.6721162	1.7933077	-0.8684491
C	1.9534678	-1.2432873	-0.9460091
H	2.9632958	-1.5765603	-0.6595421
H	1.6591788	-1.8042643	-1.8462701
C	1.9191948	0.2729687	-1.1532161
H	2.9101258	0.6769307	-1.4078381
H	1.2201078	0.5504357	-1.9542191
C	1.4231338	0.8140737	0.1887299
H	2.2354968	1.3233797	0.7439579
O	-2.9644182	1.3114297	0.3985799
C	0.3138718	1.9026997	0.1080569
H	0.8831638	2.7911157	-0.2574821
C	-0.4646172	-1.7411093	-0.1946931
H	-0.5242472	-2.6475533	-0.8334981
O	-3.1410492	-0.8942543	-1.0550341
C	-0.2540612	2.2037987	1.4811099
H	0.5631878	2.4402637	2.1815759
H	-0.9453342	3.0573787	1.4417619
H	-0.7916852	1.3328567	1.8867109
C	-1.3369732	-1.9153373	1.0338409
H	-2.3684302	-2.1802673	0.7697219
H	-0.9214602	-2.7166963	1.6647769
H	-1.3390952	-0.9856573	1.6278769
Ru	-2.2669942	0.5974407	-0.9904191
O	-2.6996372	1.3312697	-2.4689231

E_{THF} = -857.942746311

G_{THF} = -857.759317

9t

C	1.1773964	0.8774634	0.1424178
H	1.5554604	1.4905794	0.9846138
O	-0.0057716	0.1959874	0.5740688
O	1.6543434	-1.0813286	-1.1618472
O	-1.6583866	-1.1222276	-1.1481892
C	0.7661774	1.7471574	-1.0486362
H	1.1446994	2.7729874	-0.9297272
H	1.2000264	1.3395834	-1.9745682
C	-0.7655856	1.6920904	-1.0971312
H	-1.2243076	2.6912414	-1.0694172
H	-1.1079456	1.1949124	-2.0179592
C	-1.1871756	0.8632044	0.1164408
H	-1.5708796	1.5019354	0.9370728
O	0.0359704	-3.5177456	-0.0192532
C	-2.2071416	-0.2318996	-0.1981562
H	-3.0717566	0.2565864	-0.6950132
C	2.2009604	-0.2072416	-0.1950912
H	3.0642284	0.2932194	-0.6820782
C	-2.6865186	-0.9575706	1.0426788
H	-3.2008366	-0.2664396	1.7298818
H	-3.3843496	-1.7609076	0.7649778
H	-1.8393206	-1.4102096	1.5853918
C	2.6831924	-0.9559506	1.0314458
H	3.3751604	-1.7584056	0.7363858
H	3.2051804	-0.2791326	1.7270098
H	1.8370584	-1.4134026	1.5721298
Ru	0.0101224	-1.9544866	-0.7074472

E_{THF} = -707.711428183
G_{THF} = -707.532258

$9t_{HO}$

C	-1.2931547	-1.0791173	-0.0677248
H	-1.6205057	-1.8503123	0.6568232
O	-0.1032687	-0.4497283	0.4731022
O	-1.7858247	1.1086947	-0.9077678
O	1.7462293	0.8696107	-0.8627198
C	-0.8424657	-1.6884473	-1.3875598
H	-1.3948177	-2.6137823	-1.6064218
H	-1.0503207	-0.9721653	-2.1984948
C	0.6669093	-1.9108883	-1.2361428
H	0.9310013	-2.9779173	-1.1957088
H	1.2128453	-1.4623133	-2.0800228
C	1.0644893	-1.2111433	0.0666842
H	1.2804333	-1.9329823	0.8762302
C	2.2028273	-0.1978563	-0.0721798
H	2.9977303	-0.6986353	-0.6671748
C	-2.3397967	0.0232687	-0.1997698
H	-3.1688127	-0.3899393	-0.8135838

O	-0.0345537	3.2028527	-1.3781568
H	0.8622453	3.5763447	-1.4256238
O	0.7280093	2.3831937	1.2791232
H	0.2719673	3.2280147	1.4263122
C	2.7877853	0.2197557	1.2637512
H	3.2765473	-0.6423583	1.7475582
H	3.5409213	1.0060717	1.1085262
H	2.0199283	0.6252357	1.9371322
C	-2.8861037	0.4690227	1.1435672
H	-3.5904507	1.3015117	1.0012962
H	-3.4132457	-0.3536823	1.6535072
H	-2.0705247	0.8153417	1.8018792
Ru	0.0039763	1.6023497	-0.3364398

E_{THF} = -784.129042214
G_{THF} = -784.928553

9q

C	1.1768351	0.8052299	0.0405110
H	1.4620931	1.4913389	0.8632260
O	0.0000171	0.0881729	0.4461580
O	1.8481921	-1.2094641	-1.0829960
O	-1.8496549	-1.2077821	-1.0829470
C	0.7697951	1.5782669	-1.2156190
H	1.1916201	2.5939059	-1.2056470
H	1.1679981	1.0672879	-2.1075420
C	-0.7675649	1.5783569	-1.2163640
H	-1.1893019	2.5940449	-1.2077950
H	-1.1649679	1.0664779	-2.1081230
C	-1.1758749	0.8064809	0.0399790
H	-1.4604399	1.4933019	0.8623430
O	-0.0031529	-2.9941151	0.4009300
C	-2.2803139	-0.2385411	-0.1649740
H	-3.1406459	0.2965689	-0.6239860
C	2.2800411	-0.2410371	-0.1647440
H	3.1410081	0.2932919	-0.6234850
C	-2.7178929	-0.8716301	1.1415310
H	-3.1140239	-0.1135761	1.8370850
H	-3.5028989	-1.6178141	0.9521030
H	-1.8701659	-1.3836401	1.6240980
C	2.7168821	-0.8752361	1.1414770
H	3.5017731	-1.6214881	0.9518060
H	3.1129561	-0.1178831	1.8378180
H	1.8687581	-1.3874201	1.6231710
Ru	-0.0010709	-1.8730991	-0.9580150

E_{THF} = -707.676261824
G_{THF} = -707.500097

$9q_{HO}$

C	-1.2561859	-0.9838074	-0.0152900
H	-1.5469899	-1.8418314	0.6246450
O	-0.0750419	-0.3897274	0.5389380

O	-1.9194189	1.2676486	-0.5890110
O	1.8596781	1.1850166	-0.5867890
C	-0.8487479	-1.4421544	-1.4172580
H	-1.3198489	-2.4028694	-1.6701090
H	-1.1704289	-0.6965664	-2.1618200
C	0.6892031	-1.5250264	-1.3822680
H	1.0632021	-2.5438164	-1.5600110
H	1.1261161	-0.8690594	-2.1512230
C	1.0896051	-1.0369264	0.0142750
H	1.3418961	-1.8886884	0.6782690
C	2.2136611	0.0021966	0.0900660
H	3.0885981	-0.4324984	-0.4400730
C	-2.3398269	0.0962356	0.0664310
H	-3.2239089	-0.2905644	-0.4841280
O	-0.0127559	1.5361246	-2.6028910
H	0.9040691	1.5427396	-2.9215580
O	-0.0156879	2.6823156	1.0366950
H	0.8900891	2.8988916	1.3083070
C	2.5918511	0.3097516	1.5276940
H	2.9589471	-0.5901124	2.0476520
H	3.3858181	1.0707256	1.5513280
H	1.7172471	0.6949476	2.0763140
C	-2.7191059	0.4168626	1.5003990
H	-3.5100309	1.1798826	1.5149530
H	-3.0856829	-0.4804344	2.0253750
H	-1.8465129	0.8205206	2.0374150
Ru	-0.0298059	1.7102246	-0.6563280

E_{THF} = -784.118722636

G_{THF} = -783.917969

10

C	2.3912658	1.4289498	0.0098421
H	2.9686898	1.0594758	-0.8458249
O	1.0846608	-0.6338892	-0.7594309
O	-0.9932072	-1.5493242	0.3057661
C	2.5546538	0.7195348	1.3194321
H	3.5407778	0.2231078	1.3471161
H	2.5495578	1.4559438	2.1422911
C	1.4689148	-0.3221212	1.5963711
H	1.6931758	-0.8687152	2.5297741
H	0.4925638	0.1750248	1.7450791
C	1.3425868	-1.3128832	0.4523781
H	2.2997248	-1.8582282	0.3094931
C	1.6154358	2.5229698	-0.1716079
H	1.0842278	2.9306298	0.6995371
C	0.1811278	-2.2848932	0.6108121
H	0.0752808	-2.5914262	1.6715071
Ru	-0.7806842	-0.1783232	-1.0459929
O	-0.5806722	1.4641148	-0.5814119
O	-2.7075662	-0.1467382	-0.7755599
C	0.3000708	-3.4980262	-0.2843299
H	1.1538478	-4.1281332	0.0130841

H	-0.6176982	-4.1007802	-0.2272029
H	0.4447618	-3.1864802	-1.3323399
C	1.5326698	3.2939668	-1.4395019
H	2.0569178	4.2616178	-1.3469349
H	1.9857578	2.7380718	-2.2751419
H	0.4868528	3.5213708	-1.6993039
I	-4.7241302	-0.1135722	-0.4924779
O	-4.6006072	0.1848488	1.3124171
O	-5.9464882	1.2603978	-0.7655499
O	-5.5381822	-1.7070542	-0.7107159
O	-0.7635612	-0.6167192	-2.6976439
Na	-6.0507272	1.8572808	1.3860711

E_{THF} = -1181.89231658

G_{THF} = -1181.722406

11

C	-1.0545939	0.5004386	-1.2002462
O	-0.0059239	-0.3895174	-1.5243872
C	-0.2087019	-1.6280034	-0.8833252
C	-1.7241879	-1.7902414	-0.8842902
C	-2.2120669	-0.3573964	-0.6628242
C	0.4480921	-1.6416944	0.5366768
C	1.6327261	-2.5875264	0.6017748
O	0.7257971	1.9115786	-0.2567222
C	-0.6181699	1.5925196	-0.1908862
C	-1.4078089	2.8715786	-0.4367082
O	0.6972121	-0.3471184	0.9949128
O	3.2287831	-0.1579314	1.3984998
O	3.1064891	2.2874976	0.2955198
H	-1.3191199	1.0138496	-2.1440572
H	0.2887441	-2.3910884	-1.5071332
H	-2.0465319	-2.1581274	-1.8715342
H	-2.0907779	-2.5000414	-0.1262322
H	-3.1652839	-0.1542054	-1.1729392
H	-2.3705239	-0.1584284	0.4122618
H	-0.3169059	-2.0161824	1.2572968
H	2.0957211	-2.5795614	1.5987608
H	1.3032871	-3.6145764	0.3729108
H	2.3986061	-2.3084414	-0.1435762
H	-0.8635649	1.2288976	0.8286418
H	-2.4889929	2.6514236	-0.4231742
H	-1.1936259	3.6251866	0.3352668
H	-1.1478779	3.2976536	-1.4183952
O	2.6646461	0.0259486	-1.1976722
O	1.5048551	1.6582986	2.4326948
H	0.9696121	2.4190776	2.1625928
H	0.8701881	0.9252076	2.5291068
Ru	2.2999001	0.7709266	0.2871868

E_{THF} = -934.357711761

G_{THF} = -934.150660

12

C	-1.0984417	0.8673574	-0.9060064
O	-0.3687477	-0.2192036	-1.4479474
C	-0.6881477	-1.3922656	-0.7492574
C	-2.1798847	-1.2507626	-0.4745884
C	-2.3224887	0.2521534	-0.2027924
C	0.1497203	-1.5923226	0.5690076
C	0.6869223	-3.0056866	0.6498966
O	1.0764733	1.8198424	-0.4337644
C	-0.2261297	1.6950674	0.0454816
C	-0.8197407	3.0889444	0.2123846
O	1.1368093	-0.6321136	0.8081576
O	3.8812103	-0.8191996	0.3580236
O	3.3412543	1.2056014	-1.3488334
H	-1.3718827	1.5069524	-1.7650784
H	-0.4558817	-2.2307526	-1.4265514
H	-2.7395677	-1.5347916	-1.3796614
H	-2.5351017	-1.8842016	0.3537126
H	-3.2734167	0.6534314	-0.5825364
H	-2.2933547	0.4648254	0.8805966
H	-0.5535997	-1.4258686	1.4171856
H	1.1926783	-3.1783696	1.6112136
H	-0.1362947	-3.7341226	0.5518026
H	1.4051083	-3.1921636	-0.1660784
H	-0.2161067	1.1971214	1.0408906
H	-1.8653857	3.0254644	0.5584066
H	-0.2466267	3.6748124	0.9457656
H	-0.7956167	3.6227684	-0.7507244
O	2.0363383	-1.1726116	-1.6035624
O	2.6613623	1.4014484	1.2138836
H	1.8203603	1.8903954	0.5346866
H	2.2076223	0.9400674	1.9373456
Ru	2.5905563	-0.0418166	-0.4510584

E_{THF} = -934.339413340

G_{THF} = -934.134750

13

C	1.4925392	-0.5306814	-0.7426056
O	0.0694822	-0.5435494	-0.7878286
C	-0.4547488	0.7662016	-0.7445236
C	0.7336672	1.6946346	-0.9797546
C	1.8800262	0.8947376	-0.3786386
C	-1.1575618	0.9889156	0.6022754
C	-1.7914778	2.3664426	0.7298654
O	1.5781452	-2.8274454	-0.3137836
C	1.9754732	-1.5884614	0.2268214
C	3.4799912	-1.5360804	0.4154554
O	-2.0308078	-0.0516374	0.9370174
H	1.8820302	-0.8020894	-1.7477506
H	-1.2184668	0.8676226	-1.5431286
H	0.8884512	1.8221386	-2.0635486

H	0.6115912	2.6963076	-0.5427636
H	2.8685212	1.1830516	-0.7658746
H	1.9037812	1.0134146	0.7211854
H	-0.3683528	0.8833056	1.3842414
H	-2.4925298	2.3743196	1.5770234
H	-1.0215258	3.1308586	0.9185584
H	-2.3466798	2.6542336	-0.1760736
H	1.4602842	-1.3921644	1.1955194
H	3.8147542	-2.3690754	1.0551624
H	3.9873662	-1.6390224	-0.5588046
H	3.8141252	-0.6010674	0.8925604
H	1.8143162	-3.5182024	0.3158374
O	-3.6080518	-1.7156174	1.3974574
H	-2.8169858	-1.3866554	1.8762664
O	-3.7999818	0.8786036	-0.7123006
O	-5.0838578	-1.4675234	-0.4713836
O	-2.5364188	-1.4884344	-1.4417336
Ru	-3.5270978	-0.7570804	-0.2747506

E_{THF} = -934.364129903

G_{THF} = -934.160979

14

C	1.3424534	-0.7462724	-0.9227120
O	-0.0103756	-0.3244884	-1.1356700
C	-0.1697416	1.0178026	-0.7841120
C	1.1957744	1.6497086	-1.0053460
C	2.1376514	0.5184626	-0.5978070
C	-0.6709376	1.1986226	0.6918090
C	-1.3024726	2.5637126	0.8790590
O	0.4710314	-2.8456984	-0.1446220
C	1.3572294	-1.8098704	0.1700950
C	2.7308954	-2.4207444	0.3220020
O	-1.4979386	0.1650436	1.0725910
H	1.6717104	-1.2263334	-1.8646840
H	-0.9715846	1.4264106	-1.4301660
H	1.3137714	1.8927806	-2.0735930
H	1.3482254	2.5758276	-0.4298930
H	3.1035324	0.5552276	-1.1217340
H	2.3538844	0.5633046	0.4848470
H	0.2484404	1.1132026	1.3195100
H	-1.5752256	2.7204406	1.9345130
H	-0.6189616	3.3755426	0.5827600
H	-2.2183646	2.6528606	0.2703270
H	1.0600184	-1.3075214	1.1204050
H	2.7037454	-3.2109284	1.0861620
H	3.0403634	-2.8844364	-0.6296280
H	3.4879014	-1.6770794	0.6166480
H	-0.4085266	-2.4498364	-0.2597840
O	-3.6490426	-0.1279214	1.7220090
H	-2.5949596	0.2094816	1.8278450
O	-3.1562026	0.6371746	-1.1421860

O	-4.9822456	-1.2000984	-0.2282240
O	-2.3649246	-1.9737264	-0.3063340
Ru	-3.3751246	-0.6306504	-0.0240880

E_{THF} = -934.357957979

G_{THF} = -934.157902

15

C	1.1228850	-0.1223908	0.3736633
H	1.2661070	-0.2328778	1.4740753
O	-0.0000070	-0.8739228	-0.0300417
C	0.7676800	1.3284922	0.0302443
H	1.2018440	2.0436982	0.7457233
H	1.1574680	1.5854382	-0.9697927
C	-0.7676620	1.3284722	0.0300663
H	-1.2020160	2.0438032	0.7453023
H	-1.1572000	1.5852012	-0.9701247
C	-1.1228940	-0.1223578	0.3736213
H	-1.2660960	-0.2327418	1.4740483
C	2.3613620	-0.6566058	-0.3051337
H	2.1473920	-0.6634198	-1.3980917
C	-2.3613790	-0.6566358	-0.3051087
H	-2.1474030	-0.6636028	-1.3980637
C	-3.5756800	0.2065322	-0.0175307
H	-3.7427940	0.2707062	1.0711513
H	-3.4741740	1.2264312	-0.4211547
H	-4.4781380	-0.2382818	-0.4686117
C	3.5756690	0.2065092	-0.0174307
H	3.4741630	1.2264692	-0.4208987
H	3.7427890	0.2705192	1.0712593
H	4.4781250	-0.2382378	-0.4685847
O	-2.5520990	-1.9676248	0.1793073
H	-3.3129570	-2.3429748	-0.2784017
O	2.5520580	-1.9676628	0.1791053
H	3.3129570	-2.3429358	-0.2785987

E_{THF} = -539.875078467

G_{THF} = -539.677105

16

C	-2.1608036	-0.5959708	-1.0045083
H	-2.3894156	-1.0000098	-2.0071323
O	-1.5650906	0.6760212	-1.2108623
O	0.0745524	-1.5690838	-0.8225713
O	0.1216634	0.5819142	0.8262627
C	-3.4033616	-0.2931188	-0.1772783
H	-4.2073786	0.0719622	-0.8364573
H	-3.7879806	-1.1653348	0.3728197
C	-2.9024886	0.8195372	0.7392587
H	-3.7030036	1.4991672	1.0664457
H	-2.4362376	0.3986002	1.6458877
C	-1.8478436	1.5354672	-0.1074063

H	-2.2384486	2.4858092	-0.5215053
O	1.2023194	0.6596742	-2.1123253
C	-0.5341936	1.8093882	0.6409767
H	-0.7856256	2.1437412	1.6725917
C	-1.2190546	-1.5889128	-0.2951993
H	-1.1602606	-1.3113538	0.7777047
O	2.7406404	-1.2993778	-0.8090913
C	0.2923874	2.9057022	-0.0083043
H	-0.2197696	3.8738562	0.1110597
H	1.2885074	2.9674262	0.4543387
H	0.4175504	2.7231272	-1.0886593
C	-1.7105536	-3.0189078	-0.4277463
H	-1.0338796	-3.6962208	0.1115977
H	-2.7253876	-3.1382948	-0.0163203
H	-1.7245946	-3.3181898	-1.4883073
Ru	1.3071704	-0.1074188	-0.6332813
I	4.3220544	-0.2719408	0.0710237
O	4.3832594	-1.2403478	1.5848547
O	2.7181744	0.9070952	0.2166967
O	5.3651734	-0.9284538	-1.2858173
O	5.3839334	1.2058122	0.2818997
Na	6.8223074	0.7645462	-1.3603243
O	1.5312744	-1.3525068	1.6337567
H	2.4631274	-1.5619928	1.8404397
H	1.3212764	-0.5714128	2.1654837

E_{THF} = -1333.58906876

G_{THF} = -1333.377765

17

C	-2.1441749	-0.4956002	-0.9192057
H	-2.5139139	-0.6934822	-1.9416847
O	-1.6431239	0.8247808	-0.9004157
O	0.1697071	-1.1953592	-1.1902817
O	0.3702301	1.0887208	1.0308483
C	-3.2390269	-0.5241022	0.1405203
H	-4.1747359	-0.1095802	-0.2694287
H	-3.4513939	-1.5367052	0.5167963
C	-2.6533949	0.4100448	1.1925053
H	-3.4093529	0.8543428	1.8566323
H	-1.9227489	-0.1196212	1.8291843
C	-1.9471409	1.4565588	0.3402593
H	-2.6348369	2.3046218	0.1362323
O	1.5087061	1.3175308	-1.4639717
C	-0.6668559	2.0308478	0.9402903
H	-0.9123429	2.3223978	1.9868493
C	-1.0478999	-1.5315022	-0.5967117
H	-0.9167019	-1.5734542	0.5025733
O	2.6840951	-1.3025652	-1.1650077
C	-0.2011759	3.2606018	0.1887343
H	0.7746681	3.5929168	0.5726973
H	-0.0949409	3.0378398	-0.8845017
H	-0.9266839	4.0823818	0.3011653

C	-1.4241719	-2.9111072	-1.1022877
H	-0.6742749	-3.6506852	-0.7890447
H	-2.4087139	-3.2228522	-0.7172447
H	-1.4655909	-2.9057132	-2.2033477
Ru	1.5256441	-0.0313952	-0.4755797
I	4.5144591	-0.8407442	-0.2231907
O	4.6480971	-2.4301152	0.5838813
O	3.1220371	0.3061258	0.5917663
O	5.1980221	-0.6660382	-1.9127047
O	5.7978311	0.2407488	0.5089293
Na	6.8606911	0.7590608	-1.3460427
O	1.0038421	-1.0563642	1.3847893
H	1.7994241	-1.0828512	1.9399893
H	0.4957431	-0.0096822	1.5560073

E_{THF} = -1333.56600606

G_{THF} = -1333.360692

18

C	1.4688711	-1.0625553	0.9841999
H	1.2368771	-1.4680323	1.9867659
O	1.3600681	0.3514337	1.0273939
O	-0.8143169	-1.1615713	0.5726619
O	1.3041131	1.7602057	-1.4113321
C	2.9017621	-1.3644393	0.5468089
H	3.5457311	-1.4485733	1.4381999
H	2.9958001	-2.3040563	-0.0167931
C	3.2662821	-0.1248803	-0.2549671
H	4.3504251	0.0530187	-0.3153281
H	2.8651701	-0.1745503	-1.2811031
C	2.5382671	0.9670567	0.5072769
H	3.1625081	1.3266127	1.3549479
O	-1.4922389	1.5365577	-0.1426471
C	2.1275921	2.1644977	-0.3396651
H	3.0518981	2.5611147	-0.8033461
C	0.4047671	-1.6032613	0.0139919
H	0.5886601	-1.1365883	-0.9733661
O	-3.2574639	-0.5583203	0.9734309
C	1.4652211	3.2469867	0.4887839
H	2.1343021	3.6138277	1.2837619
H	1.1794071	4.0964057	-0.1495341
H	0.5553771	2.8483937	0.9687509
C	0.3676401	-3.1111673	-0.0890471
H	-0.4728159	-3.4139893	-0.7306431
H	1.2921421	-3.5166003	-0.5275291
H	0.2201931	-3.5590873	0.9075829
Ru	-2.0507879	-0.0349833	-0.3370091
I	-5.1272949	-0.2272253	0.0839439
O	-5.6832779	-1.9201983	0.2001559
O	-3.6970339	0.0523607	-1.3138191
O	-5.4976329	0.8734877	1.4971959
O	-6.2795099	0.6577097	-1.0290441
Na	-6.9470769	2.2137437	0.3972669

O	-1.4211659	-0.9288633	-1.9011451
H	-2.0837729	-0.7598213	-2.5967571
H	0.4413121	1.5553507	-1.0200441

E_{THF} = -1333.59647156

G_{THF} = -1333.388638

19

C	-1.9191169	-0.3856596	-0.6999020
H	-2.1129039	-0.6187246	-1.7685820
O	-0.7312559	0.3830354	-0.5982170
O	-0.4794469	-2.2589406	-0.4996680
O	0.4458801	1.9426914	1.5686080
C	-3.0487329	0.4616664	-0.0879220
H	-3.7309259	0.8215594	-0.8744130
H	-3.6588549	-0.1048966	0.6345920
C	-2.3023159	1.6195944	0.5641920
H	-2.8950489	2.5458514	0.6071170
H	-1.9692239	1.3697744	1.5852200
C	-1.0784719	1.7341784	-0.3193790
H	-1.3341559	2.2601434	-1.2678080
O	0.6804731	-0.9250966	1.5911390
C	0.1159311	2.4460144	0.2965020
H	-0.2103579	3.4914044	0.4651420
C	-1.7045909	-1.7080986	0.0138820
H	-1.5688319	-1.4959136	1.0938260
O	2.3577281	-1.0154496	-0.8434370
C	1.3066661	2.4331114	-0.6380050
H	1.0560991	2.8486424	-1.6282280
H	2.1310951	3.0303924	-0.2168390
H	1.6738841	1.4068854	-0.7984160
C	-2.8303749	-2.6875676	-0.2068660
H	-2.6131419	-3.6481976	0.2899010
H	-3.7768969	-2.3143906	0.2100340
H	-2.9766749	-2.8751776	-1.2842570
Ru	1.6234031	-1.9213856	0.5587660
I	4.3905621	-0.6433316	-0.1772580
O	5.3517721	-1.7936836	-1.1582080
O	3.2874301	-1.7056026	1.3118350
O	4.2285981	1.0026444	-0.9669200
O	5.4027051	-0.0023156	1.2078480
Na	5.2386941	2.1585284	0.6974110
O	1.5867191	-3.6183766	0.3569010
H	0.6112121	0.9865964	1.4772080
H	-0.5475309	-3.2199066	-0.4958000

E_{THF} = -1333.58821346

G_{THF} = -1333.378663

20

C	-2.1187231	1.1541752	-0.4884828

O	-1.2142111	0.1233622	-0.9500598
C	-1.8365811	-1.1600718	-0.8401718
C	-3.2969841	-0.8610348	-1.1242648
C	-3.5018091	0.5005012	-0.4505188
C	-1.5614431	-1.7687098	0.5606912
C	-1.2331521	-3.2441898	0.4324502
O	-0.1995351	1.6988652	0.8666362
C	-1.6097911	1.6544222	0.8582852
C	-2.1320701	3.0367132	1.1774392
O	-0.5625561	-1.0863928	1.2438132
O	2.0666229	-0.3537868	1.2905312
O	1.5993669	0.4688582	-1.1573978
H	-2.0435981	1.9662702	-1.2336258
H	-1.3597241	-1.7830958	-1.6166808
H	-3.4584211	-0.7847478	-2.2109348
H	-3.9695091	-1.6416558	-0.7353838
H	-4.2644561	1.1061012	-0.9605138
H	-3.8290731	0.3771872	0.5965952
H	-2.4911061	-1.6632748	1.1677182
H	-1.1091611	-3.7009218	1.4246672
H	-2.0257381	-3.7880368	-0.1107588
H	-0.2854571	-3.3603358	-0.1218178
H	-1.9321351	0.9323782	1.6403712
H	-1.7667261	3.3668152	2.1599992
H	-1.7882301	3.7586422	0.4190552
H	-3.2349761	3.0414402	1.1956682
C	3.8014239	0.5053432	-0.8357958
H	3.8142469	-0.0447838	-1.7832438
C	4.0100759	-0.2025388	0.3234192
H	4.2775509	0.3606582	1.2243892
C	4.2220689	-1.6749868	0.3424332
H	3.8042649	-2.1257738	1.2555042
H	3.7405139	-2.1509898	-0.5276438
H	5.2986419	-1.9218558	0.3155702
C	3.8566689	1.9912232	-0.8962338
H	4.8637359	2.3386442	-1.1903008
H	3.1456569	2.3917992	-1.6348758
H	3.6177689	2.4328842	0.0850772
Ru	0.7065579	0.1108982	0.2883922

E_{THF} = -939.945160867

G_{THF} = -939.663917

21

C	-1.8638291	1.3578975	-0.3718545
O	-1.0036851	0.3233826	-0.9068945
C	-1.6783651	-0.9463725	-0.9622615
C	-3.1303591	-0.5576604	-1.1802955
C	-3.2776711	0.7726755	-0.4269585
C	-1.3863521	-1.7304945	0.3156965
C	-1.5558961	-3.2187255	0.1100215
O	-0.0061361	1.5981666	1.2372905

C	-1.3997931	1.7417296	1.0410075
C	-1.8038041	3.1612786	1.3703225
O	-0.0632661	-1.4951915	0.7879675
O	2.4485089	0.1998156	1.3569435
O	1.8872569	0.1033256	-1.2049695
H	-1.7273241	2.2197186	-1.0487365
H	-1.2297861	-1.4750485	-1.8216615
H	-3.3153111	-0.4166844	-2.2560335
H	-3.8309811	-1.3269875	-0.8202305
H	-3.9875601	1.4472336	-0.9264605
H	-3.6547701	0.6067885	0.5966705
H	-2.0872291	-1.3898875	1.1099745
H	-1.3422071	-3.7556005	1.0448855
H	-2.5813781	-3.4682294	-0.2083605
H	-0.8505191	-3.5734454	-0.6590785
H	-1.8990381	1.0509685	1.7575955
H	-1.5052881	3.4107145	2.3980525
H	-1.3025701	3.8634706	0.6846115
H	-2.8951131	3.2940566	1.2791945
C	3.2886439	0.1636656	-0.8661115
H	3.7919109	-0.5042795	-1.5948395
C	3.4661499	-0.3599514	0.5579655
H	4.4328379	0.0179006	0.9555235
C	3.4676369	-1.8783505	0.6314905
H	3.5033059	-2.1998865	1.6831675
H	2.5510199	-2.2996545	0.1838795
H	4.3354519	-2.3057975	0.1012775
C	3.7682489	1.5872776	-1.0381615
H	4.8639359	1.6488825	-0.9368455
H	3.4850369	1.9763985	-2.0276755
H	3.3128059	2.2260335	-0.2625305
Ru	0.7754809	0.1308666	0.3164225

E_{THF} = -940.057106772

G_{THF} = -939.768939

21_{NaIO4}

C	-1.3391455	-1.5258185	1.1307170
O	-1.6762775	-0.2488025	0.5149780
C	-2.7870615	-0.3440575	-0.4053480
C	-3.4640965	-1.6499605	-0.0251110
C	-2.3310665	-2.5168615	0.5325590
C	-2.2001045	-0.2447165	-1.8108120
C	-3.2356285	0.1453675	-2.8425400
O	0.9190615	-0.6792465	0.8515260
C	0.1258695	-1.8557295	0.8282900
C	0.6986895	-2.8486325	1.8132180
O	-1.1678525	0.7094615	-1.8385410
O	1.8096715	1.4534515	-0.7216210
O	0.0083605	1.9003245	1.1215310
H	-1.4799475	-1.3755125	2.2163410
H	-3.4166685	0.5424585	-0.2112990
H	-4.2279045	-1.4648875	0.7462590

H	-3.9676495	-2.1217345	-0.8835400
H	-2.6907095	-3.2463195	1.2726610
H	-1.8400155	-3.0823035	-0.2780320
H	-1.7615115	-1.2354445	-2.0813480
H	-2.7635885	0.2215435	-3.8319660
H	-4.0484015	-0.5964955	-2.9005780
H	-3.6673985	1.1275585	-2.5902280
H	0.1627045	-2.2863245	-0.1936300
H	1.7182945	-3.1195105	1.4998780
H	0.7278125	-2.4113845	2.8241070
H	0.0837045	-3.7641385	1.8368160
C	1.1923445	2.6793775	1.2667030
H	0.8692655	3.7200455	1.4801610
C	2.0037945	2.6929085	-0.0386030
H	3.0831525	2.7642615	0.1969870
C	1.5849825	3.8035125	-0.9786210
H	2.1080055	3.7127325	-1.9416420
H	0.4986705	3.7495655	-1.1688220
H	1.8101125	4.7904685	-0.5423460
C	1.9812075	2.1270355	2.4379970
H	2.8077115	2.8085875	2.7009590
H	1.3258085	2.0140035	3.3142220
H	2.4121425	1.1467065	2.1756510
Ru	0.0440755	0.6681735	-0.3392470
I	2.7809765	-0.7272745	-0.8339750
O	3.8094545	-0.1171645	0.5698370
O	3.0729265	-2.5057605	-0.5539440
O	1.0622905	-0.7007695	-1.6398590
O	3.9724425	-0.4396805	-2.1711930
Na	5.3914955	-1.6690125	-0.5085540

E_{THF} = -1414.33539591

G_{THF} = -1414.042063

$21_{[ox]}$

C	-1.9120641	1.1166586	-0.8275680
O	-1.3721781	-0.1333724	-1.2669690
C	-2.1479621	-1.1849764	-0.6731210
C	-3.5672251	-0.6547904	-0.7714200
C	-3.3922181	0.8530896	-0.5288990
C	-1.7072771	-1.4650274	0.7768200
C	-1.9762601	-2.9210934	1.1164860
O	0.2383529	1.3062046	0.1220550
C	-1.0922741	1.5910196	0.3816520
C	-1.2421931	3.0847066	0.5910100
O	-0.3447201	-1.2322324	1.0227940
O	2.2702929	-0.8880354	0.8500340
O	2.2084859	0.6204266	-1.1846320
H	-1.7453721	1.8243636	-1.6571820
H	-1.9586481	-2.0748804	-1.2955020
H	-3.9663761	-0.8427604	-1.7797120
H	-4.2460781	-1.1310714	-0.0467820
H	-4.0552281	1.4481456	-1.1729470

H	-3.6263691	1.1257816	0.5144240
H	-2.3096561	-0.8229474	1.4577480
H	-1.7291011	-3.1225464	2.1679910
H	-3.0352431	-3.1811174	0.9460140
H	-1.3470961	-3.5666454	0.4808180
H	-1.4427081	1.0553036	1.2890740
H	-0.6618731	3.4103816	1.4659130
H	-0.8696721	3.6271766	-0.2925410
H	-2.2993681	3.3528066	0.7558970
O	0.7348399	-1.7857494	-1.4404840
C	3.4220629	0.6947866	-0.4701430
H	4.2309219	0.7644556	-1.2290260
C	3.5663479	-0.6034764	0.3103500
H	4.2206469	-0.4692744	1.1939280
C	4.0521529	-1.7607414	-0.5335620
H	3.9819669	-2.7051584	0.0259610
H	3.4492429	-1.8513964	-1.4519170
H	5.1029039	-1.6042314	-0.8261750
C	3.4314649	1.9265256	0.4144340
H	4.4231449	2.0752736	0.8721140
H	3.1715149	2.8167556	-0.1764730
H	2.6812369	1.8181176	1.2136330
Ru	0.8615829	-0.5104544	-0.3440930

E_{THF} = -1015.21161683

G_{THF} = -1014.919096

22

C	-1.7515109	-0.8720835	-0.1448789
H	-1.7213839	-1.8779885	-0.6143659
O	-0.6578939	-0.1117645	-0.6261299
O	-0.3368429	-1.6470505	1.6282141
O	0.0155141	2.6632125	-0.6950459
C	-3.0265649	-0.1007785	-0.5390679
H	-3.6256939	-0.6854225	-1.2547699
H	-3.6725359	0.1075305	0.3287461
C	-2.4908469	1.1790715	-1.1738479
H	-3.1323099	1.5720075	-1.9766149
H	-2.3496029	1.9722905	-0.4211229
C	-1.1196789	0.7524595	-1.6578699
H	-1.2031449	0.1790135	-2.6091339
O	0.7090891	0.9623075	1.6010311
C	-0.1037329	1.8677815	-1.8516139
H	-0.5193049	2.5377135	-2.6295289
C	-1.5977349	-1.0750325	1.3571081
H	-1.6781389	-0.0731875	1.8390451
O	2.2813551	-1.1847435	0.3126411
C	1.2377231	1.3297015	-2.3083839
H	1.1485611	0.7834125	-3.2617529
H	1.9486221	2.1582025	-2.4500179
H	1.6654961	0.6306805	-1.5705119
C	-2.6488849	-2.0231755	1.9000601
H	-2.5108459	-2.1676485	2.9820401

H	-3.6675029	-1.6392895	1.7360721
H	-2.5582809	-3.0053745	1.4086821
Ru	1.4863551	-0.5238015	1.8084431
I	4.3571661	-0.5939625	0.5817411
O	5.0551411	-2.2408015	0.5418591
O	3.2625821	-0.1150895	2.2627481
O	4.1917191	0.2471405	-1.0363099
O	5.6502991	0.5556875	1.1702461
Na	5.6833281	1.8967005	-0.6128619
O	1.2327281	-1.6373005	3.2132301
H	0.2750441	2.0684565	0.0282161
H	0.1717141	-1.8888755	2.7337051

E_{THF} = -1333.55597994

G_{THF} = -1333.354110

23

C	-2.2899884	1.1657086	-0.9562198
O	-1.8682354	-0.0858584	-1.4624218
C	-2.5136454	-1.1197824	-0.7510498
C	-3.9187034	-0.5662044	-0.5250018
C	-3.6540284	0.9269166	-0.2879948
C	-1.8230844	-1.4650924	0.5773812
C	-2.2697884	-2.8363124	1.0541312
O	0.0438686	1.5505646	-0.5708478
C	-1.2231184	1.7259916	-0.0004578
C	-1.4178654	3.2072186	0.2503882
O	-0.4151684	-1.4834294	0.5135262
O	2.4257596	-1.1600844	0.4255072
O	2.4697066	1.1099156	-0.6485928
H	-2.3509614	1.8502776	-1.8218958
H	-2.4879084	-2.0091654	-1.4055538
H	-4.5209244	-0.7146964	-1.4345248
H	-4.4522894	-1.0434864	0.3116572
H	-4.4452614	1.5611006	-0.7134458
H	-3.6062894	1.1556646	0.7909472
H	-2.1419954	-0.7076844	1.3304632
H	-1.8324084	-3.0649704	2.0368872
H	-3.3666734	-2.9019874	1.1396292
H	-1.9241174	-3.6021324	0.3410602
H	-1.2826464	1.1830796	0.9644402
H	-0.6728934	3.5763786	0.9692532
H	-1.2937734	3.7640376	-0.6925468
H	-2.4244874	3.4147236	0.6498552
O	0.7674516	-0.9309344	-1.8770158
C	3.7618516	0.6403486	-0.2978838
H	4.4260696	0.8863506	-1.1525948
C	3.6881416	-0.8819124	-0.1432998
H	4.4439186	-1.2109834	0.5997092
C	3.9025426	-1.6188024	-1.4480418
H	3.7024506	-2.6927374	-1.3189748
H	3.2364596	-1.2391044	-2.2411208
H	4.9430196	-1.4949314	-1.7909158

C	4.2173266	1.3732536	0.9451022
H	5.2681156	1.1387376	1.1783342
H	4.1207746	2.4592496	0.8042342
H	3.5925016	1.0848306	1.8062152
O	0.6589526	0.1555696	1.7298152
H	1.4631626	-0.2016304	2.1372052
H	0.0425636	-0.7900034	1.4300592
Ru	1.0216166	-0.1079914	-0.4454008

E_{THF} = -1091.61095991
G_{THF} = -1091.296972

24

C	-1.7349861	1.2876349	-0.7603245
O	-1.6660951	-0.1184341	-0.9510585
C	-2.9507901	-0.7230791	-0.7966545
C	-3.9410571	0.4321539	-0.8793355
C	-3.1467511	1.5808979	-0.2705705
C	-3.0052351	-1.4931201	0.5237315
C	-4.2072561	-2.4076781	0.5848745
O	0.6254099	1.4268679	-0.3656195
C	-0.6358211	1.7101149	0.2033345
C	-0.6515231	3.2006409	0.4803535
O	-1.8691851	-2.3002921	0.6717675
O	2.7912329	-1.3108681	0.6414865
O	3.0029879	0.8092619	-0.6908485
O	1.0054099	-1.1389401	-1.6866505
C	4.2494719	0.3362829	-0.1927295
C	4.0983719	-1.1542901	0.0987205
C	4.2998809	-2.0319481	-1.1158965
C	4.6257999	1.1480369	1.0263715
O	0.4499469	-0.6900171	1.2315475
H	-1.5416111	1.7882039	-1.7336125
H	-3.0679041	-1.4526991	-1.6198015
H	-4.1832191	0.6516289	-1.9321795
H	-4.8863681	0.2309679	-0.3522325
H	-3.5049941	2.5756709	-0.5749245
H	-3.1803121	1.5345579	0.8334495
H	-3.0671761	-0.7457231	1.3517955
H	-4.2097611	-2.9616421	1.5349805
H	-5.1590061	-1.8612161	0.4989185
H	-4.1494781	-3.1452571	-0.2330775
H	-0.7794831	1.1367639	1.1410165
H	0.2069389	3.4749489	1.1099815
H	-0.5752671	3.7658039	-0.4631985
H	-1.5742111	3.5027819	1.0005975
H	-1.0986841	-1.7062151	0.6927205
H	4.9880009	0.4840909	-1.0070195
H	4.7991179	-1.4505481	0.9043045
H	4.0386829	-3.0755871	-0.8859665
H	3.6740449	-1.6973511	-1.9602935
H	5.3523789	-2.0004371	-1.4407435
H	5.6435699	0.9005089	1.3679305

H	4.5813259	2.2226869	0.7992415
H	3.9196119	0.9376249	1.8470395
H	0.9527389	-1.3814931	1.7044455
Ru	1.4812509	-0.2912941	-0.3358705

E_{THF} = -1091.64940909

G_{THF} = -1091.336133

25

C	-2.0263441	1.2699585	-0.6665434
O	-1.7218971	-0.0743005	-0.9844294
C	-2.8754381	-0.9107065	-0.8270084
C	-4.0504041	0.0554945	-0.7471524
C	-3.4266611	1.2670435	-0.0681804
C	-2.6983931	-1.7922375	0.4078836
C	-3.7883401	-2.8351925	0.5153886
O	0.3262879	1.7810245	-0.3945244
C	-0.9602771	1.8422305	0.2450296
C	-1.2383501	3.2717835	0.6502756
O	-1.4844361	-2.4850255	0.3432946
O	2.9992509	-1.5297905	-0.4061304
O	3.1622179	0.9649985	0.2064066
O	1.4912439	0.0625055	-2.1038644
C	4.3083989	0.1874225	0.5938246
C	4.3421949	-1.0414195	-0.2986654
C	4.9090559	-0.7642305	-1.6749384
C	4.2231829	-0.1437655	2.0666306
O	0.7233749	-0.6404495	0.8589646
H	-2.0230281	1.8712205	-1.6087634
H	-2.9186161	-1.5737825	-1.7106954
H	-4.3941991	0.3228505	-1.7599014
H	-4.9108951	-0.3544855	-0.1981114
H	-3.9703851	2.2060445	-0.2499204
H	-3.3691601	1.1160775	1.0251716
H	-2.7293331	-1.1283275	1.3064196
H	-3.5929911	-3.4820495	1.3828426
H	-4.7911421	-2.3955225	0.6281756
H	-3.7805801	-3.4731855	-0.3844724
H	-0.8676101	1.1820575	1.1263986
H	-0.3815821	3.6782685	1.2059186
H	-1.4022151	3.9064395	-0.2384434
H	-2.1309771	3.3435625	1.2905446
H	-0.7658311	-1.8329505	0.3954966
H	5.1830039	0.8372945	0.3927706
H	4.9122629	-1.8566125	0.1895496
H	4.7756649	-1.6396195	-2.3269834
H	4.3998019	0.0943655	-2.1426094
H	5.9850659	-0.5351675	-1.6100794
H	5.1542339	-0.6208715	2.4124346
H	4.0591489	0.7698955	2.6564746
H	3.3879769	-0.8377595	2.2573916
Ru	1.7302799	-0.1063315	-0.4263494
H	0.2264379	2.0232465	-1.3295204

E_{THF} = -1091.63417140
G_{THF} = -1091.323205

26

C	2.4781032	-1.6288514	-0.6171998
O	2.4810682	-0.3861774	-1.2743578
C	2.7964772	0.6531116	-0.3427128
C	3.3998062	-0.0400244	0.8850832
C	3.5650162	-1.4965954	0.4429852
C	1.5382412	1.4688306	-0.0530228
C	1.8566552	2.7501456	0.6776712
O	0.0898882	-1.3475854	-0.7490038
C	1.1105092	-1.9736664	0.0117402
C	0.8945912	-3.4647604	0.1230272
O	0.9125342	1.8122646	-1.2655738
O	-3.7107278	-0.4682454	-0.6408638
O	-1.6265948	0.6436896	0.2587082
O	-2.1287278	-2.3206454	0.9267702
C	-2.6843048	1.5594206	-0.0307138
C	-3.9778288	0.7463976	0.0539842
C	-4.4230578	0.4812466	1.4769602
C	-2.4544478	2.1878096	-1.3860348
O	-1.7506168	-1.6338454	-1.9969538
H	2.7072742	-2.3926044	-1.3828428
H	3.5206862	1.3151246	-0.8548418
H	4.3511082	0.4133046	1.1993272
H	2.7101992	0.0335676	1.7451272
H	4.5507702	-1.6554844	-0.0216628
H	3.4618862	-2.2164924	1.2708872
H	0.8510782	0.8459446	0.5633062
H	0.9315932	3.3109716	0.8799132
H	2.3610442	2.5596196	1.6384492
H	2.5099522	3.3851856	0.0560132
H	1.0520962	-1.5087624	1.0167392
H	0.8595102	-3.9202784	-0.8814248
H	1.7157642	-3.9415504	0.6821122
H	-0.0491158	-3.6920034	0.6430442
H	0.7538972	0.9679656	-1.7161468
H	-2.6523898	2.3211596	0.7735262
H	-4.7829988	1.2507596	-0.5148038
H	-5.2608708	-0.2310274	1.4918282
H	-3.6004498	0.0632316	2.0806672
H	-4.7542988	1.4173736	1.9541482
H	-1.4252638	2.5732616	-1.4464878
H	-2.5907788	1.4306426	-2.1774718
H	-3.1679718	3.0081156	-1.5638258
H	-0.4498318	-1.7345374	-1.6637588
Ru	-1.9694728	-1.1460074	-0.2723148

E_{THF} = -1091.60472549
G_{THF} = -1091.292626

27

O	-0.0000000	-1.2717620	0.7828439
O	-0.0000000	1.2717620	0.7828439
C	-0.2995440	-0.6961030	-0.5022731
H	0.2151410	-1.3482870	-1.2340501
C	0.2995440	0.6961030	-0.5022731
H	-0.2151410	1.3482870	-1.2340501
Ru	-0.0000000	0.0000000	2.1900529
O	-1.5116570	-0.0164540	2.9563679
O	1.5116570	0.0164540	2.9563679
C	1.7936910	0.7113130	-0.7314771
H	2.0312700	0.3914540	-1.7583611
H	2.1956890	1.7231540	-0.5784931
H	2.2985570	0.0266710	-0.0295841
C	-1.7936910	-0.7113130	-0.7314771
H	-2.0312700	-0.3914540	-1.7583611
H	-2.1956890	-1.7231540	-0.5784931
H	-2.2985570	-0.0266710	-0.0295841

E_{THF} = -551.735855870

G_{THF} = -551.645124

28

C	-2.4531463	1.0741217	-0.9568493
O	-1.9785223	-0.1539453	-1.4668083
C	-2.5335803	-1.1975963	-0.6886693
C	-3.9689623	-0.7417943	-0.4473903
C	-3.8281353	0.7842737	-0.3305803
C	-1.7614703	-1.4128243	0.6205307
C	-2.0687593	-2.7880043	1.1957317
O	-0.1424813	1.5070647	-0.4396563
C	-1.4456863	1.6608577	0.0491797
C	-1.6707283	3.1455067	0.2518847
O	2.5390447	-1.3553993	0.2367877
O	2.3223157	1.1742257	-0.5834763
O	0.8544657	-0.8442183	-1.9279743
C	3.6311967	0.7547507	-0.2506073
C	3.7453797	-0.7801143	-0.2719613
C	4.0146117	-1.3296183	-1.6532713
C	4.0686847	1.4007827	1.0509667
O	1.3807447	0.0396837	1.6836247
H	-2.5036173	1.7697387	-1.8130573
H	-2.4561073	-2.1144673	-1.2983933
H	-4.5943693	-1.0102473	-1.3122923
H	-4.4235743	-1.1972463	0.4464567
H	-4.6394533	1.3119017	-0.8525323
H	-3.8587243	1.1122237	0.7226817
H	-1.6994513	-3.5647613	0.5072507
H	-1.5669753	-2.9230923	2.1645827
H	-3.1524353	-2.9285303	1.3408447
H	-1.5439473	1.1378607	1.0223057
H	-0.9683993	3.5447817	0.9967547

H	-1.5049673	3.6778157	-0.6984043
H	-2.6994513	3.3470837	0.5930137
H	2.2134327	-0.8458473	1.1880027
H	4.2708107	1.1447197	-1.0730113
H	4.5632497	-1.0859873	0.4118327
H	3.9749917	-2.4285653	-1.6436323
H	3.2681667	-0.9639653	-2.3779023
H	5.0119087	-1.0168893	-2.0023173
H	5.1354507	1.1999967	1.2421657
H	3.9239887	2.4893027	0.9921027
H	3.4657867	1.0243297	1.8902557
H	0.6816377	-0.5070613	2.0769267
H	-2.1087263	-0.6549133	1.3611957
O	-0.3763803	-1.3622893	0.4717057
Ru	0.8821857	-0.0936443	-0.4279973

E_{THF} = -1091.59729511

G_{THF} = -1091.283281

29

C	-2.3388974	0.9585324	-1.0741344
O	-1.8671564	-0.3565426	-1.3011944
C	-2.5995554	-1.2317476	-0.4650004
C	-4.0260104	-0.7028546	-0.5626014
C	-3.8158484	0.8175944	-0.6662964
C	-2.0848394	-1.2288866	0.9831466
C	-2.5129184	-2.5031506	1.6925016
O	-0.1162224	1.3640074	-0.1990704
C	-1.4777814	1.6468664	-0.0053494
C	-1.6048554	3.1561354	-0.0889904
O	3.7835816	-1.7421986	0.0258626
O	2.2049166	0.8622594	-0.3764194
O	0.8184056	-1.3783176	-1.3211414
C	3.5786696	0.7251574	-0.0802464
C	4.2313846	-0.5598086	-0.5946054
C	4.0484046	-0.7080586	-2.0919394
C	3.9089926	1.0612814	1.3669466
O	1.6607756	-0.9058596	1.5550856
H	-2.1992974	1.5050274	-2.0233754
H	-2.4663024	-2.2423056	-0.8886014
H	-4.5048314	-1.0929556	-1.4733754
H	-4.6540614	-0.9909016	0.2951046
H	-4.4931434	1.2733774	-1.4026174
H	-4.0069574	1.3194044	0.2980296
H	-2.0434484	-3.3746396	1.2086436
H	-2.2046504	-2.4826516	2.7475166
H	-3.6077184	-2.6265176	1.6533676
H	-1.7943904	1.3166374	1.0028796
H	-1.0122724	3.6396644	0.7001356
H	-1.2335204	3.5080074	-1.0644194
H	-2.6577554	3.4647124	0.0212776
H	3.2740786	-1.5266446	0.8226376
H	4.0231196	1.5355924	-0.7015714

H	5.3180386	-0.4238506	-0.3832714
H	4.5152576	-1.6432826	-2.4347364
H	2.9777036	-0.7427296	-2.3537064
H	4.5117336	0.1326894	-2.6335144
H	4.9932616	1.2296944	1.4645116
H	3.3858966	1.9823654	1.6644576
H	3.6149486	0.2638174	2.0609356
H	0.9679086	-1.4126266	2.0294066
H	-2.5442204	-0.3716356	1.5206326
O	-0.6885244	-1.1696066	1.0904936
Ru	0.7381026	-0.3450516	-0.0173944

E_{THF} = -1091.61724118

G_{THF} = -1091.301181

30

C	-2.3784723	0.9855834	-0.9184535
O	-2.0347463	-0.3382366	-1.2821575
C	-2.8375723	-1.2384406	-0.5392525
C	-4.1974253	-0.5501616	-0.4669145
C	-3.8419563	0.9443984	-0.4504855
C	-2.2210913	-1.5292676	0.8338945
C	-2.8598343	-2.7488366	1.4759935
O	-0.1086153	1.1185404	-0.0960165
C	-1.4274253	1.5180444	0.1620935
C	-1.4351623	3.0340784	0.1932945
O	3.7205747	-1.6552856	0.3681125
O	2.3612527	0.6432284	-0.6910065
O	0.8136717	-1.4998846	-1.3628435
C	3.7131437	0.7365104	-0.2182145
C	4.3695627	-0.6348086	-0.3503725
C	4.4473017	-1.0875816	-1.7920235
C	3.7801447	1.3317344	1.1730505
O	1.3972177	-0.7032206	1.6094595
H	-2.2325903	1.6000944	-1.8251495
H	-2.8524793	-2.1833976	-1.1098245
H	-4.7840683	-0.7991246	-1.3638605
H	-4.7896093	-0.8559586	0.4095415
H	-4.5024803	1.5266184	-1.1090765
H	-3.9437023	1.3714634	0.5622295
H	-2.6976743	-3.6314006	0.8368175
H	-2.4011183	-2.9454956	2.4550085
H	-3.9430093	-2.6071646	1.6179145
H	-1.7453303	1.1385724	1.1557965
H	-0.7941723	3.4126574	1.0023915
H	-1.0588063	3.4273834	-0.7652045
H	-2.4562563	3.4191044	0.3488275
H	3.2482587	-1.2971296	1.1354495
H	4.2583637	1.4022174	-0.9183975
H	5.4047687	-0.4881756	0.0382475
H	4.9299717	-2.0743576	-1.8436085
H	3.4338887	-1.1790106	-2.2118395
H	5.0306747	-0.3805326	-2.4030845

H	4.8299387	1.4783744	1.4722645
H	3.2861967	2.3173394	1.2002395
H	3.2849867	0.6952164	1.9217335
H	-2.3835673	-0.6553936	1.5045965
O	-0.8605853	-1.8289016	0.7326825
Ru	0.5685017	-0.6876946	0.1032215
H	1.9093307	1.4983004	-0.5950745

E_{THF} = -1091.61695140

G_{THF} = -1091.301695

31

C	-1.2479015	1.3298942	-0.4515174
O	-1.2238145	0.0247882	-1.0346424
C	-2.5232035	-0.5533138	-0.9026764
C	-3.4583105	0.6187342	-1.1550614
C	-2.6988525	1.8128272	-0.5543564
C	-2.7077915	-1.1884068	0.4809866
C	-3.8336065	-2.2055558	0.4643246
O	0.3414495	0.3328352	1.0123186
C	-0.7203575	1.2388542	0.9895966
C	-0.2041275	2.5814122	1.4672616
O	-1.5574925	-1.8626818	0.9317186
O	2.3400525	-1.2930908	0.5095866
H	-0.5371475	1.9322542	-1.0440104
H	-2.5812395	-1.3429538	-1.6716304
H	-3.6002875	0.7528312	-2.2377264
H	-4.4518215	0.4712122	-0.7033354
H	-2.7905005	2.7092242	-1.1835944
H	-3.0867515	2.0791052	0.4438156
H	-2.9655215	-0.3918858	1.2122616
H	-3.9745385	-2.6347038	1.4659646
H	-4.7808295	-1.7409158	0.1443676
H	-3.5887335	-3.0245748	-0.2307394
H	-1.5344435	0.9019232	1.6635416
H	0.1441785	2.5141892	2.5076736
H	0.6405065	2.9065372	0.8367426
H	-0.9979985	3.3451812	1.4127666
O	0.2474955	-2.2918528	-1.1710474
C	3.4048825	-0.9784088	-0.3821054
H	4.3255885	-1.3734108	0.0935966
C	3.5053495	0.5506662	-0.4363084
H	4.2596425	0.7991872	-1.2079734
C	3.9232635	1.1417902	0.8956956
H	3.9753495	2.2386262	0.8226066
H	3.1851345	0.8798952	1.6720856
H	4.9082785	0.7677032	1.2203816
C	3.2135065	-1.6018008	-1.7436454
H	4.0991205	-1.4173248	-2.3729074
H	3.0613445	-2.6890538	-1.6680714
H	2.3391275	-1.1550458	-2.2429914
O	0.8995875	-2.5539528	1.6454776
H	2.0833395	-2.1446378	1.2220746

O	2.2874315	1.1052822	-0.8792124
H	1.6433095	0.9278682	-0.1653514
Ru	0.2373335	-1.5192488	0.3240596

E_{THF} = -1091.59623599

G_{THF} = -1091.282925

32

C	0.4356756	0.6188898	-0.2208737
H	1.3061996	0.4603728	-0.8987927
C	-0.0575934	-0.7707252	0.1558303
H	0.8366256	-1.3209152	0.5302332
C	-0.6371444	-1.5083852	-1.0322918
H	0.0966056	-1.5887162	-1.8504678
H	-0.9375244	-2.5317352	-0.7502448
H	-1.5182504	-0.9670452	-1.4068458
C	0.8826006	1.4098108	0.9900573
H	1.6716686	0.8785918	1.5463233
H	1.2872446	2.3912888	0.6900773
H	0.0270026	1.5659158	1.6633103
O	-1.0103714	-0.6256942	1.1889883
H	-1.4246014	-1.4846772	1.3276782
O	-0.6079434	1.2755948	-0.9106787
H	-0.3501934	2.1974288	-1.0223027

E_{THF} = -308.739012248

G_{THF} = -308.629976

$NaIO_4$

I	-0.5875062	-0.0123668	0.0102888
O	-1.5876572	1.4615232	0.1189148
O	-1.5269012	-1.5277538	-0.0644672
O	0.6062818	0.0961112	-1.3651232
O	0.6572238	-0.0689528	1.3431858
Na	2.4385588	0.0514392	-0.0427992

E_{THF} = -474.283927618

G_{THF} = -474.304476

$NaIO_3$

I	-0.6369028	-0.1625548	0.8892466
O	-0.0616838	1.5322262	0.4678246
O	0.9942582	-1.0019368	0.7732386
O	-1.2566758	-0.6173888	-0.7810124
Na	0.9610042	0.2496542	-1.3492974

E_{THF} = -399.169922227

G_{THF} = -399.193133

H_2O

O	0.0000000	0.0000000	0.4003193

H	0.0000000	0.7534980	-0.2001597
H	0.0000000	-0.7534980	-0.2001597

E_{THF} = -76.4129602233
G_{THF} = -76.409081

2-*E*-Buten

C	-0.4642843	-0.4793494	-0.0136133
H	-1.4941273	-0.2127644	0.2659717
C	0.4642847	0.4793486	0.0136137
H	1.4941237	0.2127686	-0.2659873
C	-0.2175993	-1.8982384	-0.3962253
H	-0.4773393	-2.5917884	0.4222947
H	-0.8328853	-2.1994454	-1.2617763
H	0.8392577	-2.0646014	-0.6581483
C	0.2176067	1.8982306	0.3962597
H	-0.8392393	2.0645806	0.6582357
H	0.8329837	2.1994956	1.2617087
H	0.4772187	2.5917636	-0.4223333

E_{THF} = -157.098882759
G_{THF} = -157.018849

(b) Absolute energies and cartesian coordinates for the regioselectivity of Ru-catalysed oxidative cyclisation of methyl 1,5-dienoate (**5a**). All energies are in Hartree.

Here, due to the difficulty in locating the TS **6a** using the DFT functional M06 (M06/cc-pVDZ/LANL2DZ), both TSs **6a** and **d-6a** have been optimised in gas phase with M06-2X (M06-2X/cc-pVDZ/LANL2DZ) followed by single point energy calculations in THF with the M06 functional ((SMD)-M06//aug-cc-pVDZ/LANL2DZ) in order to compare them directly. So, only **5a**, **RuO_4**, **6a** and **d-6a** are optimised with M06-2X/cc-pVDZ/LANL2DZ then single point energy with M06/aug-cc-pVDZ/LANL2DZ.

5a

C	-0.7827026	-0.8445225	0.4304432
C	-1.9968156	-1.2618645	0.0582412
H	-2.2052136	-2.3097745	-0.1569368
H	-0.6382766	0.2176935	0.6366242
C	0.4066174	-1.7441855	0.5623292
H	0.8525914	-1.6119595	1.5586642
H	0.0873774	-2.7901085	0.4684132
C	1.4895864	-1.4457215	-0.4963788
H	2.3050504	-2.1705635	-0.3750108
H	1.0491484	-1.6055495	-1.4913348

C	2.0450674	-0.0534395	-0.4019188
C	3.3060984	0.2330055	-0.0727938
H	1.3604014	0.7720385	-0.6206198
C	3.8729124	1.6173895	0.0276402
H	3.9927074	-0.5940515	0.1350522
H	4.6915464	1.7573335	-0.6914008
H	3.1032304	2.3721645	-0.1720218
H	4.2883814	1.7996055	1.0279972
C	-3.1682506	-0.3709365	-0.1056608
O	-4.2573606	-0.7577295	-0.4630868
O	-2.9076846	0.9204995	0.1785562
C	-4.0221926	1.7998845	0.0185472
H	-3.6587846	2.7914355	0.2965662
H	-4.3665286	1.7891955	-1.0215138
H	-4.8469056	1.4901605	0.6696022

E_{THF} = -501.516503571

G_{THF} = -501.342774

RuO_4

O	0.9722320	0.9722320	0.9722320
O	-0.9722320	-0.9722320	0.9722320
O	-0.9722320	0.9722320	-0.9722320
O	0.9722320	-0.9722320	-0.9722320
Ru	0.0000000	0.0000000	0.0000000

E_{THF} = -394.514781651

G_{THF} = -394.528209

d-6a

C	-2.4459822	0.3284001	0.2516494
C	-3.5484322	-0.4172549	0.1614044
H	-4.2441452	-0.2284219	-0.6624336
H	-1.7517852	0.1358091	1.0750654
O	0.2384468	-1.1580869	0.1541514
O	2.3953778	-2.7789559	0.8324614
O	2.3328618	-1.2015129	-1.4595316
C	-2.0706832	1.4064391	-0.7253736
H	-1.9339452	2.3636321	-0.1992186
H	-2.8895252	1.5451031	-1.4426066
C	-0.7848332	1.0849431	-1.4983276
H	-0.6225862	1.8361521	-2.2835256
H	-0.9004532	0.1170671	-2.0071776
C	0.4409998	1.0282141	-0.6302736
C	1.7045828	1.0356551	-1.1360196
H	0.3216938	1.1187021	0.4489014
H	1.8953558	1.1553331	-2.2009586
O	0.7003998	-3.4416349	-1.3420116
Ru	1.4324048	-2.2247749	-0.4339856
C	-3.9148872	-1.5161169	1.1126524
H	-4.0151322	-2.4730869	0.5826824
H	-4.8799482	-1.3133659	1.5964374
H	-3.1513882	-1.6301569	1.8909634

C	2.9149338	1.0785001	-0.2789606
O	2.6798548	0.5761521	0.9485324
O	3.9907718	1.4850171	-0.6435096
C	3.8222208	0.5342721	1.8102384
H	4.6068388	-0.0820559	1.3585834
H	3.4693768	0.0904461	2.7430894
H	4.2076078	1.5455871	1.9771014

E_{THF} = -896.041976051

G_{THF} = -895.863242

6a

C	1.1627201	1.4386145	0.1230582
C	2.1349671	1.0133135	-0.6894518
H	2.3077511	1.4604635	-1.6685458
H	1.0518031	0.9622815	1.0968822
O	-0.4485939	-0.8558555	0.7582782
O	-0.7673399	-3.5298325	0.0706282
O	-1.7914769	-1.4297435	-1.4347318
C	0.1662841	2.4922735	-0.2643678
H	-0.0650649	3.1300785	0.5999902
H	0.5924911	3.1323875	-1.0468018
C	-1.1367549	1.8746175	-0.7991228
H	-1.7873119	2.6872935	-1.1560108
H	-0.9073579	1.2491005	-1.6740558
C	-1.9020919	1.0505195	0.2012402
C	-2.9668259	0.2820115	-0.1389688
H	-1.6374309	1.1424395	1.2568112
C	-3.7359339	-0.5509375	0.8344692
H	-3.3327149	0.3210055	-1.1662998
H	-3.7350869	-1.6039935	0.5196892
H	-3.2990129	-0.4860715	1.8372342
H	-4.7856329	-0.2314465	0.8792402
O	0.9617811	-1.8320545	-1.4160448
Ru	-0.4608279	-1.9784365	-0.5207978
C	3.0475001	-0.1079975	-0.3669868
O	3.9823931	-0.4339255	-1.0600728
O	2.7167581	-0.7492125	0.7724202
C	3.5165341	-1.8981085	1.0560782
H	3.1314191	-2.3021205	1.9947932
H	3.4168041	-2.6297995	0.2458502
H	4.5702531	-1.6168655	1.1555962

E_{THF} = -896.048541757

G_{THF} = -895.868330

d-7a

C	-2.6511416	0.0473059	-0.1869924
C	-3.4074726	-0.8365041	-0.8436164
H	-3.6232726	-0.6491291	-1.9066044
H	-2.4257746	-0.1322411	0.8725846

O	0.0631164	0.0283669	0.8593306
O	1.5919574	-2.3260201	1.7945636
O	1.8135744	-0.8382101	-0.7638614
C	-2.0260486	1.2477569	-0.8321404
H	-2.0644526	2.1197889	-0.1526274
H	-2.6161486	1.5213139	-1.7242054
C	-0.5787646	1.0301999	-1.2789004
H	-0.2672356	1.8520799	-1.9493834
H	-0.5088266	0.0956109	-1.8676014
C	0.4303694	0.9873989	-0.1455704
C	1.8150684	0.5706199	-0.6097314
H	0.4621784	1.9633219	0.3757916
H	2.0581834	1.0084909	-1.5964464
O	-0.5402186	-2.5821301	-0.3033634
Ru	0.6881274	-1.7290841	0.4922936
C	-3.9788136	-2.0779281	-0.2526764
H	-3.6175256	-2.9738251	-0.7859214
H	-5.0800696	-2.0948851	-0.3211524
H	-3.6965756	-2.1817401	0.8070796
C	2.8652774	1.0869109	0.3634046
O	3.5366794	0.1120269	0.9681416
O	3.0313154	2.2662609	0.5499856
C	4.4996574	0.5459869	1.9278616
H	5.2798044	1.1508459	1.4429726
H	4.9284024	-0.3653061	2.3578916
H	4.0186284	1.1527169	2.7088936

E_{THF} = -896.142330227

G_{THF} = -895.958877

7a

C	1.3999294	0.9308101	-0.3930308
C	2.3273454	0.7285611	-1.3345218
H	2.3927824	1.3622771	-2.2256518
H	1.3758184	0.2617451	0.4741372
O	-0.8824126	-0.0761859	1.2186252
O	-1.6813286	-2.8573179	1.8162122
O	-2.7955126	-1.0148409	-0.1688278
C	0.3635944	2.0037401	-0.4664518
H	0.3979204	2.6149161	0.4561802
H	0.6067114	2.6803311	-1.3029048
C	-1.0626726	1.4781071	-0.6508908
H	-1.7070186	2.2992801	-1.0130888
H	-1.0831346	0.6959351	-1.4338468
C	-1.7051316	0.9349581	0.6138752
C	-3.0567736	0.2966711	0.3643452
H	-1.7728966	1.7385361	1.3754822
C	-3.9110936	0.1828621	1.6061092
H	-3.6029516	0.8269091	-0.4394738
H	-4.8073406	-0.4193929	1.3995072
H	-3.3466376	-0.3017199	2.4201182
H	-4.2301896	1.1790231	1.9510272

O	-0.1344326	-2.1701749	-0.6862508
Ru	-1.2366886	-1.8204349	0.5509872
C	3.3330064	-0.3481939	-1.2992718
O	4.1422194	-0.5424179	-2.1760908
O	3.2578064	-1.1016759	-0.1841928
C	4.1800324	-2.1800349	-0.1341248
H	3.9930064	-2.7004579	0.8126332
H	4.0280034	-2.8666269	-0.9811398
H	5.2180404	-1.8151869	-0.1694808

E_{THF} = -896.154419214

G_{THF} = -895.970475

d-7a$_{NaIO4}$

C	-1.6388149	2.1428081	1.2780935
H	-1.8660409	2.4364211	0.2462365
O	-0.8610319	0.1607831	-0.1690005
O	0.2185081	-1.9098009	0.8276485
C	-2.5656919	1.1721271	1.9457245
H	-3.5613179	1.2201931	1.4712695
H	-2.7059269	1.4551491	3.0038305
C	-2.0563709	-0.2704189	1.8954675
H	-2.7920029	-0.9581329	2.3489785
H	-1.1269589	-0.3567649	2.4871805
C	-1.7802109	-0.7074789	0.4680345
H	-2.7117889	-0.7126359	-0.1316515
C	-0.5574129	2.6920961	1.8704185
H	-0.3621679	2.4523631	2.9257025
C	-1.0954219	-2.0738739	0.3754445
H	-1.6008439	-2.8336309	0.9998085
Ru	0.9852301	-0.2378609	0.2828995
O	1.2390571	0.8643051	1.5306815
O	2.6774601	-1.1758359	0.0926485
I	3.4439761	-0.4876029	-1.5971065
O	2.9408711	-1.3354699	-3.0919555
O	5.0807241	-1.1734499	-1.1558215
O	4.0970321	1.2129381	-1.7921475
O	1.5237571	0.4138941	-1.3439735
Na	6.2316231	0.7120401	-1.2815295
C	0.3398401	3.6827971	1.2155255
H	1.4002071	3.4463201	1.3979555
H	0.1774401	3.7053991	0.1261315
H	0.1685471	4.6998261	1.6107005
C	-1.1561329	-2.5283129	-1.0785925
O	0.0043511	-2.3260429	-1.6990085
O	-2.1625749	-2.9511209	-1.5888695
C	0.0116961	-2.5658589	-3.1123445
H	0.9927081	-2.2184609	-3.4585475
H	-0.1266019	-3.6392089	-3.3087905
H	-0.8057169	-2.0074969	-3.5910415

E_{THF} = -1370.46172646

G_{THF} = -1370.272344

7a$_{NaIO4}$

C	-2.1935765	1.4234565	0.2486158
H	-1.8413775	1.3715275	1.2832158
O	-0.6594715	-0.6602405	0.6544118
O	0.1252225	-2.2357465	-1.1235232
C	-3.2510675	0.4624185	-0.1884602
H	-3.9081735	0.1959625	0.6574518
H	-3.8878005	0.9216865	-0.9639662
C	-2.6262565	-0.8142215	-0.7668292
H	-3.4217315	-1.5212315	-1.0634662
H	-2.0620855	-0.5657795	-1.6856362
C	-1.6977215	-1.5165135	0.2124888
H	-2.2629635	-1.8182655	1.1186868
C	-1.5823385	2.2863975	-0.5798012
H	-1.9122755	2.4325585	-1.6145672
C	-0.9861935	-2.7312855	-0.3855772
H	-1.6417115	-3.2327015	-1.1254312
Ru	0.8179295	-0.5457155	-0.5757662
O	0.4410545	0.7582395	-1.5613792
O	2.5251365	-1.1856375	-1.2134822
C	-0.5056705	-3.7087195	0.6624398
H	-1.3555255	-4.1919305	1.1700468
H	0.1164005	-4.4878365	0.1993948
H	0.1005105	-3.1830565	1.4191568
I	3.8501505	-0.4403835	0.0749978
O	4.3231725	-1.4332645	1.4849788
O	5.1662385	-0.6509725	-1.1762402
O	4.0956945	1.3723195	0.1800658
O	1.8883625	-0.0664895	0.8409608
Na	5.7001315	1.4904555	-1.4087162
C	-0.3726835	3.0479425	-0.2090282
O	0.1410025	3.8976395	-0.8992442
O	0.1349225	2.6190945	0.9587228
C	1.4357595	3.1003495	1.2777148
H	2.1427225	2.8520315	0.4709938
H	1.4261905	4.1894885	1.4391418
H	1.7380225	2.5684225	2.1876278

E_{gas} = -1370.42993459

G_{gas} = -1370.240109

E_{THF} = -1370.47073000

G_{THF} = -1370.280905

d-8a$_{NaIO4}$

C	-1.9162655	2.0255220	-0.2587817
H	-1.8588375	1.9537250	-1.3495407
O	-0.8831645	0.0304400	-0.4547697
O	-0.1469405	-1.4405570	1.5227473
C	-3.0889605	1.3968730	0.4263843
H	-3.8851215	1.2015100	-0.3113547

H	-3.5047335	2.0904660	1.1777063
C	-2.6997715	0.0825260	1.1092733
H	-3.5907775	-0.4614400	1.4658603
H	-2.0645565	0.2852600	1.9896763
C	-1.9210995	-0.7530610	0.1103363
H	-2.5800315	-1.1065670	-0.7068367
C	-1.0187785	2.8614020	0.3698843
H	-1.2316285	3.1521710	1.4056663
C	-1.1891925	-1.9439700	0.7391693
H	-1.8662865	-2.5454110	1.3747233
Ru	0.7527065	0.0130850	0.6564033
O	0.4733345	1.5655590	1.3156833
O	2.4407885	-0.5124000	1.5148073
I	3.7727355	-0.4169170	0.0744303
O	3.9629225	-1.8559290	-0.9797027
O	5.1528385	-0.5173650	1.2713923
O	4.3498775	1.1872260	-0.6061937
O	1.8525595	0.0597190	-0.7946117
Na	6.1384665	1.3731130	0.7482773
C	0.0101095	3.6336010	-0.3780887
H	0.8807715	3.8566240	0.2555873
H	0.3607685	3.0711270	-1.2590777
H	-0.3998005	4.5979180	-0.7275737
C	-0.6912235	-2.8319360	-0.3979027
O	-1.4281765	-3.4941460	-1.0842657
O	0.6241075	-2.7140960	-0.5566367
C	1.1906635	-3.3488110	-1.7087187
H	2.2338485	-3.0106890	-1.7386487
H	1.1254755	-4.4418350	-1.6033127
H	0.6433725	-3.0427380	-2.6119917

E_{gas} = -1370.41822307
G_{gas} = -1370.228095
E_{THF} = -1370.46016232
G_{THF} = -1370.270034

8a$_{NaIO4}$

C	-2.2842454	0.9141148	0.1415229
H	-2.1480434	1.1369398	1.2018119
O	-0.7507344	-0.5621962	0.5807119
O	0.4725946	-2.1411152	-1.0299381
C	-3.2691414	-0.1333372	-0.2716161
H	-3.9074544	-0.4102152	0.5833999
H	-3.9291424	0.2598268	-1.0634341
C	-2.5308484	-1.3763692	-0.7772461
H	-3.2278384	-2.2138172	-0.9489191
H	-2.0281954	-1.1631462	-1.7385151
C	-1.4892004	-1.7305042	0.2684079
H	-1.9948174	-2.0711262	1.1962799
C	-1.7263754	1.7927168	-0.7717551
H	-2.1066274	1.8424718	-1.7957221
C	-0.4657614	-2.7798512	-0.1743821

H	-0.9674424	-3.5545552	-0.7891391
Ru	0.7864706	-0.3097822	-0.6401491
O	0.0053356	0.8973538	-1.5752931
O	2.5371706	-0.3841412	-1.5568151
C	0.2531256	-3.4107932	0.9977619
H	-0.4430664	-3.9845142	1.6299979
H	1.0393016	-4.0902022	0.6379129
H	0.7246796	-2.6277962	1.6155759
I	3.7698626	0.4921998	-0.3175761
O	4.4835266	-0.4496782	1.0850519
O	5.1983126	0.1565438	-1.4065791
O	3.6959796	2.2778968	-0.1543301
O	1.8510066	0.3015138	0.6959459
Na	6.3632546	-1.0769702	-0.0280231
C	-0.8620514	2.9311298	-0.3755461
O	-0.6442794	3.8841178	-1.0811141
O	-0.3228704	2.7177538	0.8314519
C	0.7722326	3.5680088	1.1828139
H	1.6614656	3.2894208	0.5928349
H	0.5185586	4.6232948	1.0085859
H	0.9652586	3.3848078	2.2460259

E_{gas} = -1370.41999481
G_{gas} = -1370.228920
E_{THF} = -1370.46415077
G_{THF} = -1370.273076

9a$_{NaIO4}$

C	-1.5084722	-1.0185949	1.2720414
H	-2.5258672	-1.2781869	0.9377334
O	-1.1806952	0.2925031	0.7400014
O	0.7915358	-1.4673439	0.7301364
O	0.9889978	1.8078311	1.1783864
C	-1.3982712	-0.9046229	2.7963104
H	-2.3837802	-1.0735139	3.2558764
H	-0.7096812	-1.6602859	3.2033114
C	-0.8950482	0.5138961	3.0580574
H	-1.3386682	0.9698901	3.9548954
H	0.2007628	0.5274851	3.1775444
C	-1.2608142	1.2800631	1.7990424
H	-2.2980922	1.6653171	1.8285744
C	-0.2878952	2.3859841	1.4163484
H	-0.1568162	3.0367641	2.3048504
C	-0.5103352	-1.9643989	0.6117444
H	-0.5556562	-2.9423159	1.1331214
O	2.8347438	0.2305661	-0.2914246
C	-0.7489092	3.2109371	0.2341904
H	-1.6939102	3.7282121	0.4645804
H	0.0115788	3.9638661	-0.0170556
H	-0.9037012	2.5754561	-0.6526686
Ru	0.9645568	0.3052911	0.0374914
I	3.0578158	0.5516201	-2.3055976

O	3.0911838	2.1816981	-3.0660036
O	0.8414578	0.6765121	-1.6893206
O	4.8053978	0.0140681	-2.2105226
O	2.5929398	-0.7973929	-3.4827036
Na	4.6352838	-1.7574169	-3.4868986
C	-0.9539132	-2.2297729	-0.8287386
O	0.0435058	-2.0845529	-1.6865136
O	-2.0916702	-2.5195759	-1.1098976
C	-0.3057642	-2.0638719	-3.0765096
H	-0.5060862	-3.0872759	-3.4285366
H	-1.2079902	-1.4530559	-3.2241176
H	0.5622758	-1.6157809	-3.5777276

E_{gas} = -1370.49923130
G_{gas} = -1370.303617
E_{THF} = -1370.54325062
G_{THF} = -1370.347636