Supplementary Material (ESI) for Dalton Transactions

Supporting Information for –

Computational Study of Ethene Hydroarylation at $[Ir(\kappa^2\text{-}OAc)(PMe_3)Cp]^+$. †

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Contents:

Computed Cartesian coordinates (Å), SCF energies and enthalpies (0 K and 298.15 K) and free energies (298.15 K) in atomic units for all stationary points including unique imaginary eigenvalues for all transition states. Species are numbered according to the numbering scheme in the main text.

Computed Energies and Cartesian Coordinates.

Benzene

BP86 Energy = -232.242073665
Enthalpy 0K= -232.144364
Enthalpy 298K= -232.139833
Free Energy 298K= -232.171907

C	1.21660	-0.70237	0.00000
C	1.21681	0.70215	0.00000
C	0.00000	1.40468	0.00000
C	-1.21651	0.70256	0.00000
C	-1.21666	-0.70240	0.00000
C	-0.00027	-1.40470	0.00000
H	2.16517	1.25021	0.00000
H	0.00029	2.50002	0.00000
H	-2.16506	1.25033	0.00000
H	-2.16543	-1.24977	0.00000
H	0.00024	-2.50004	0.00000
H	2.16504	-1.25027	0.00000

Ethene

BP86 Energy = -78.5835139052
Enthalpy 0K= -78.533855
Enthalpy 298K= -78.530778
Free Energy 298K= -78.556069

C	0.00001	-0.67005	0.00000
C	0.00001	0.67001	0.00000
H	0.93080	1.24730	0.00000
H	0.93069	-1.24728	0.00000
H	-0.93097	1.24741	0.00000
H	-0.93065	-1.24720	0.00000

Acetic Acid
BP86 Energy = -229.088712434
Enthalpy 0K= -229.028684
Enthalpy 298K= -229.023986
Free Energy 298K= -229.056384

H	-1.72200	-0.80724	0.00004
O	-0.65941	1.20856	0.00000
C	-0.09255	0.12629	-0.00002
C	1.40379	-0.10154	-0.00001
H	1.69814	-0.68571	0.88738
H	1.69805	-0.68665	-0.88679
H	1.92130	0.86612	-0.00050
O	-0.77346	-1.06294	-0.00000

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BP86 Energy = -879.678005697
Enthalpy (0K) = -879.541490
Enthalpy (298K) = -879.523606
Free Energy (298K) = -879.589787

Ir	0.05681	0.13182	-0.00593
C	2.18507	0.59532	0.60159
C	1.69548	-0.65391	1.21700
C	2.13901	0.43428	-0.82193
C	1.42206	-1.59864	0.14842
C	1.61647	-0.91105	-1.12400
C	2.65363	1.79848	1.36525
C	1.68711	-0.94064	2.68985
C	2.52121	1.44802	-1.85773
C	1.14591	-3.06303	0.32665
C	1.55034	-1.52435	-2.49289
P	-2.00710	-1.00611	-0.00214
C	-2.20165	-2.32725	-1.29394
C	-2.39596	-1.86397	1.59800
C	-3.50813	0.04965	-0.28552
O	-0.97262	1.74757	1.09526
C	-1.27383	2.35475	-0.00317
C	-1.96885	3.68436	-0.00876
H	-1.21356	4.48663	0.06024
H	-2.53034	3.82391	-0.94363
H	-2.63429	3.77478	0.86235
O	-0.92693	1.76324	-1.09803
H	-3.21531	-2.75698	-1.24052
H	-2.04540	-1.88405	-2.28935
H	-1.46745	-3.13047	-1.13566
H	-4.40668	-0.58761	-0.29241
H	-3.59744	0.78905	0.52412
H	-3.41712	0.57054	-1.24981
H	-3.38133	-2.35467	1.53988
H	-1.62780	-2.62163	1.81268
H	-2.40240	-1.12025	2.40947
H	2.53651	-1.93562	-2.77793
H	0.82068	-2.34729	-2.53539
H	1.26699	-0.78081	-3.25390
H	2.10762	-3.59906	0.42736
H	0.56140	-3.27213	1.23573
H	0.62443	-3.49826	-0.53902
H	2.70723	-1.19772	3.03082
H	1.35295	-0.06581	3.26920
H	1.02900	-1.78716	2.93817
H	3.69435	1.64771	1.70587
H	2.63357	2.70941	0.74842
H	2.03403	1.97632	2.25815
H	3.51309	1.19892	-2.27713
H	1.80072	1.46160	-2.69088
H	2.57830	2.46355	-1.43889

TS(1-2)

BP86 Energy = -1081.54130357
Enthalpy (0K) = -1081.064107
Enthalpy (298K) = -1081.029823
Free Energy (298K) = -1081.133152
Nimag=1 (-131.7791 cm^{-1})

Ir	-0.88858	0.08094	0.00861
C	-0.49267	-1.83162	-1.11972
C	-1.87617	-1.81957	-0.73618
C	-0.21578	-0.64097	-1.95807
C	-2.46745	-0.60128	-1.29847
C	-1.44942	0.08144	-2.11847
C	0.52921	-2.86415	-0.77947
C	-2.59117	-2.85470	0.08081

```
C    1.08690 -0.37617 -2.65332
C   -3.90375 -0.19780 -1.18853
C   -1.71116  1.23471 -3.04074
P   -0.18223  2.27832  0.46789
C   -1.49439  3.24111  1.35631
C    1.26225  2.27456  1.63162
C    0.35041  3.37943 -0.92411
H    3.93291 -2.44939  1.22815
C    4.23972 -1.55780  0.67165
C    4.39054 -0.33105  1.34188
C    4.51277 -1.64309 -0.70526
C    4.81299  0.80915  0.63529
C    4.93038 -0.50112 -1.41321
C    5.07949  0.72527 -0.74310
H    4.20240 -0.27170  2.41898
H    4.42803 -2.60548 -1.22173
H    4.96287  1.75687  1.16411
H    5.16456 -0.57350 -2.48065
H    5.42804  1.60852 -1.28880
O   -1.31851  0.11270  2.05730
C   -0.82586 -0.97071  2.65589
C   -1.26587 -1.14685  4.09670
H   -2.32698 -1.44784  4.12600
H   -0.65824 -1.92064  4.58450
H   -1.18418 -0.19673  4.64766
O   -0.06486 -1.76108  2.06950
H   -1.08666  4.19946  1.71671
H   -2.33662  3.43329  0.67409
H   -1.84650  2.63503  2.20402
H    0.62735  4.36883 -0.52522
H    1.22219  2.94208 -1.43386
H   -0.47269  3.49944 -1.64373
H    1.53927  3.30870  1.89497
H    0.97183  1.72341  2.53827
H    2.11935  1.76520  1.16324
H   -4.48739 -0.69055 -1.98978
H   -4.33907 -0.50122 -0.22443
H   -4.03055  0.88936 -1.30313
H   -2.13512  0.85779 -3.98982
H   -2.43694  1.94787 -2.61857
H   -0.78726  1.77845 -3.28730
H    1.15912 -1.00281 -3.56200
H    1.17511  0.67449 -2.96968
H    1.95122 -0.61774 -2.01394
H    0.68441 -3.51682 -1.66034
H    1.49837 -2.39932 -0.53561
H    0.22151 -3.48262  0.07324
H   -3.00351 -3.64278 -0.57499
H   -1.90993 -3.32680  0.80359
H   -3.43144 -2.41593  0.64111
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BP86 Energy = -1081.54682332
Enthalpy (0K)  = -1081.069214
Enthalpy (298K) = -1081.034260
Free Energy (298K) = -1081.140331

Ir -0.89971  0.01294  0.00839
C  -0.15070 -1.86467 -1.02190
C  -1.56055 -1.99737 -0.84128
C   0.09743 -0.63897 -1.82075
C  -2.20144 -0.84729 -1.51177
C  -1.17985 -0.07508 -2.20039
C   0.91037 -2.79868 -0.53692
C  -2.28595 -3.11897 -0.16393
C   1.44247 -0.19484 -2.30563
C  -3.68034 -0.63226 -1.60863
C  -1.42193  1.00943 -3.20947
P  -0.78316  2.33386  0.45254
C  -2.26861  2.92548  1.39320
C   0.65505  2.74892  1.54710
C  -0.62653  3.52892 -0.95657
H   4.37663 -2.31060  0.99604
C   4.52745 -1.32030  0.55319
C   4.32091 -0.16557  1.32884
C   4.96099 -1.20325 -0.77970
C   4.55026  1.10488  0.77168
C   5.18705  0.06783 -1.33734
C   4.98176  1.22201 -0.56169
H   4.00739 -0.25817  2.37401
H   5.14469 -2.10284 -1.37677
H   4.42208  2.00293  1.38606
H   5.54290  0.15745 -2.36910
H   5.18059  2.21066 -0.98896
O  -0.84295 -0.01703  2.02672
C  -0.73198 -1.17475  2.74422
C  -0.88485 -0.93095  4.23310
H  -1.87224 -0.48850  4.44611
H  -0.77698 -1.87691  4.77972
H  -0.12535 -0.21158  4.58139
O  -0.51953 -2.27199  2.24102
H  -2.14422  3.98143  1.68342
H  -3.16758  2.81879  0.76703
H  -2.37857  2.29970  2.29115
H  -0.56057  4.55477 -0.55917
H   0.28509  3.30929 -1.53288
H  -1.50121  3.45609 -1.61898
H   0.63179  3.81643  1.82042
H   0.58478  2.12432  2.44893
H   1.59507  2.51801  1.02245
H  -4.09400 -1.27108 -2.41207
H  -4.19292 -0.90675 -0.67364
H  -3.92904  0.41173 -1.85203
H  -1.57428  0.55418 -4.20526
H  -2.32357  1.59814 -2.97914
H  -0.56779  1.69754 -3.29090
H   1.71579 -0.76803 -3.21193
H   1.44569  0.87203 -2.57607
H   2.23242 -0.36564 -1.55764
H   1.08311 -3.58244 -1.29900
H   1.86612 -2.27571 -0.37533
H   0.61131 -3.27903  0.40473
H  -2.50820 -3.91374 -0.90040
H  -1.68420 -3.54719  0.64901
H  -3.24573 -2.78461  0.26006
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TS(2-3)

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BP86 Energy  = -1081.52460413
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Enthalpy (0K) = -1081.049988
Enthalpy (298K) = -1081.017042
Free Energy (298K) = -1081.110811
Nimag=1(-804.2257 cm^{-1})

Ir	-0.34324	-0.01466	-0.03434
C	-1.43960	1.15973	1.59560
C	-2.20552	1.22674	0.37910
C	-1.32011	-0.25603	1.96793
C	-2.58460	-0.12888	-0.02248
C	-2.06118	-1.03207	0.99188
C	-0.94350	2.33271	2.38993
C	-2.61063	2.47716	-0.34306
C	-0.84971	-0.79780	3.29007
C	-3.53523	-0.47095	-1.13449
C	-2.42198	-2.47841	1.17942
P	0.49127	-1.90045	-1.18279
C	-0.77977	-3.10935	-1.80890
C	1.40557	-1.56012	-2.76824
C	1.64865	-2.99211	-0.22274
H	1.14322	1.54652	0.19263
C	1.79851	0.45260	0.55605
C	2.87948	0.38438	-0.37451
C	2.14524	0.30190	1.92882
C	4.19899	0.14332	0.02701
C	3.46173	0.05176	2.33956
C	4.49316	-0.04105	1.38961
H	2.67775	0.57970	-1.43189
H	1.37277	0.38279	2.69485
H	5.00133	0.11361	-0.71753
H	3.68646	-0.06216	3.40505
H	5.52206	-0.23214	1.71044
O	0.06387	1.10652	-1.83578
C	0.52226	2.30838	-1.64409
C	0.61211	3.21436	-2.85145
H	0.13062	4.17848	-2.62288
H	1.67274	3.42842	-3.06438
H	0.14258	2.75630	-3.73196
O	0.91156	2.73327	-0.50755
H	-0.26564	-3.91556	-2.35696
H	-1.34285	-3.55304	-0.97820
H	-1.47231	-2.59713	-2.49418
H	1.99810	-3.82596	-0.85324
H	2.50956	-2.39713	0.11641
H	1.12647	-3.39783	0.65788
H	1.54868	-2.50983	-3.30827
H	0.81473	-0.86390	-3.38094
H	2.38778	-1.11458	-2.56276
H	-4.58041	-0.30802	-0.81208
H	-3.36127	0.15488	-2.02385
H	-3.44507	-1.52443	-1.43969
H	-3.15807	-2.55304	2.00153
H	-2.89285	-2.91279	0.28617
H	-1.55641	-3.09678	1.46589
H	-1.72652	-1.04245	3.91856
H	-0.25334	-1.71660	3.17869
H	-0.25191	-0.06527	3.85213
H	-1.72756	2.67654	3.08923
H	-0.05642	2.07922	2.99059
H	-0.67260	3.17719	1.73842
H	-3.61132	2.79504	0.00314
H	-1.91170	3.30430	-0.15035
H	-2.67456	2.31504	-1.43003

3
BP86 Energy = -1081.54529765
Enthalpy (0K) = -1081.066288
Enthalpy (298K) = -1081.033514
Free Energy (298K) = -1081.126467

Ir	0.29052	-0.02141	0.01637
C	1.10933	0.16985	-2.11174
C	1.80408	1.13323	-1.30824
C	1.35639	-1.15304	-1.52511
C	2.57391	0.42435	-0.27119
C	2.33694	-0.97079	-0.43603
C	0.34273	0.43604	-3.37378
C	1.93590	2.60442	-1.58605
C	1.08072	-2.46984	-2.19851
C	3.52172	1.08191	0.69167
C	3.06854	-2.09608	0.23662
P	-0.33685	-1.43635	1.78362
C	0.97526	-1.66575	3.08308
C	-1.78144	-0.90492	2.82026
C	-0.79378	-3.15968	1.27412
H	-0.91301	2.11858	-0.61711
C	-1.74952	-0.13807	-0.50891
C	-2.78331	0.61546	0.10832
C	-2.16725	-1.03429	-1.52803
C	-4.12548	0.53213	-0.30845
C	-3.50702	-1.13060	-1.94365
C	-4.49594	-0.33615	-1.34445
H	-2.56172	1.27111	0.95627
H	-1.43666	-1.69802	-1.99866
H	-4.88151	1.14734	0.19179
H	-3.77454	-1.83863	-2.73582
H	-5.53885	-0.40486	-1.66822
O	-0.10555	1.64049	1.47931
C	-0.49000	2.77466	1.08995
C	-0.54677	3.95815	2.01016
H	-0.07052	4.83036	1.53452
H	-1.60206	4.22642	2.19028
H	-0.05794	3.72523	2.96432
O	-0.89298	3.00794	-0.15209
H	0.59628	-2.30786	3.89502
H	1.87338	-2.12640	2.64971
H	1.23863	-0.67798	3.49197
H	-1.08825	-3.75564	2.15307
H	-1.63354	-3.10361	0.56423
H	0.06177	-3.64442	0.77947
H	-1.91135	-1.61939	3.64905
H	-1.58410	0.09747	3.22865
H	-2.69215	-0.87389	2.20660
H	4.46366	1.35973	0.18378
H	3.09529	2.00480	1.11725
H	3.77898	0.41620	1.52961
H	3.87124	-2.45642	-0.43353
H	3.54691	-1.78121	1.17609

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H    2.41500 -2.95870  0.44254
H    1.96906 -2.78492 -2.77761
H    0.85620 -3.27125 -1.47738
H    0.24161 -2.40380 -2.90701
H    0.94296  0.13066 -4.25006
H   -0.60538 -0.12478 -3.40164
H    0.10411  1.50432 -3.48988
H    2.86671  2.78329 -2.15572
H    1.10223  3.00014 -2.18414
H    2.00839  3.19654 -0.66045
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BP86 Energy              = -734.455784738
Enthalpy 0K         =  -734.118654
Enthalpy 298K       =  -734.096607
Free Energy 298K    =  -734.167749

Ir -0.53252 -0.38862  0.14503
C  -1.13838 -2.63008 -0.03013
C  -2.30888 -1.85126 -0.38435
C  -1.99831 -1.07126 -1.53782
C  -0.62214 -1.34116 -1.90173
C  -0.11350 -2.33993 -0.98288
H  -3.26511 -1.86246  0.13910
H  -1.06339 -3.33597  0.79737
H   0.88907 -2.76619 -0.99617
H  -0.10498 -0.96365 -2.78244
H  -2.68142 -0.40108 -2.05929
P  -0.60419  1.93151 -0.18554
C  -2.33855  2.60507 -0.25273
C   0.11342  2.60858 -1.75798
C   0.24670  2.93045  1.12341
C   1.60017 -0.17600  0.11568
C   2.45465 -0.51664  1.18791
C   3.85496 -0.49790  1.04082
C   4.44437 -0.14768 -0.18144
C   3.61435  0.16808 -1.26556
C   2.21485  0.15036 -1.11774
H   1.60553  0.37611 -1.99685
H   4.04665  0.42289 -2.23924
H   5.53284 -0.13387 -0.29107
H   4.48125 -0.77006  1.89703
H   2.05906 -0.82645  2.15683
C  -1.61657  0.08368  2.00667
C  -0.29841 -0.34519  2.32038
H  -0.12494 -1.36059  2.69293
H   0.43871  0.39322  2.64614
H  -1.89173  1.13525  2.13031
H  -2.46083 -0.60436  2.11559
H  -2.30688  3.70424 -0.32729
H  -2.84632  2.20095 -1.14213
H  -2.91272  2.31994  0.64029
H   0.17075  4.00178  0.87815
H  -0.21086  2.75738  2.10920
H   1.30489  2.63131  1.15739
H  -0.15417  3.67541 -1.82978
H   1.20678  2.50747 -1.74746
H  -0.29792  2.07485 -2.62820
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TS(4-5)

```
BP86 Energy              = -734.423552772
Enthalpy 0K         =  -734.087819
Enthalpy 298K       =  -734.066153
Free Energy 298K    =  -734.136659
Nimag=1(-319.0442 cm-1)

Ir -0.36534 -0.48587  0.17613
C   0.07462 -2.74484  0.00871
C  -1.34261 -2.51347  0.10825
C  -1.73992 -1.73551 -1.03851
C  -0.57042 -1.55169 -1.89532
C   0.52996 -2.15544 -1.23593
H  -2.00103 -2.85501  0.90697
H   0.68230 -3.32110  0.70606
H   1.56353 -2.13640 -1.58185
H  -0.54709 -1.04949 -2.86152
H  -2.76266 -1.45019 -1.28240
P  -1.49659  1.51336 -0.24901
C  -3.34643  1.31609 -0.19410
C  -1.19975  2.22979 -1.93802
C  -1.27422  2.96748  0.89874
C   1.67352  0.38155  0.40392
C   2.72386 -0.57815  0.46050
C   3.98057 -0.31784 -0.09982
C   4.24437  0.92420 -0.70320
C   3.24146  1.90739 -0.71924
C   1.98159  1.64530 -0.16204
H   1.23451  2.44192 -0.16794
H   3.44153  2.89018 -1.15825
H   5.23020  1.13368 -1.12854
H   4.76333 -1.08130 -0.04456
H   2.55354 -1.53533  0.96550
C  -0.62477 -0.14169  2.25160
C   0.73265  0.39832  2.12542
H   1.52230 -0.16838  2.62560
H   0.84450  1.47906  2.25546
H  -1.42346  0.55746  2.52748
H  -0.72049 -1.09866  2.78128
H  -3.83621  2.29389 -0.33041
H  -3.67953  0.63952 -0.99495
H  -3.64244  0.89143  0.77746
H  -1.92778  3.78606  0.55666
H  -1.56798  2.69007  1.92255
H  -0.23577  3.32780  0.91116
H  -1.74830  3.17806 -2.05851
H  -0.12249  2.39826 -2.08303
H  -1.54723  1.51144 -2.69669
```

5

```
BP86 Energy              = -734.460911465
Enthalpy 0K         =  -734.123407
Enthalpy 298K       =  -734.101595
Free Energy 298K    =  -734.172516

Ir -0.10514  0.36065 -0.17066
C   0.80833  2.27085 -0.98426
C  -0.62063  2.40934 -0.79555
C  -0.87206  2.32665  0.64152
```

```
C    0.36505   2.11991   1.32209
C    1.39152   2.03543   0.30439
H   -1.35676   2.64496  -1.56360
H    1.34046   2.30508  -1.93434
H    2.44420   1.81882   0.48816
H    0.50983   2.01735   2.39612
H   -1.84897   2.44097   1.11358
P   -2.06988  -0.76780   0.36156
C   -3.55461  -0.00235  -0.45270
C   -2.49359  -0.74557   2.17173
C   -2.26699  -2.56591  -0.08004
C    1.65993  -1.37764  -0.65055
C    3.00209  -0.91386  -0.80582
C    3.79114  -0.62792   0.30306
C    3.26455  -0.74314   1.61999
C    1.96207  -1.18337   1.80601
C    1.13230  -1.51600   0.68092
H    0.30677  -2.21099   0.85630
H    1.57197  -1.34251   2.81657
H    3.90279  -0.52838   2.48238
H    4.83549  -0.32969   0.16349
H    3.41981  -0.84155  -1.81554
C   -0.16474  -0.66421  -2.06002
C    0.82866  -1.81754  -1.85233
H    1.47014  -2.00413  -2.73162
H    0.32118  -2.77064  -1.61973
H   -1.16490  -0.99460  -2.38394
H    0.20671   0.05410  -2.80810
H   -4.47645  -0.52217  -0.14573
H   -3.62537   1.05916  -0.17125
H   -3.44309  -0.07076  -1.54584
H   -3.29107  -2.88416   0.17382
H   -2.10303  -2.71484  -1.15762
H   -1.55813  -3.19235   0.48241
H   -3.46449  -1.23675   2.34750
H   -1.71031  -1.27289   2.73751
H   -2.54060   0.29512   2.52589
```

6

```
BP86 Energy              = -963.574257633
Enthalpy 0K        =  -963.175092
Enthalpy 298K      =  -963.147469
Free Energy 298K   =  -963.232912

Ir   0.58819  -0.13043   0.32360
C   -0.96541  -1.41879   1.20480
C    0.34594  -1.95142   1.50100
C    0.99490  -1.05208   2.45638
C    0.12907   0.04511   2.66176
C   -1.09408  -0.15788   1.88957
H    0.71345  -2.92946   1.18942
H   -1.72663  -1.87998   0.57557
H   -2.01165   0.42931   1.94842
H    0.34709   0.91540   3.28322
H    1.98051  -1.18542   2.90067
P    2.56659  -0.78426  -0.74814
C    2.39369  -2.23225  -1.89650
C    3.91290  -1.32053   0.41585
C    3.39326   0.51131  -1.78650
C   -2.85142   0.06043  -1.21336
C   -3.30970  -1.25579  -1.44519
C   -4.47192  -1.73652  -0.82147
C   -5.20577  -0.90524   0.04308
C   -4.77642   0.41224   0.26515
C   -3.61073   0.88853  -0.36124
H   -3.30361   1.93114  -0.20997
H   -5.35618   1.07687   0.91417
H   -6.11616  -1.27694   0.52323
H   -4.81542  -2.75650  -1.02296
H   -2.76232  -1.90587  -2.13879
C   -0.28324  -0.19120  -1.63868
C   -1.60012   0.57808  -1.90104
H   -1.47836   1.65339  -1.67767
O    1.17969   1.88444  -0.23219
H    0.46244   0.19610  -2.35807
H   -0.43296  -1.25939  -1.87573
C    0.47102   2.89129   0.04201
C    0.90611   4.28286  -0.30070
O   -0.70166   2.79072   0.65048
H   -1.76718   0.53297  -2.99845
H    0.17979   4.73315  -0.99795
H    0.91060   4.90611   0.60867
H    1.90393   4.27125  -0.75591
H   -0.88480   1.80556   0.75902
H    4.30442   0.09146  -2.24194
H    2.70784   0.84718  -2.57874
H    3.65386   1.37299  -1.15574
H    4.81829  -1.59453  -0.15006
H    4.14831  -0.49612   1.10606
H    3.57739  -2.19279   0.99727
H    3.37125  -2.48337  -2.33842
H    2.01188  -3.10076  -1.33817
H    1.68215  -1.98496  -2.69809
```

TS(6-7)

```
BP86 Energy              = -963.545355295
Enthalpy 0K        =  -963.150678
Enthalpy 298K      =  -963.124463
Free Energy 298K   =  -963.205982
Nimag=1(-1022.749023 cm-1)

Ir  -0.57698  -0.11591  -0.38488
C    1.23160  -1.14513  -1.22119
C    0.07528  -1.98564  -1.37516
C   -0.86458  -1.29456  -2.25381
C   -0.26497  -0.03852  -2.61906
C    1.02597   0.06556  -1.98825
H   -0.04275  -2.98602  -0.96055
H    2.11288  -1.37346  -0.61929
H    1.72623   0.89464  -2.06813
H   -0.73932   0.72821  -3.23349
H   -1.81438  -1.67754  -2.62419
P   -2.39819  -0.99884   0.83518
C   -2.19011  -1.33986   2.65132
C   -2.98395  -2.64850   0.20664
C   -3.93009   0.04429   0.76461
C    3.02944   0.33058   1.25266
C    3.50344  -0.97176   1.52594
```

```
C   4.54109 -1.53471  0.76536
C   5.12766 -0.79835 -0.27967
C   4.68091  0.50656 -0.54660
C   3.64125  1.06596  0.21591
H   3.30829  2.09178  0.01904
H   5.15315  1.09586 -1.33951
H   5.94299 -1.23186 -0.86703
H   4.90481 -2.54077  0.99830
H   3.06671 -1.54348  2.35431
C   0.47043  0.34729  1.69288
C   1.88515  0.91721  2.04934
H   1.88466  2.01485  1.96331
O  -1.67496  1.71360 -0.35618
H  -0.27526  0.74670  2.39894
H   0.51793 -0.74164  1.83232
C  -0.98510  2.76394 -0.01943
C  -1.65431  4.10865 -0.17167
O   0.19846  2.67970  0.43147
H   2.02489  0.68017  3.12182
H  -1.74453  4.58251  0.81957
H  -1.01496  4.76335 -0.78519
H  -2.64630  4.01408 -0.63214
H   0.29673  1.30614  0.68736
H  -4.74543 -0.45948  1.30864
H  -3.73037  1.02695  1.21403
H  -4.22044  0.19615 -0.28565
H  -3.86345 -2.96975  0.78784
H  -3.26853 -2.57290 -0.85327
H  -2.19053 -3.40299  0.31816
H  -3.10555 -1.82276  3.02946
H  -1.33361 -2.01111  2.81679
H  -2.02588 -0.40450  3.20549
```

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```
BP86 Energy              = -963.568631295
Enthalpy 0K        =  -963.171312
Enthalpy 298K      =  -963.141858
Free Energy 298K   =  -963.238239

Ir -1.00303 -0.10748 -0.46433
C   0.64615 -1.52207 -0.67996
C  -0.47811 -2.03870 -1.41086
C  -0.81824 -1.05113 -2.40831
C   0.19612  0.00756 -2.38146
C   1.08731 -0.27702 -1.31964
H  -1.00958 -2.96865 -1.21574
H   1.14209 -1.99059  0.16971
H   1.91546  0.34592 -0.97690
H   0.20124  0.90447 -2.99876
H  -1.65316 -1.11069 -3.10779
P  -2.74660 -0.77591  0.96445
C  -2.47545 -0.23564  2.71610
C  -3.08770 -2.59418  1.06830
C  -4.36176 -0.00781  0.47841
C   4.15369 -0.12003  1.25425
C   4.22054 -1.38814  0.63631
C   4.41630 -1.50975 -0.74981
C   4.55275 -0.35839 -1.54733
C   4.48437  0.91172 -0.94752
C   4.28079  1.02634  0.43864
H   4.25062  2.01968  0.90143
H   4.60892  1.81406 -1.55524
H   4.73401 -0.45150 -2.62292
H   4.49546 -2.50314 -1.20444
H   4.15550 -2.29078  1.25643
C   2.47283 -0.05442  3.18196
C   3.95560  0.00430  2.75421
H   4.39562  0.95459  3.10480
O  -1.46869  1.69222  0.23733
H   2.37394  0.02866  4.27727
H   2.01168 -1.00968  2.87288
C  -0.81318  2.82097 -0.23855
C  -1.27255  4.06767  0.48272
O   0.01777  2.78367 -1.13171
H   4.51004 -0.80407  3.26416
H  -1.09881  3.96674  1.56686
H  -0.73087  4.94101  0.09692
H  -2.35686  4.20880  0.33969
H   1.89697  0.76864  2.72400
H  -5.14093 -0.25982  1.21603
H  -4.22561  1.08285  0.43399
H  -4.66142 -0.37436 -0.51516
H  -3.91874 -2.77562  1.76915
H  -3.36692 -2.98248  0.07673
H  -2.19280 -3.12370  1.42965
H  -3.35167 -0.49627  3.33170
H  -1.57861 -0.72805  3.12140
H  -2.32302  0.85362  2.72135
```

Ethylbenzene

```
BP86 Energy =    -310.871657820
Enthalpy 0K=             -310.719058
Enthalpy 298K=           -310.711541
Free Energy 298K=        -310.751256

C  -0.43993 -0.00009 -0.33070
C   0.26930  1.20999 -0.18573
C   1.64433  1.21322  0.09598
C   2.33723  0.00009  0.23851
C   1.64447 -1.21312  0.09609
C   0.26943 -1.21007 -0.18565
C  -2.77053  0.00009  0.70449
C  -1.93512 -0.00013 -0.59441
H  -0.26463  2.16118 -0.30094
H   2.17670  2.16505  0.19931
H   3.41083  0.00016  0.45438
H   2.17693 -2.16489  0.19948
H  -0.26434 -2.16136 -0.30076
H  -3.85144  0.00001  0.48200
H  -2.54674  0.88994  1.31707
H  -2.54667 -0.88949  1.31743
H  -2.20288 -0.88584 -1.19956
H  -2.20287  0.88538 -1.19985
```

TS(1-8)

```
BP86 Energy =    -731.274216509
Enthalpy 0K=             -730.978791
Enthalpy 298K=           -730.956692
```

Free Energy 298K= -731.030662
Nimag=1 (-139.4989cm^{-1})

Ir	-0.34687	-0.24024	-0.10040
C	-2.41000	-1.23137	0.03991
C	-2.24969	-0.68405	-1.26149
C	-1.33098	-2.18128	0.29766
C	-1.04913	-1.27061	-1.85107
C	-0.51891	-2.23658	-0.89343
P	2.00022	-0.28620	0.03348
C	2.72262	-0.27120	-1.67270
C	2.83213	1.14333	0.87057
C	2.73877	-1.78382	0.84347
O	0.14834	1.64343	-1.03871
C	-0.47924	2.52908	-0.30099
C	-0.43917	3.96855	-0.75765
O	-1.09861	2.14673	0.72291
H	-3.18475	-0.94317	0.75006
H	-2.87146	0.08753	-1.71509
H	-1.21248	-2.79329	1.19014
H	-0.67914	-1.08908	-2.86080
H	0.32451	-2.90540	-1.06552
H	3.82321	-0.25222	-1.62132
H	2.40073	-1.16833	-2.22310
H	2.35495	0.62500	-2.19432
H	3.92270	1.05839	0.73566
H	2.47854	2.07827	0.41252
H	2.60162	1.14882	1.94558
H	3.83836	-1.73015	0.78939
H	2.43121	-1.83200	1.89881
H	2.40064	-2.69776	0.33235
H	-1.36849	4.19295	-1.30898
H	-0.40104	4.63780	0.11450
H	0.41241	4.15773	-1.42657
C	-1.41446	0.05942	2.79903
C	-0.06694	0.18113	2.69004
H	-2.06937	0.90606	2.57812
H	-1.87779	-0.87160	3.14442
H	0.60119	-0.63143	2.99396
H	0.37257	1.15602	2.46474

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BP86 Energy = -731.307844589
Enthalpy 0K= -731.008285
Enthalpy 298K= -730.987451
Free Energy 298K= -731.056850

Ir	0.54422	-0.18926	0.11227
C	2.55555	-1.24307	-0.28103
C	2.03578	-0.85160	-1.55436
C	2.73933	-0.03692	0.51372
C	1.86336	0.57385	-1.56282
C	2.33132	1.08812	-0.27799
P	-1.04679	1.59376	-0.07995
C	-0.18026	3.20953	-0.42212
C	-2.18399	1.43344	-1.53605
C	-2.14970	2.08042	1.32781
H	2.78165	-2.26261	0.03016
H	1.73012	-1.53144	-2.35073
H	3.15273	0.00924	1.52217
H	1.52386	1.16372	-2.41396
H	2.42008	2.13443	0.00916
H	-0.94105	3.99598	-0.55471
H	0.46323	3.48483	0.42731
H	0.42450	3.15041	-1.33927
H	-2.61732	2.42197	-1.75829
H	-1.62808	1.06602	-2.41073
H	-2.98390	0.72610	-1.28148
H	-2.74731	2.94464	0.99397
H	-2.81386	1.24283	1.57743
H	-1.55051	2.37883	2.20099
H	-1.13333	0.01559	2.33691
C	-0.07167	-0.21732	2.25012
C	0.27282	-1.52985	1.85348
H	0.61954	0.38255	2.85271
H	1.24197	-1.95768	2.12912
H	-0.51133	-2.25443	1.62189
O	-0.86996	-1.45934	-0.77336
C	-2.11155	-1.58355	-0.31686
C	-2.87202	-2.71518	-0.99460
O	-2.60818	-0.87430	0.57203
H	-2.72688	-3.63903	-0.40829
H	-3.94634	-2.48259	-0.99933
H	-2.50907	-2.90078	-2.01551

TS(8-9)

BP86 Energy = -731.278655320
Enthalpy 0K= -730.984307
Enthalpy 298K= -730.963605
Free Energy 298K= -731.032928
Nimag=1 (-232.6491cm^{-1})

Ir	0.49672	-0.14199	-0.04091
C	2.39853	-1.40543	-0.24191
C	2.03502	-0.90223	-1.53324
C	2.62486	-0.25596	0.61972
C	2.04340	0.54059	-1.49936
C	2.43021	0.93870	-0.15112
P	-0.89521	1.74627	0.11951
C	0.02120	3.34719	-0.10258
C	-2.22449	1.83112	-1.17265
C	-1.81044	2.00934	1.71116
H	2.48891	-2.45338	0.03889
H	1.73575	-1.50940	-2.38897
H	2.91361	-0.29288	1.66985
H	1.86983	1.20122	-2.34853
H	2.58765	1.95645	0.20232
H	-0.69530	4.18436	-0.08891
H	0.74065	3.48246	0.71927
H	0.55690	3.35096	-1.06382
H	-2.72417	2.81177	-1.11661
H	-1.78792	1.69333	-2.17283
H	-2.96427	1.03992	-0.98656
H	-2.42475	2.92041	1.62793
H	-2.46069	1.14379	1.90548
H	-1.09857	2.13244	2.54165
H	-1.13145	-0.89835	1.33138
C	-0.09208	-0.84841	1.97810

```
C   0.28536 -2.10884  2.35915
H  -0.06405 -0.06530  2.74617
H   0.63784 -2.33355  3.37399
H   0.20437 -2.96109  1.67425
O  -1.02146 -1.19142 -1.04440
C  -2.15948 -1.50004 -0.47887
C  -3.09727 -2.34096 -1.31944
O  -2.47298 -1.15748  0.69649
H  -2.91986 -3.40514 -1.08617
H  -4.14040 -2.11077 -1.05962
H  -2.91674 -2.18731 -2.39238
```

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```
BP86 Energy =    -731.300380866
Enthalpy 0K=             -731.003377
Enthalpy 298K=           -730.981632
Free Energy 298K=        -731.055572

Ir  0.10743 -0.42090  0.01170
C  -0.53790 -2.53782 -0.56563
C   0.07446 -1.97692 -1.76519
C   0.46783 -2.55872  0.45700
C   1.42245 -1.64881 -1.48727
C   1.66858 -1.94851 -0.07511
P   1.42586  1.51590  0.07339
C   3.19617  1.22667  0.54365
C   1.51318  2.33193 -1.59165
C   0.90590  2.90358  1.19490
H  -1.54941 -2.93508 -0.48787
H  -0.43741 -1.80901 -2.71395
H   0.35048 -2.93079  1.47455
H   2.13945 -1.22532 -2.19013
H   2.62398 -1.87698  0.44365
H   3.75081  2.17891  0.53747
H   3.23840  0.78515  1.55120
H   3.66446  0.53471 -0.17257
H   2.12282  3.24879 -1.54282
H   1.95617  1.63460 -2.31862
H   0.49228  2.57987 -1.91848
H   1.52854  3.78830  0.98613
H  -0.15067  3.15564  1.01767
H   1.03836  2.61829  2.24933
H  -2.37807  0.09606  1.22526
C  -0.55086 -0.05472  1.92589
C  -1.27214 -0.89411  2.71553
H  -0.32025  0.92108  2.38028
H  -1.56951 -0.59501  3.72918
H  -1.58847 -1.89780  2.40612
O  -1.43101  0.88686 -0.81679
C  -2.64304  0.97701 -0.46168
C  -3.64232  1.66980 -1.34333
O  -3.12708  0.48483  0.65708
H  -4.39365  0.93510 -1.68018
H  -4.18108  2.43973 -0.76825
H  -3.14639  2.11523 -2.21461
```

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```
BP86 Energy =    -580.805468908
Enthalpy 0K=             -580.515701
Enthalpy 298K=           -580.496908
Free Energy 298K=        -580.561647

Ir  0.39466  0.07057  0.10183
C   2.67152 -0.36578  0.29952
C   1.98876 -1.60116  0.63066
C   1.24497 -2.01802 -0.51219
C   1.43700 -1.03432 -1.55912
C   2.36165 -0.03591 -1.05686
P  -1.88024 -0.41076 -0.11093
C  -2.43944 -1.90942  0.83311
C  -2.40582 -0.79514 -1.84821
C  -3.02937  0.94163  0.41897
C  -0.08844  1.67624 -1.16549
C   0.11761  2.99832 -1.03513
C  -0.05081  0.33901  2.24303
C   0.29775  1.59220  1.66716
H   3.33115  0.19729  0.96047
H   2.03854 -2.12247  1.58682
H   0.64327 -2.92366 -0.58793
H   1.05693 -1.09543 -2.57862
H   2.72746  0.83121 -1.60580
H  -3.52319 -2.05387  0.69387
H  -1.90680 -2.79786  0.46071
H  -2.22514 -1.79108  1.90535
H  -3.48566 -1.01446 -1.86746
H  -2.20323  0.06323 -2.50541
H  -1.85329 -1.67305 -2.21682
H  -4.07284  0.63107  0.25083
H  -2.89001  1.16780  1.48717
H  -2.80620  1.84351 -0.17032
H  -0.46657  1.32554 -2.13808
H  -0.10184  3.66922 -1.87599
H   0.51270  3.48076 -0.13595
H  -1.08769  0.14043  2.53206
H   0.68317 -0.22189  2.83111
H   1.29546  2.01360  1.83101
H  -0.48358  2.33195  1.47328
```

TS(10-11)

```
BP86 Energy =    -580.774884521
Enthalpy 0K=             -580.485804
Enthalpy 298K=           -580.467628
Free Energy 298K=        -580.531599
Nimag=1 (-363.0397cm-1)

Ir -0.36510 -0.00853 -0.13398
C  -2.55159 -0.70321 -0.39940
C  -1.65454 -1.63801 -1.02603
C  -0.79993 -2.17921  0.00315
C  -1.22742 -1.63574  1.28896
C  -2.27892 -0.71792  1.02365
P   1.92615 -0.22863  0.17618
C   2.72782 -1.39822 -1.02363
C   2.40827 -0.89780  1.84048
C   2.98525  1.29415  0.02747
C  -0.33516  1.94196  0.84682
C  -1.43677  2.49949  1.42252
C   0.05329  1.07805 -1.90590
```

```
C  -0.29350  2.20297 -1.02134
H  -3.33053 -0.12563 -0.89712
H  -1.61626 -1.88916 -2.08608
H  -0.05304 -2.95974 -0.14458
H  -0.81976 -1.88580  2.26717
H  -2.77722 -0.09502  1.76671
H   3.80922 -1.47077 -0.82410
H   2.27445 -2.39630 -0.92671
H   2.56950 -1.03876 -2.05186
H   3.50536 -0.96854  1.92010
H   2.02560 -0.22963  2.62711
H   1.97259 -1.89878  1.98124
H   4.04102  1.00625  0.15597
H   2.86655  1.75881 -0.96305
H   2.72629  2.02768  0.80580
H   0.63204  2.19562  1.29763
H  -1.35215  3.09284  2.33982
H  -2.43858  2.41138  0.98760
H   1.07986  1.03508 -2.29013
H  -0.68190  0.82737 -2.68105
H  -1.28127  2.64587 -1.18087
H   0.48764  2.96435 -0.89050
```

11

```
BP86 Energy =    -580.821367641
Enthalpy 0K=             -580.528659
Enthalpy 298K=           -580.510919
Free Energy 298K=        -580.573182

Ir -0.42329  0.11651 -0.01210
C  -2.19653 -0.69219 -1.19695
C  -1.26681 -1.75769 -0.93444
C  -1.28818 -2.02497  0.50562
C  -2.14529 -1.08099  1.11190
C  -2.69788 -0.22627  0.05906
P   1.80968 -0.59141  0.04506
C   2.09521 -2.18347 -0.87444
C   2.42259 -0.98659  1.75615
C   3.15574  0.48924 -0.64501
C   0.48859  2.02511  0.84377
C  -0.79286  1.83085  1.38672
C  -0.00027  1.66842 -1.43347
C   0.63436  2.72569 -0.50537
H  -2.43105 -0.27857 -2.17796
H  -0.75323 -2.34856 -1.69134
H  -0.73478 -2.81115  1.01951
H  -2.36423 -1.00016  2.17653
H  -3.43024  0.56802  0.20120
H   3.14787 -2.49037 -0.76372
H   1.44821 -2.97784 -0.47313
H   1.87137 -2.03816 -1.94234
H   3.45887 -1.36016  1.71364
H   2.38841 -0.08722  2.39013
H   1.77507 -1.75533  2.20432
H   4.10576 -0.06859 -0.62083
H   2.92636  0.76435 -1.68540
H   3.26776  1.40296 -0.04345
H   1.36191  1.85134  1.48385
H  -0.90355  1.47689  2.41659
H  -1.64431  2.38637  0.97876
H   0.65997  1.32838 -2.24504
H  -0.95841  1.99098 -1.87010
H   0.11459  3.70031 -0.51108
H   1.68989  2.92333 -0.74571
```

TS(11-12)

```
BP86 Energy =    -580.783269065
Enthalpy 0K=             -580.493666
Enthalpy 298K=           -580.475376
Free Energy 298K=        -580.540268
Nimag=1 (-97.5279cm-1)

Ir  0.49653 -0.25644 -0.03950
C   2.29473 -1.61320  0.32996
C   2.38408 -0.97596 -0.93380
C   2.39693  0.47674 -0.68559
C   2.49303  0.69243  0.75411
C   2.32605 -0.56948  1.36513
H   2.40329 -1.45393 -1.91339
H   2.22572 -2.68559  0.51400
H   2.24241 -0.75430  2.43735
H   2.57228  1.65287  1.26118
H   2.50329  1.24197 -1.45554
P  -0.88197  1.63823 -0.03458
C   0.03200  3.15371 -0.60061
C  -1.48153  2.10273  1.66414
C  -2.41056  1.65301 -1.08245
C  -2.82889 -1.52481  0.65377
C  -4.08152 -1.76550  0.22770
H  -4.94957 -1.28711  0.69149
H  -2.67896 -0.83626  1.49751
H  -4.28600 -2.46670 -0.59017
C  -0.86688 -1.38839 -1.09148
C  -1.59527 -2.17514  0.07420
H  -0.89181 -2.43893  0.89324
H  -1.86537 -3.15252 -0.37343
H  -1.61413 -0.86052 -1.70077
H  -0.33621 -2.10926 -1.73610
H  -0.63512  4.02927 -0.54953
H   0.90718  3.33019  0.04236
H   0.36584  3.01491 -1.64020
H  -2.93294  2.61548 -0.95881
H  -2.13274  1.52443 -2.14019
H  -3.07488  0.82806 -0.78162
H  -2.04142  3.05118  1.61626
H  -2.13947  1.31485  2.05989
H  -0.61780  2.21734  2.33648
```

12

```
BP86 Energy =    -580.827179018
Enthalpy 0K=             -580.538559
Enthalpy 298K=           -580.520009
Free Energy 298K=        -580.585202

Ir  0.27009 -0.26806 -0.03513
C   0.79725 -2.29284  1.10839
C  -0.34075 -2.50242  0.27746
C   0.03907 -2.22791 -1.09868
```

```
C   1.44492 -1.88392 -1.10329
C   1.89885 -1.89336  0.25873
H  -1.32582 -2.82569  0.61487
H   0.83396 -2.40837  2.19177
H   2.91325 -1.67346  0.59325
H   2.05007 -1.66267 -1.98204
H  -0.58691 -2.36718 -1.97909
P  -1.87915  0.61806 -0.05728
C  -2.84376  0.38599  1.51195
C  -2.95010 -0.16286 -1.35590
C  -2.03707  2.42801 -0.42743
C   1.70691  2.61812 -0.14779
C   2.83296  3.07936 -0.73110
H   2.84804  4.02901 -1.27238
H   0.78177  3.20443 -0.21446
H   3.77828  2.52823 -0.67389
C   0.65084  1.10217  1.62650
C   1.65688  1.38030  0.64498
H   0.34653  0.67126 -1.30821
H   2.63112  0.88987  0.76851
H  -0.11628  1.86234  1.81314
H   0.91470  0.51667  2.51362
H  -3.85267  0.81588  1.40107
H  -2.93055 -0.68817  1.73575
H  -2.32768  0.88035  2.34836
H  -3.10346  2.70283 -0.46826
H  -1.54471  3.02858  0.35149
H  -1.56611  2.64100 -1.39909
H  -3.96193  0.27259 -1.32095
H  -2.50898  0.01635 -2.34824
H  -3.01798 -1.24767 -1.18357
```

TS(12-13)

BP86 Energy = -580.788982417
Enthalpy 0K= -580.499758
Enthalpy 298K= -580.481055
Free Energy 298K= -580.547296
Nimag=1 (-134.6875cm^{-1})

```
Ir -0.26634 -0.24853  0.09297
P   2.02754  0.19057 -0.10798
C   2.46568  1.21162 -1.59737
C   3.09078 -1.32026 -0.27784
C   2.79012  1.11129  1.31412
H   0.00953  1.60613  2.53040
H   3.55616  1.36787 -1.63538
H   2.13741  0.68968 -2.50899
H   1.95833  2.18631 -1.54419
H   4.15028 -1.02879 -0.36172
H   2.96083 -1.96520  0.60462
H   2.79723 -1.87731 -1.18061
H   3.85832  1.29054  1.11029
H   2.28035  2.07647  1.45236
H   2.68932  0.51633  2.23471
C  -2.20189 -1.08215 -0.66482
C  -1.04204 -1.69266 -1.34309
C  -0.35493 -2.54662 -0.40584
C  -0.90598 -2.25929  0.87409
C  -2.10218 -1.41031  0.70515
H  -2.95366 -0.45413 -1.14082
H  -0.83324 -1.61378 -2.41112
H   0.52389 -3.15561 -0.61056
H  -0.55247 -2.65311  1.82822
H  -2.77268 -1.09757  1.50558
C  -1.85858  2.19776 -0.38548
C  -1.83627  2.87478 -1.55441
C  -0.84541  1.97648  1.93897
C  -0.65275  1.80494  0.40991
H  -2.83217  1.91788  0.04551
H  -2.75750  3.14855 -2.07654
H  -0.89535  3.19589 -2.01627
H  -1.75212  1.46066  2.29669
H  -0.96302  3.05237  2.17207
H   0.20631  2.42190  0.08661
```

13

BP86 Energy = -580.852428174
Enthalpy 0K= -580.559948
Enthalpy 298K= -580.541938
Free Energy 298K= -580.604582

```
Ir -0.39316 -0.02265 -0.15883
P   1.91665 -0.27405  0.10384
C   3.08457  0.69390 -0.97240
C   2.50734 -2.01541 -0.16680
C   2.50494  0.12484  1.82072
H  -0.31901  2.52618  2.39966
H   4.11539  0.48409 -0.64473
H   2.97542  0.38490 -2.02326
H   2.90535  1.77687 -0.89228
H   3.59285 -2.07697  0.01382
H   1.99212 -2.70410  0.51977
H   2.29449 -2.31411 -1.20464
H   3.58771 -0.05990  1.91105
H   2.29670  1.18137  2.04755
H   1.96505 -0.50129  2.54698
C  -2.60732 -0.57134  0.15117
C  -2.03847 -1.48577 -0.81092
C  -0.97846 -2.20387 -0.17090
C  -0.90067 -1.73338  1.21208
C  -1.92091 -0.74730  1.40798
H  -3.44094  0.10709 -0.03169
H  -2.35063 -1.59868 -1.84928
H  -0.38496 -3.00049 -0.61697
H  -0.23863 -2.12321  1.98570
H  -2.13261 -0.21724  2.33632
C  -0.76158  1.92888 -0.97368
C  -0.10457  1.14884 -1.99118
C  -0.75917  2.83114  1.43658
C  -0.07262  2.15632  0.26951
H  -1.83105  2.16181 -1.05170
H  -0.69459  0.83964 -2.86020
H   0.95057  1.32774 -2.21013
H  -1.83796  2.60736  1.46565
H  -0.64341  3.92860  1.36042
H   1.00338  2.36420  0.19728
```

TS(4-4b)

BP86 Energy = -734.416860009
Enthalpy 0K= -734.084080
Enthalpy 298K= -734.062143
Free Energy 298K= -734.134986
Nimag=1 (-223.6383cm^{-1})

C	0.14986	1.11010	2.95460
C	-0.60591	0.06911	2.52023
Ir	-0.47445	-0.43185	0.10389
P	-0.74098	1.84052	-0.35890
C	1.58419	-0.22072	-0.07326
C	-1.02646	2.19313	-2.16199
C	0.62616	3.01240	0.08303
C	-2.24050	2.59001	0.44497
C	2.19319	0.19217	-1.28155
C	3.59267	0.22574	-1.42332
C	4.42203	-0.15524	-0.35752
C	3.83792	-0.58390	0.84321
C	2.43732	-0.62314	0.98249
H	1.21727	1.17099	2.71857
H	-0.27543	1.91298	3.56818
H	-1.65348	-0.04002	2.81170
H	-0.07205	-0.84958	2.16654
H	-1.20154	3.27166	-2.30579
H	-0.14451	1.89359	-2.74719
H	-1.90544	1.63725	-2.52204
H	0.36611	4.02362	-0.26864
H	0.76225	3.03388	1.17406
H	1.56138	2.67520	-0.38661
H	-2.33807	3.64869	0.15411
H	-3.14133	2.04104	0.13116
H	-2.14470	2.51965	1.53830
H	1.57370	0.48114	-2.13837
H	4.03044	0.54734	-2.37443
H	5.51044	-0.12910	-0.46525
H	4.46808	-0.90213	1.68066
H	2.02785	-0.99417	1.93001
C	-0.36335	-2.36648	-1.01684
C	-1.17437	-1.37200	-1.70911
C	-2.41093	-1.19758	-0.93313
C	-2.28806	-1.95896	0.24781
C	-1.01482	-2.68340	0.20825
H	0.60239	-2.74466	-1.35187
H	-0.98716	-0.99085	-2.71307
H	-3.25680	-0.56881	-1.21071
H	-3.01446	-2.00314	1.06027
H	-0.65127	-3.37731	0.96687

4b
BP86 Energy = -734.418142412
Enthalpy 0K= -734.084915
Enthalpy 298K= -734.062778
Free Energy 298K= -734.135572

C	0.14570	1.29836	2.96739
C	-0.62322	0.36601	2.35473
Ir	-0.49424	-0.43061	0.16207
P	-0.68559	1.82450	-0.45463
C	1.57978	-0.26276	-0.03629
C	-0.90524	2.06202	-2.28534
C	0.70476	2.98068	-0.05144
C	-2.18571	2.65652	0.25596
C	2.16657	0.01383	-1.29301
C	3.56336	0.02341	-1.46286
C	4.41045	-0.24749	-0.37762
C	3.84699	-0.53890	0.87298
C	2.44930	-0.54945	1.04230
H	1.18926	1.45975	2.67936
H	-0.24590	1.90023	3.79520
H	-1.63081	0.14402	2.71547
H	0.00592	-0.52795	1.92307
H	-1.02605	3.13561	-2.50368
H	-0.02118	1.68599	-2.82188
H	-1.79884	1.52440	-2.63656
H	0.48206	3.97127	-0.47936
H	0.80971	3.07412	1.03872
H	1.64062	2.58649	-0.47314
H	-2.26330	3.68761	-0.12550
H	-3.08817	2.09337	-0.02612
H	-2.10661	2.67814	1.35245
H	1.53134	0.21473	-2.16324
H	3.98442	0.23867	-2.45081
H	5.49671	-0.24137	-0.50770
H	4.49127	-0.76944	1.72814
H	2.05646	-0.80711	2.03365
C	-0.40634	-2.42994	-0.88236
C	-1.12662	-1.44677	-1.66983
C	-2.38389	-1.16266	-0.96811
C	-2.37517	-1.87556	0.25375
C	-1.14091	-2.65253	0.32081
H	0.55877	-2.86729	-1.13742
H	-0.86413	-1.12518	-2.67717
H	-3.18125	-0.50963	-1.32395
H	-3.15055	-1.84796	1.02015
H	-0.84833	-3.31774	1.13393

TS(4b-14)
BP86 Energy = -734.409739507
Enthalpy 0K= -734.078778
Enthalpy 298K= -734.057352
Free Energy 298K= -734.128317
Nimag=1 (-341.6648cm^{-1})

C	-0.46373	1.56569	2.80067
C	-1.14792	0.78744	1.93970
Ir	-0.57140	-0.35245	0.23164
P	-0.24679	1.79915	-0.69299
C	1.54371	-0.43539	0.13172
C	0.09407	1.74477	-2.51599
C	1.12648	2.84169	-0.02832
C	-1.75013	2.87947	-0.56911
C	2.16497	-0.74700	-1.10034
C	3.56420	-0.86877	-1.19729
C	4.37414	-0.68285	-0.06796
C	3.77125	-0.38450	1.16287
C	2.37321	-0.26341	1.26255
H	0.61904	1.71812	2.74921
H	-0.98826	2.07418	3.61853

H -2.22327 0.64778 2.11236
H -0.04358 -0.47500 1.72837
H 0.17461 2.77475 -2.90001
H 1.04070 1.21439 -2.69380
H -0.72446 1.22725 -3.03835
H 1.16877 3.77398 -0.61431
H 0.92985 3.08315 1.02504
H 2.07796 2.29846 -0.11268
H -1.55017 3.84518 -1.06106
H -2.60235 2.38945 -1.06390
H -1.99404 3.04869 0.48953
H 1.56813 -0.91139 -2.00315
H 4.01339 -1.11445 -2.16545
H 5.46142 -0.77672 -0.14443
H 4.38453 -0.24918 2.05987
H 1.94164 -0.04004 2.24457
C -0.68472 -2.49005 -0.57986
C -1.14559 -1.59140 -1.60663
C -2.38853 -0.99627 -1.14565
C -2.66271 -1.49877 0.15820
C -1.60357 -2.41167 0.52339
H 0.21678 -3.10128 -0.61806
H -0.70217 -1.46663 -2.59419
H -3.01623 -0.30540 -1.70937
H -3.51122 -1.22535 0.78655
H -1.53231 -2.97230 1.45572

14

BP86 Energy = -734.411930571
Enthalpy 0K= -734.078348
Enthalpy 298K= -734.056885
Free Energy 298K= -734.127806

C -1.55859 1.40045 2.62782
C -1.80073 0.82105 1.43951
Ir -0.56887 -0.35474 0.19981
P -0.19523 1.80433 -0.68716
C 1.57746 -0.32716 0.23272
C 0.68751 1.82944 -2.31732
C 0.77008 2.95753 0.38411
C -1.75661 2.73372 -1.07487
C 2.28679 -0.71188 -0.93003
C 3.69159 -0.80107 -0.92499
C 4.42059 -0.50097 0.23455
C 3.73154 -0.11148 1.39201
C 2.32735 -0.02471 1.39243
H -0.58541 1.37365 3.13015
H -2.36188 1.92998 3.15578
H -2.81040 0.90069 1.01289
H -0.03108 -0.28744 1.66869
H 0.74043 2.87120 -2.67321
H 1.70248 1.42628 -2.19949
H 0.13381 1.22393 -3.05113
H 0.85862 3.93059 -0.12495
H 0.24163 3.08598 1.33981
H 1.76845 2.53537 0.56601
H -1.49246 3.67599 -1.58189
H -2.39614 2.13413 -1.74054
H -2.30288 2.96118 -0.14930
H 1.75899 -0.95046 -1.85884
H 4.20897 -1.11031 -1.83941
H 5.51237 -0.57034 0.23559
H 4.28076 0.12593 2.30893
H 1.82588 0.28294 2.31619
C -0.36192 -2.49777 -0.75060
C -1.04439 -1.66244 -1.69933
C -2.28939 -1.24312 -1.10132
C -2.36047 -1.82818 0.21302
C -1.16602 -2.59777 0.43567
H 0.61645 -2.95697 -0.88821
H -0.70599 -1.43419 -2.71000
H -3.06455 -0.64224 -1.57686
H -3.17245 -1.70173 0.92937
H -0.92309 -3.16746 1.33212

TS(14-15)

BP86 Energy = -734.407951857
Enthalpy 0K= -734.076648
Enthalpy 298K= -734.055286
Free Energy 298K= -734.126282
Nimag=1 (-251.6320cm^{-1})

C -0.43167 0.42100 3.20177
C -0.91853 0.69331 1.97757
Ir -0.60796 -0.31219 0.17696
P 0.02272 1.84045 -0.59622
C 1.54684 -0.58196 0.09822
C 0.93026 1.83475 -2.21099
C 1.05484 2.90644 0.50703
C -1.47468 2.88961 -0.92628
C 2.09388 -1.32055 -0.97817
C 3.48496 -1.48936 -1.09255
C 4.35465 -0.94166 -0.13581
C 3.82172 -0.22633 0.94567
C 2.43077 -0.05214 1.06588
H 0.30045 -0.36870 3.40668
H -0.77148 0.99703 4.07227
H -1.66510 1.49981 1.89506
H 0.34828 -1.03640 1.22242
H 1.17486 2.87105 -2.49549
H 1.85423 1.24744 -2.10742
H 0.30100 1.38247 -2.99253
H 1.12302 3.90832 0.05352
H 0.59013 2.97258 1.50114
H 2.05975 2.47318 0.60222
H -1.16102 3.89263 -1.25843
H -2.09016 2.42780 -1.71252
H -2.07286 2.98680 -0.00734
H 1.44878 -1.75741 -1.74388
H 3.88478 -2.05685 -1.93939
H 5.43575 -1.08107 -0.22906
H 4.48272 0.19118 1.71222
H 2.03192 0.48653 1.93080
C -1.29955 -2.05114 -1.32341
C -1.96267 -0.84664 -1.68901
C -2.76669 -0.40587 -0.55709
C -2.60222 -1.37328 0.49325
C -1.66419 -2.36788 0.03792

```
H  -0.62775 -2.63493 -1.95176
H  -1.90691 -0.35886 -2.66292
H  -3.44993  0.44252 -0.54122
H  -3.07600 -1.34614  1.47431
H  -1.32894 -3.23688  0.60476
```

15

```
BP86 Energy =    -734.422041123
Enthalpy 0K=             -734.088249
Enthalpy 298K=           -734.066185
Free Energy 298K=        -734.139415

C  -0.44454 -0.82378  3.08050
C  -0.70598  0.09691  2.13000
Ir -0.71882 -0.24144  0.09963
P   0.22143  1.87441 -0.22654
C   1.62590 -1.11802  0.18413
C   1.38993  1.97138 -1.66490
C   1.16551  2.66983  1.15764
C  -1.06835  3.15333 -0.62087
C   2.10694 -1.55053 -1.07473
C   3.45930 -1.37562 -1.39710
C   4.33479 -0.78749 -0.46395
C   3.86481 -0.38639  0.80015
C   2.51153 -0.55177  1.12972
H  -0.13442 -1.85290  2.85843
H  -0.53086 -0.57251  4.14593
H  -1.02642  1.09488  2.46744
H   0.65408 -1.55556  0.59031
H   1.70794  3.01470 -1.82446
H   2.26992  1.34231 -1.46356
H   0.88621  1.59735 -2.56925
H   1.47588  3.68045  0.84710
H   0.53673  2.74033  2.05694
H   2.05554  2.06768  1.38728
H  -0.58869  4.13315 -0.77638
H  -1.61389  2.87439 -1.53490
H  -1.77950  3.22800  0.21593
H   1.43071 -2.03387 -1.78455
H   3.83764 -1.71071 -2.36763
H   5.39192 -0.65929 -0.71736
H   4.55768  0.04114  1.53160
H   2.12947 -0.26988  2.11511
C  -1.59325 -1.53402 -1.70417
C  -2.09595 -0.21808 -1.78144
C  -2.77301  0.08286 -0.51301
C  -2.76829 -1.13855  0.27922
C  -1.99291 -2.10815 -0.41762
H  -1.01106 -2.04409 -2.47188
H  -1.97993  0.46660 -2.62178
H  -3.34687  0.98171 -0.28807
H  -3.21806 -1.26040  1.26431
H  -1.77518 -3.12032 -0.07521
```

TS(5-20)

```
BP86 Energy =    -734.443918383
Enthalpy 0K=             -734.107246
Enthalpy 298K=           -734.086764
Free Energy 298K=        -734.157023
```

Nimag=1 (-51.0598cm^{-1})

```
Ir  1.02439 -0.26243 -0.06986
C   2.49369 -1.91640  0.47910
C   2.91528 -1.21979 -0.68170
C   3.10158  0.19120 -0.29633
C   2.96008  0.29138  1.15087
C   2.48775 -0.96236  1.59798
H   3.04492 -1.62682 -1.68464
H   2.23297 -2.97265  0.54530
H   2.17675 -1.20022  2.61664
H   3.08992  1.18838  1.75439
H   3.45990  0.97886 -0.96040
P  -0.05858  1.81371 -0.12133
C   1.14371  3.22513 -0.25322
C  -1.00667  2.18155  1.43390
C  -1.27509  2.16817 -1.47342
C  -2.49211 -1.26562 -0.16768
C  -3.46504 -0.82035 -1.08915
C  -4.64323 -0.19641 -0.64680
C  -4.87238 -0.01359  0.72758
C  -3.91964 -0.46449  1.65546
C  -2.73909 -1.08521  1.20833
H  -2.01374 -1.46120  1.94113
H  -4.10170 -0.35054  2.72915
H  -5.79628  0.46011  1.07319
H  -5.39135  0.13091 -1.37594
H  -3.31065 -0.98667 -2.16223
C  -0.23211 -1.10105 -1.49286
C  -1.23970 -1.96932 -0.65646
H  -0.74199 -2.46753  0.20047
H  -1.52954 -2.80548 -1.32597
H  -0.78541 -0.39788 -2.13339
H   0.36150 -1.76112 -2.14816
H   0.59319  4.17942 -0.22427
H   1.85603  3.19719  0.58461
H   1.69502  3.15871 -1.20354
H  -1.63990  3.20307 -1.37189
H  -0.79256  2.04737 -2.45550
H  -2.12423  1.47119 -1.39333
H  -1.42610  3.19969  1.37534
H  -1.82345  1.45093  1.54170
H  -0.33488  2.10907  2.30269
```

20

```
BP86 Energy =    -734.481014230
Enthalpy 0K=             -734.145391
Enthalpy 298K=           -734.124609
Free Energy 298K=        -734.195753

Ir -0.85204 -0.30717 -0.00404
C  -2.26336 -2.12634  0.21913
C  -2.90008 -1.05663  0.96311
C  -3.18948  0.00067  0.05689
C  -2.71931 -0.38704 -1.26069
C  -2.18519 -1.73095 -1.15625
H  -3.11691 -1.06286  2.03149
H  -1.93783 -3.08292  0.62942
H  -1.79683 -2.33275 -1.97753
```

```
H  -2.86197  0.17172 -2.18482
H  -3.68286  0.93916  0.30902
P  -0.16059  1.91648 -0.13073
C  -1.50072  3.02834 -0.78036
C   1.24967  2.22630 -1.29213
C   0.35908  2.78347  1.42874
C   2.32066 -0.94761  0.38203
C   3.15012 -0.02994  1.06601
C   4.44048  0.25950  0.59303
C   4.92528 -0.36692 -0.56629
C   4.11903 -1.30010 -1.24242
C   2.83347 -1.59041 -0.76905
H   2.21140 -2.32327 -1.29616
H   4.49786 -1.80863 -2.13437
H   5.93290 -0.14494 -0.93056
H   5.07482  0.96129  1.14368
H   2.80885  0.42612  2.00152
C   0.23860 -0.58518  1.87447
C   0.96225 -1.30746  0.87597
H   0.18192 -0.36837 -1.19905
H   0.72581 -2.37342  0.75993
H   0.66353  0.32289  2.30814
H  -0.41483 -1.13614  2.55880
H  -1.10054  4.04649 -0.91475
H  -1.85976  2.65247 -1.74983
H  -2.33878  3.06291 -0.06818
H   1.32779  2.39072  1.77129
H   0.47055  3.85956  1.21859
H  -0.39750  2.64043  2.21511
H   1.50018  3.29960 -1.30552
H   2.12438  1.64377 -0.96380
H   0.96090  1.90279 -2.30393
```

21

```
BP86 Energy =    -424.771828867
Enthalpy 0K=             -424.569955
Enthalpy 298K=           -424.556316
Free Energy 298K=        -424.611044

Ir  0.38507 -0.34784 -0.06985
C   2.60748 -0.23286 -0.59123
C   2.43388 -0.40060  0.80332
C   1.61801  0.73041  1.26910
C   1.47141  1.67491  0.14935
C   2.01724  1.05565 -0.99038
P  -1.89034  0.13202  0.01673
H  -0.06044 -1.76545  0.53352
C  -2.76066 -0.48485  1.53031
C  -2.75976 -0.70339 -1.40038
C  -2.36613  1.91819 -0.11572
H   3.09835 -0.93539 -1.26599
H   2.77210 -1.23944  1.41056
H   1.32980  0.91853  2.30455
H   0.96882  2.64050  0.19160
H   2.00261  1.44748 -2.00815
H  -3.83487 -0.24622  1.47047
H  -2.62294 -1.57380  1.60438
H  -2.32782 -0.00958  2.42359
H  -3.84180 -0.50255 -1.33046
H  -2.38151 -0.31682 -2.35907
H  -2.58812 -1.78957 -1.35229
H  -3.46350  2.01810 -0.14073
H  -1.97544  2.46699  0.75503
H  -1.93953  2.34590 -1.03572
```

Styrene

```
BP86 Energy =    -309.639907320
Enthalpy 0K=             -309.510366
Enthalpy 298K=           -309.503378
Free Energy 298K=        -309.542016

C   0.00000  0.56543  0.00000
C   1.34634  0.13098  0.00000
C   1.67103 -1.23289  0.00000
C   0.65159 -2.19740  0.00000
C  -0.69305 -1.78356  0.00000
C  -1.01539 -0.42191  0.00000
H   2.14572  0.88145  0.00000
H   2.72156 -1.54252  0.00000
H   0.89975 -3.26384  0.00000
H  -1.49489 -2.52974  0.00000
H  -2.06765 -0.11883  0.00000
C  -0.27977  2.01245  0.00000
C  -1.48534  2.61894  0.00000
H   0.61678  2.64843  0.00000
H  -1.56490  3.70961  0.00000
H  -2.42885  2.06326  0.00000
```

17

```
BP86 Energy =    -966.699632898
Enthalpy 0K=             -966.262849
Enthalpy 298K=           -966.235974
Free Energy 298K=        -966.319608

C   3.62150 -0.05052  1.57569
C   3.13335  1.00278  0.77263
C   3.97221  1.50491 -0.24615
C   5.24624  0.95818 -0.47450
C   5.70815 -0.10336  0.31978
C   4.89315 -0.60149  1.34992
C   1.76987  1.62906  1.02151
C   0.56501  0.69252  1.26603
Ir -0.40972 -0.26118 -0.42667
C  -0.40026 -1.48322 -2.49085
C  -0.16203 -2.34747 -1.39306
C   1.03864 -1.89233 -0.69609
C   1.57787 -0.77571 -1.44942
C   0.65630 -0.48307 -2.49659
P  -1.83946 -1.10337  1.21239
C  -1.02167  1.98997 -0.88918
C  -3.42992 -1.82428  0.57837
C  -2.39264 -0.05288  2.64026
C  -1.05530 -2.54598  2.08884
H  -0.76643 -3.21383 -1.12234
H   1.53503 -2.39988  0.13015
H   2.49907 -0.23917 -1.22448
H   0.75534  0.32755 -3.22063
H  -1.22975 -1.54979 -3.19472
```

```
H  -0.21017  1.27974  1.78150
H   0.87308 -0.11769  1.95246
H   1.55236  2.34205  0.20656
H   1.85684  2.25507  1.93610
H   3.62330  2.34197 -0.86380
H   5.87830  1.36549 -1.27022
H   6.70013 -0.53139  0.14585
H   5.25390 -1.41491  1.98806
H   3.01197 -0.43513  2.40204
C  -2.07940  1.17618 -1.42542
C  -3.40871  1.30993 -0.89576
C  -3.66967  2.20263  0.12989
C  -2.61726  2.99845  0.67989
C  -1.33050  2.90104  0.18140
H  -1.98853  0.76443 -2.43392
H  -4.22670  0.76158 -1.37439
H  -4.69420  2.33900  0.49144
H  -2.84665  3.72776  1.46337
H  -0.54610  3.56527  0.55683
H  -0.14073  2.21421 -1.49950
H  -1.72896 -2.92416  2.87487
H  -0.84582 -3.35832  1.37661
H  -0.10885 -2.22405  2.54950
H  -3.97070 -2.31968  1.40122
H  -4.05216 -1.01807  0.16515
H  -3.22077 -2.55752 -0.21483
H  -3.08336 -0.64217  3.26489
H  -1.52360  0.24425  3.24480
H  -2.90477  0.84685  2.27185
```

TS(17-22)

BP86 Energy = -966.686714872
Enthalpy 0K= -966.253783
Enthalpy 298K= -966.227274
Free Energy 298K= -966.310552
Nimag=1 (-384.3564cm^{-1})

```
C   3.96828 -0.23410  1.39057
C   2.95868  0.74182  1.24214
C   3.14798  1.76309  0.28875
C   4.30047  1.79587 -0.51585
C   5.28631  0.80582 -0.37365
C   5.12057 -0.20636  0.58815
C   1.69655  0.67580  2.08006
C   0.69766 -0.44627  1.71270
Ir -0.20297 -0.42843 -0.26678
C  -0.13187 -0.88763 -2.62472
C  -0.31726 -2.11768 -1.93197
C   0.80805 -2.32378 -1.03888
C   1.70328 -1.20874 -1.20547
C   1.09932 -0.30146 -2.15287
P  -2.12883 -1.27049  0.83201
C  -1.35380  1.41905 -0.21638
C  -3.59944 -1.35044 -0.29469
C  -2.81985 -0.44430  2.34288
C  -1.86505 -3.01785  1.40415
H  -1.15374 -2.80428 -2.07039
H   0.98547 -3.20386 -0.42141
H   2.65961 -1.06283 -0.70247
H   1.53312  0.64118 -2.48671
H  -0.80315 -0.46403 -3.37098
H  -0.09390 -0.45417  2.47951
H   1.20501 -1.42604  1.76389
H   1.19069  1.65879  2.06019
H   1.98044  0.50406  3.13916
H   2.39387  2.55401  0.18959
H   4.43519  2.60439 -1.24197
H   6.18801  0.83347 -0.99320
H   5.89729 -0.96599  0.72374
H   3.85722 -1.01635  2.15149
C  -1.96129  1.87363 -1.41294
C  -2.75088  3.03656 -1.41837
C  -2.93914  3.78131 -0.24313
C  -2.32357  3.35693  0.94316
C  -1.53621  2.19171  0.95469
H  -1.83434  1.32347 -2.34811
H  -3.21822  3.35902 -2.35470
H  -3.54980  4.68895 -0.25615
H  -2.44089  3.93585  1.86509
H  -1.04642  1.89292  1.88677
H   0.23138  1.08127  0.01682
H  -2.76173 -3.39089  1.92490
H  -1.64959 -3.66743  0.54269
H  -1.00545 -3.04079  2.09164
H  -4.46929 -1.75966  0.24421
H  -3.82662 -0.33345 -0.64958
H  -3.37290 -1.98905 -1.16155
H  -3.66153 -1.05812  2.70263
H  -2.06434 -0.37432  3.13895
H  -3.17720  0.56246  2.08760
```

22

BP86 Energy = -655.826460064
Enthalpy 0K= -655.544585
Enthalpy 298K= -655.525670
Free Energy 298K= -655.593280

```
Ir -0.35789 -0.42131  0.06943
C  -0.38263 -2.62241  0.51378
C  -0.69941 -2.41589 -0.85743
C  -1.94794 -1.64303 -0.92195
C  -2.42701 -1.44453  0.41144
C  -1.41772 -1.94801  1.29938
P  -1.04010  1.81991 -0.13932
C   1.61182 -0.02569 -0.08861
C  -2.79020  1.97532 -0.74717
C  -0.09616  2.87349 -1.34084
C  -1.07601  2.79684  1.44549
C   2.50417 -0.98184 -0.67340
C   3.89090 -0.82501 -0.61159
C   4.44895  0.27421  0.07258
C   3.60676  1.22823  0.66715
C   2.21549  1.10209  0.55011
H   0.47997 -3.15169  0.91702
H  -0.13357 -2.76593 -1.72108
H  -2.45055 -1.34567 -1.84252
H  -3.33339 -0.91867  0.70661
H  -1.44057 -1.88977  2.38865
```

```
H  -3.05428  3.04078 -0.84550
H  -2.88651  1.48918 -1.72967
H  -3.48164  1.49833 -0.03662
H  -0.50796  3.89562 -1.35245
H   0.96715  2.90053 -1.06355
H  -0.18395  2.42903 -2.34419
H  -1.47429  3.80586  1.24911
H  -1.72453  2.28034  2.16952
H  -0.06788  2.88257  1.87665
H   2.09987 -1.85187 -1.19944
H   4.54537 -1.56389 -1.08489
H   5.53583  0.38834  0.13246
H   4.03421  2.08264  1.20153
H   1.59008  1.87371  1.00860
```

18

```
BP86 Energy =    -813.084343744
Enthalpy 0K=             -812.692184
Enthalpy 298K=           -812.668526
Free Energy 298K=        -812.744701

Ir -0.60128  0.33784  0.16383
C   1.17749  1.30426 -0.93072
C   0.00268  1.30668 -1.77623
C  -0.96830  2.20109 -1.17527
C  -0.41966  2.68864  0.04764
C   0.90311  2.12089  0.21063
H  -0.08361  0.82612 -2.75034
H   2.10054  0.75417 -1.11305
H   1.58895  2.30992  1.03617
H  -0.91438  3.36983  0.74038
H  -1.93983  2.46849 -1.59048
P  -2.57484 -0.78155 -0.35741
C  -2.59119 -1.51156 -2.06306
C  -4.08672  0.29880 -0.33826
C  -3.06576 -2.20561  0.73275
C   2.87772 -1.27375  0.18588
C   3.51501 -1.34726 -1.07271
C   4.67395 -0.60020 -1.33946
C   5.22328  0.22849 -0.34544
C   4.61520  0.29154  0.91873
C   3.45443 -0.45659  1.17972
H   3.00168 -0.42287  2.17826
H   5.05325  0.91135  1.70801
H   6.13092  0.80486 -0.54921
H   5.15801 -0.67652 -2.31846
H   3.10705 -2.00779 -1.84774
C   0.32704 -1.60201 -0.27704
C   1.61078 -2.06253  0.45310
H   1.44108 -2.12997  1.54081
C  -1.44112  0.54942  2.17963
H  -0.42518 -2.39462 -0.12809
H   0.52161 -1.54887 -1.36317
C  -0.37226 -0.39344  2.20137
H   0.60643 -0.09866  2.59286
H  -0.59685 -1.45994  2.29940
H  -1.27689  1.57120  2.53708
H  -2.47755  0.21328  2.28921
H   1.77716 -3.10752  0.11724
H  -4.98355 -0.30466 -0.55356
H  -4.19692  0.77684  0.64671
H  -3.99029  1.08335 -1.10344
H  -4.01626 -2.62636  0.36726
H  -2.29657 -2.99177  0.71095
H  -3.20349 -1.86803  1.77091
H  -3.54473 -2.03400 -2.24197
H  -2.47449 -0.70694 -2.80505
H  -1.75846 -2.22222 -2.17200
```

TS(18-23)

```
BP86 Energy =    -813.033212436
Enthalpy 0K=             -812.646876
Enthalpy 298K=           -812.622752
Free Energy 298K=        -812.700689
Nimag=1 (-513.4464cm-1)

Ir -0.54770  0.29231  0.16853
C   0.81219  1.66447 -1.23731
C  -0.50643  2.19513 -1.23438
C  -0.85320  2.53129  0.13494
C   0.30930  2.26110  0.95653
C   1.31881  1.68803  0.12232
H  -1.15009  2.32365 -2.10512
H   1.35828  1.29060 -2.10320
H   2.30721  1.35368  0.43863
H   0.38747  2.42856  2.03072
H  -1.76894  3.02297  0.46344
P  -2.57613 -0.61380 -0.55939
C  -3.07662 -2.27320  0.09992
C  -2.67004 -0.82003 -2.40346
C  -4.03139  0.46147 -0.15556
C   2.89505 -1.37520 -0.14027
C   3.46330 -0.91016 -1.34585
C   4.56665 -0.04244 -1.33230
C   5.12559  0.36742 -0.10882
C   4.58310 -0.10654  1.09722
C   3.47560 -0.97264  1.07929
H   3.06264 -1.34655  2.02349
H   5.02717  0.18898  2.05314
H   5.99123  1.03685 -0.09761
H   5.00242  0.30063 -2.27624
H   3.05280 -1.24764 -2.30610
C   0.37567 -1.63597 -0.68785
C   1.68246 -2.28416 -0.16183
H   1.52317 -2.72248  0.83999
C  -1.38885 -0.00305  2.05084
H  -0.41456 -2.39697 -0.73713
H   0.54456 -1.22937 -1.69566
C  -1.27097 -1.03191  2.91059
H  -1.73966 -0.98680  3.90212
H  -0.70620 -1.94536  2.68852
H  -1.97896  0.86908  2.37294
H   0.14644 -1.02629  0.74869
H   1.87417 -3.13800 -0.84295
H  -3.64891 -1.23852 -2.68893
H  -2.53470  0.15687 -2.89197
H  -1.87401 -1.50049 -2.74275
H  -4.95544  0.00404 -0.54470
```

```
H  -4.11081  0.56877  0.93665
H  -3.90009  1.45571 -0.60857
H  -4.08743 -2.51245 -0.26733
H  -2.38123 -3.05571 -0.23878
H  -3.07331 -2.23597  1.19867
```

23

```
BP86 Energy =    -502.171745706
Enthalpy 0K=             -501.936917
Enthalpy 298K=           -501.920553
Free Energy 298K=        -501.982867

Ir  0.42832  0.22474  0.03440
C   2.67521  0.15373  0.33821
C   2.34877 -0.14673 -1.01300
C   1.50833 -1.35019 -1.00126
C   1.45592 -1.85326  0.36090
C   2.09256 -0.89245  1.18466
P  -1.82218 -0.45147 -0.01889
C   0.05698  2.09418 -0.47505
C  -2.94714  0.45581 -1.18084
C  -2.68699 -0.39631  1.62804
C  -2.02180 -2.22128 -0.54474
C  -0.80895  2.77885  0.33129
H   3.25907  1.00297  0.69325
H   2.63278  0.42054 -1.89957
H   1.12242 -1.85292 -1.88843
H   0.94855 -2.75610  0.69728
H   2.15268 -0.92058  2.27354
H   0.78151  2.66161 -1.07842
H  -3.97152  0.05831 -1.09801
H  -2.94592  1.53017 -0.94877
H  -2.57989  0.32125 -2.20981
H  -3.71049 -0.79295  1.52433
H  -2.12831 -1.00689  2.35368
H  -2.73763  0.63701  2.00324
H  -3.09294 -2.47831 -0.57426
H  -1.59307 -2.36022 -1.54871
H  -1.51138 -2.88810  0.16601
H  -0.68608  3.85592  0.51518
H  -1.62503  2.30135  0.88483
```

TS(18-24)

```
BP86 Energy =    -813.037065327
Enthalpy 0K=             -812.645546
Enthalpy 298K=           -812.622396
Free Energy 298K=        -812.698351
Nimag=1 (-404.1132cm-1)

Ir -0.66927 -0.33181 -0.21863
C   1.05675 -1.81670  0.31102
C   0.05031 -1.92223  1.33374
C  -1.18040 -2.27825  0.67289
C  -0.92186 -2.45162 -0.75153
C   0.47981 -2.16674 -0.95860
H   0.18941 -1.76399  2.40230
H   2.08995 -1.50104  0.46839
H   1.00923 -2.19968 -1.91071
H  -1.63253 -2.80737 -1.49672
H  -2.13251 -2.47958  1.16527
P  -2.66757  0.66812  0.40632
C  -3.03061  0.61248  2.23010
C  -4.14721 -0.15341 -0.36145
C  -2.94444  2.46326 -0.00347
C   3.10408  1.29768  0.31376
C   3.48482  0.57075  1.46350
C   4.50757 -0.38902  1.40307
C   5.17097 -0.63636  0.18763
C   4.81665  0.09336 -0.95797
C   3.79471  1.05621 -0.89200
H   3.55379  1.64841 -1.78310
H   5.34676 -0.07269 -1.90117
H   5.97474 -1.37757  0.14136
H   4.80068 -0.93111  2.30798
H   2.99058  0.77540  2.42148
C   0.56269  1.71094  0.52697
C   1.97950  2.31262  0.39038
H   2.03243  3.01381 -0.46218
C  -0.80044  0.65136 -2.07324
H  -0.18104  2.48643  0.74659
H   0.58962  1.00255  1.36701
C   0.23994  1.47747 -1.44427
H   1.26705  1.22382 -1.72318
H   0.04690  2.55708 -1.43510
H  -0.46405 -0.02405 -2.87114
H  -1.74200  1.15137 -2.33255
H   2.11263  2.92823  1.30261
H  -5.07907  0.32513 -0.01917
H  -4.07536 -0.07618 -1.45722
H  -4.16483 -1.21894 -0.08556
H  -3.97939  2.73453  0.25989
H  -2.25639  3.09970  0.57328
H  -2.79148  2.64648 -1.07733
H  -4.01022  1.07104  2.44284
H  -3.03847 -0.43264  2.57497
H  -2.24611  1.15792  2.77726
```

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```
BP86 Energy =    -813.076569477
Enthalpy 0K=             -812.683927
Enthalpy 298K=           -812.660680
Free Energy 298K=        -812.736885

Ir -0.65997 -0.30691 -0.21878
C   1.13855 -1.75191 -0.36856
C   0.45622 -2.06394  0.89091
C  -0.86614 -2.45224  0.59155
C  -1.06118 -2.31851 -0.86068
C   0.23447 -1.97487 -1.44033
H   0.90441 -1.99503  1.88132
H   2.17473 -1.41889 -0.45432
H   0.44492 -1.85091 -2.50263
H  -1.94725 -2.62419 -1.41767
H  -1.62792 -2.75620  1.30847
P  -2.68001  0.53899  0.55534
C  -3.28713 -0.22604  2.13652
C  -4.09105  0.27816 -0.62381
C  -2.76502  2.35940  0.92696
```

C	3.07109	1.29789	0.46065
C	3.22749	0.48747	1.60662
C	4.11433	-0.60123	1.60569
C	4.86198	-0.89845	0.45261
C	4.72931	-0.08985	-0.68921
C	3.84542	1.00285	-0.68209
H	3.77573	1.64756	-1.56554
H	5.32938	-0.29730	-1.58099
H	5.56220	-1.73957	0.45240
H	4.23851	-1.20511	2.51061
H	2.66479	0.72934	2.51667
C	0.66450	2.08702	-0.05763
C	2.07632	2.44186	0.47533
H	2.44192	3.27571	-0.15549
C	-0.75301	1.06825	-1.83523
H	-0.06391	2.85403	0.25598
H	0.34630	1.15161	0.57198
C	0.54819	1.83999	-1.58017
H	1.41149	1.23923	-1.91507
H	0.60257	2.80775	-2.11877
H	-0.76674	0.54485	-2.80483
H	-1.62938	1.73863	-1.80415
H	1.98219	2.83700	1.50169
H	-5.02687	0.67309	-0.19648
H	-3.87733	0.78999	-1.57431
H	-4.20627	-0.79860	-0.82041
H	-3.78628	2.62056	1.24879
H	-2.05919	2.60776	1.73451
H	-2.51274	2.94480	0.02991
H	-4.22841	0.25329	2.45137
H	-3.46711	-1.30125	1.98606
H	-2.52754	-0.09617	2.92231