Electronic Supplementary Material (ESI) for RSC Advances
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Supporting Information

for

Elucidating Active Species and Mechanism of the Direct Oxidation of Benzene to Phenol with Hydrogen Peroxide Catalyzed by Vanadium-Based Catalysts using DFT Calculations

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Content

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1. Figures and Tables

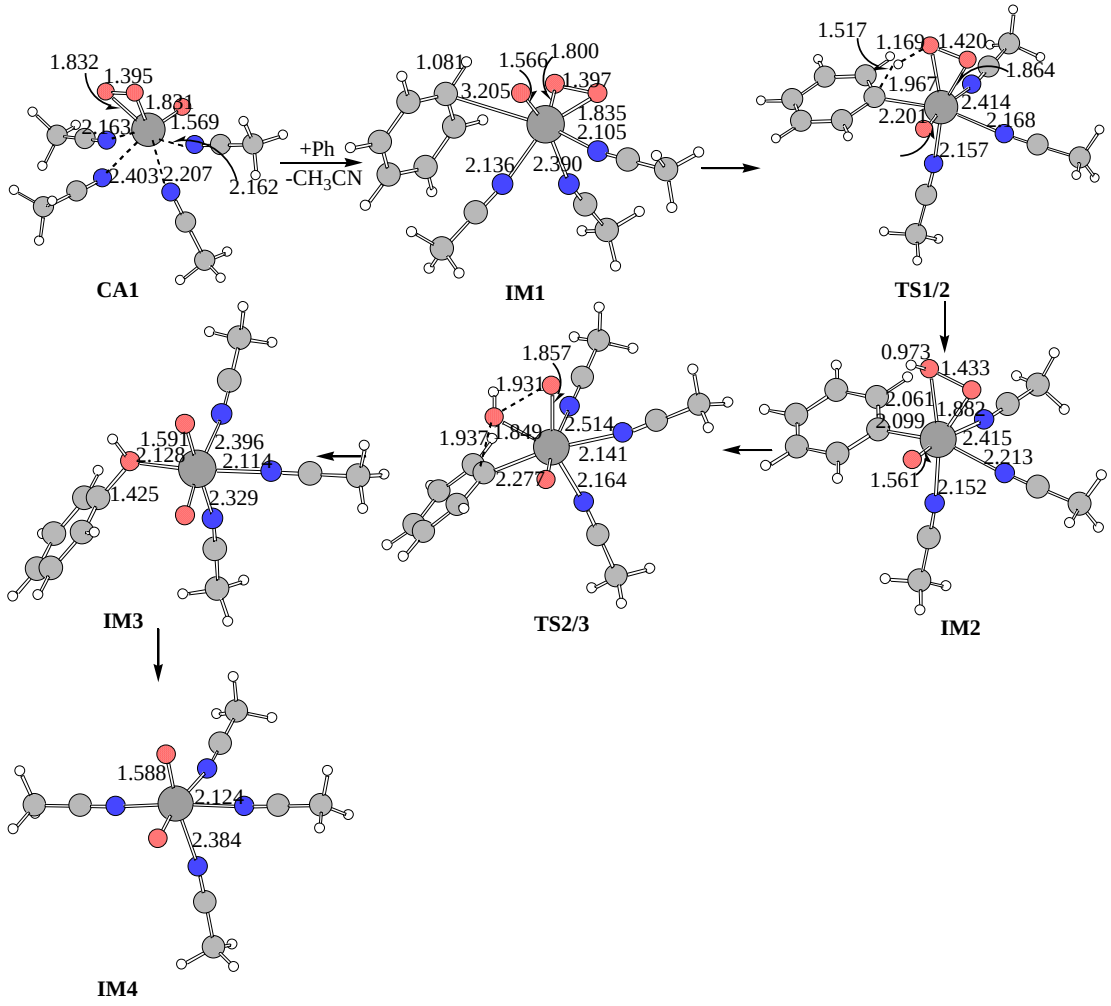

Fig. S1 The optimized structures involved in hydroxylation of benzene with $VO(O_2)(CH_3CN)_4^+$ as catalyst and selected parameters. The bond lengthens are in angstrom.

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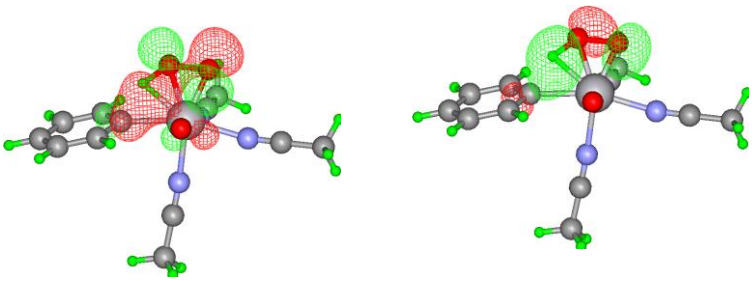
TS1/2



TS2/3

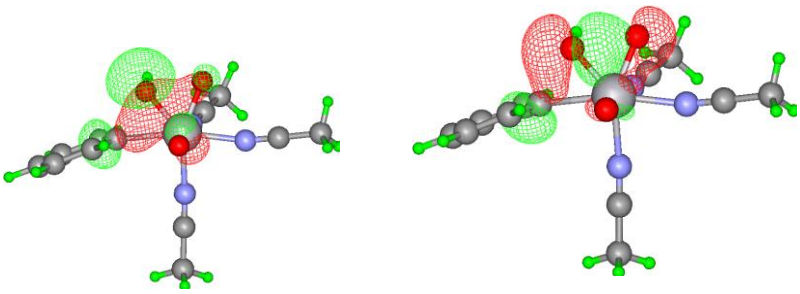


Fig. S2 The selected molecular orbitals of the C-H bond activation and hydroxyl transfer transition states(Cutoff=0.025).

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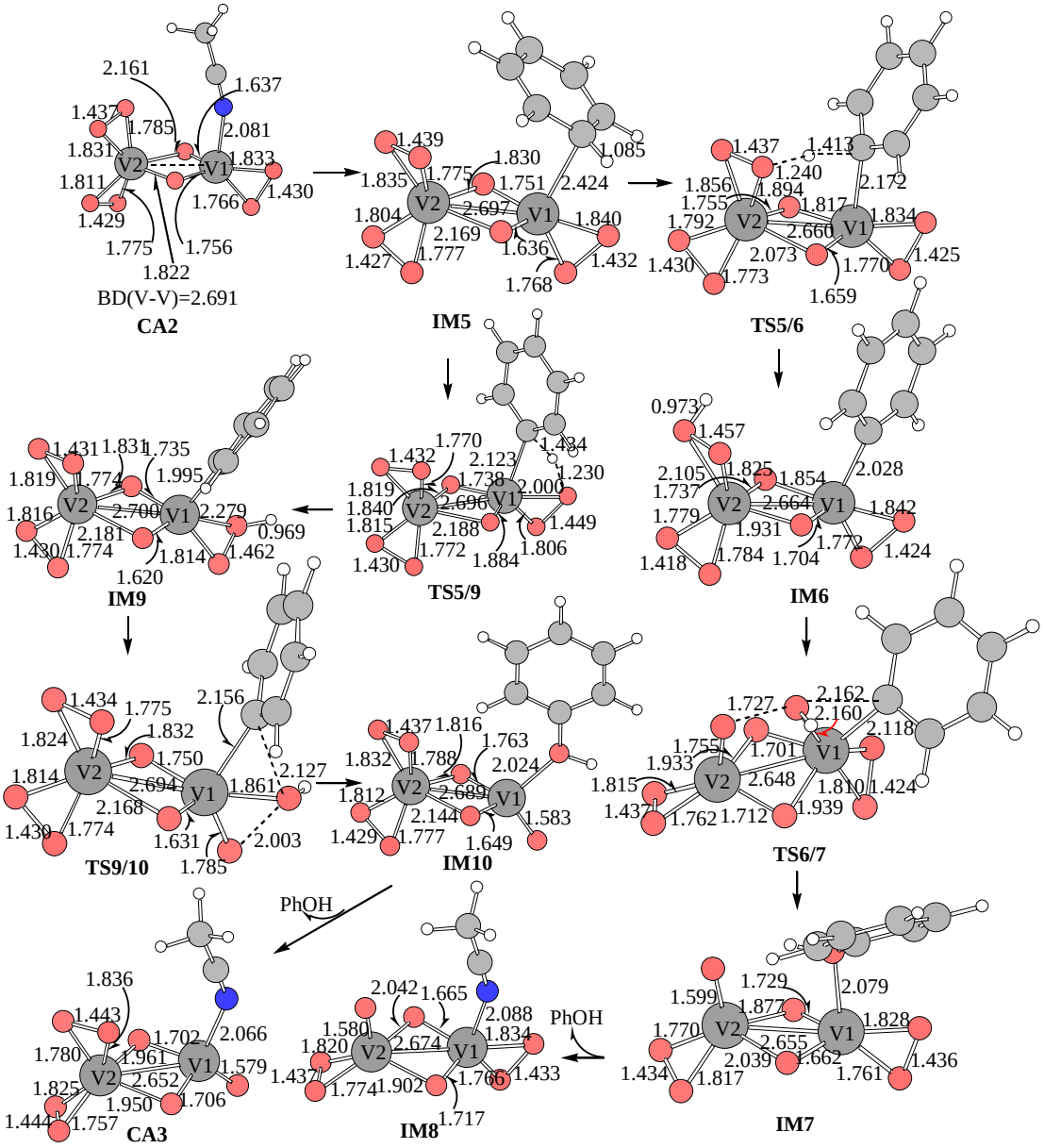

Fig. S3 The optimized structures involved in hydroxylation of benzene with $V(O_2)_2(\mu\text{-}O)_2V(O_2)(CH_3CN)$ as the catalyst and selected parameters. The bond lengths are in angstrom.

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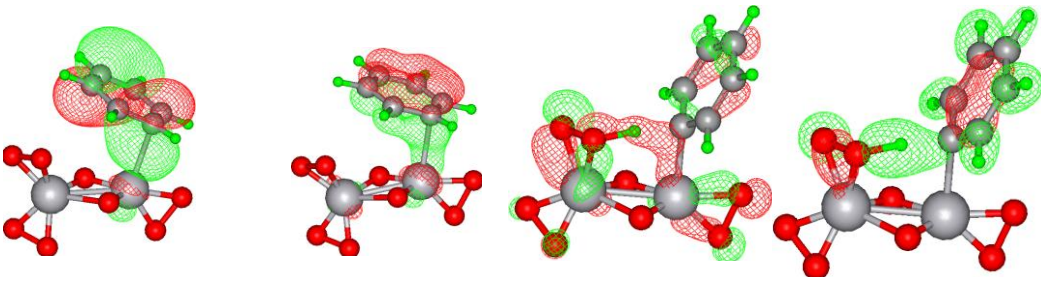
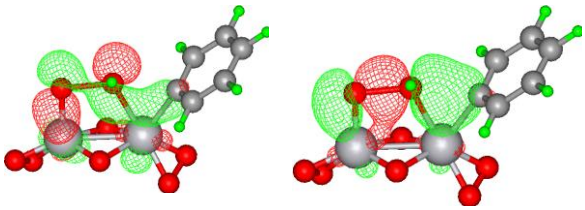
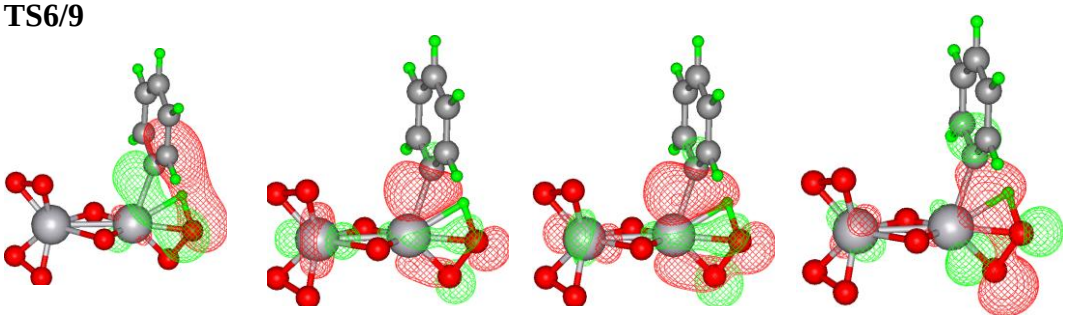
IM5 **TS5/6**



TS6/7



TS6/9



TS9/10

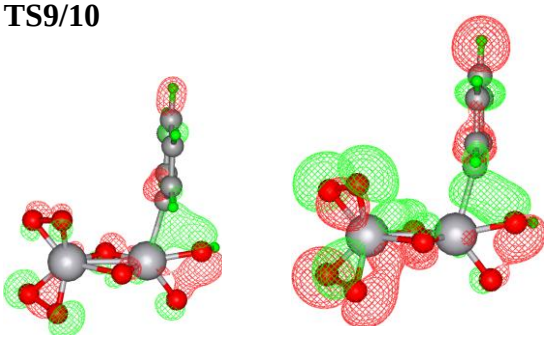


Fig. S4 The selected molecular orbitals of the C-H bond activation and hydroxyl transfer transition states with $V(O_2)_2(\mu\text{-}O)_2V(O_2)(CH_3CN)$ as the catalyst(Cutoff=0.025).

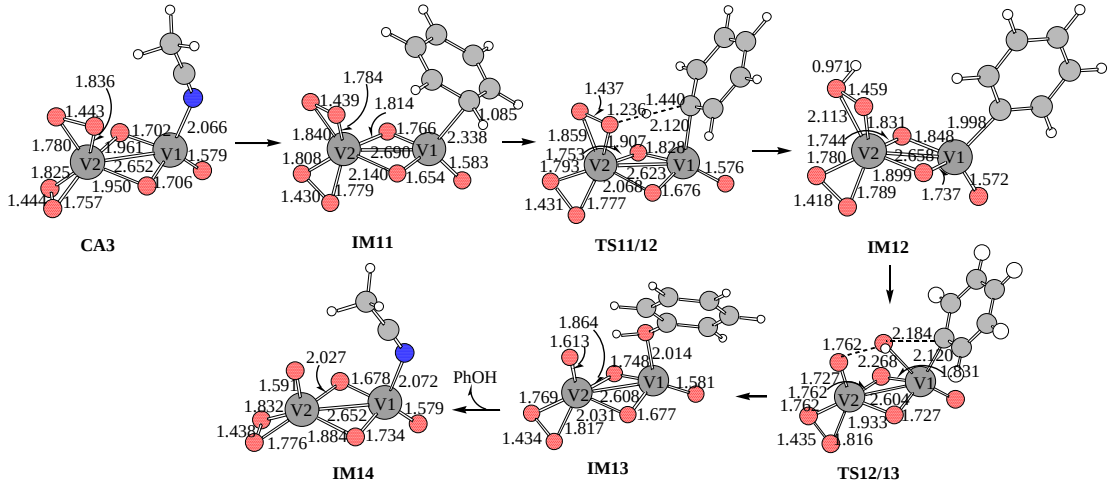
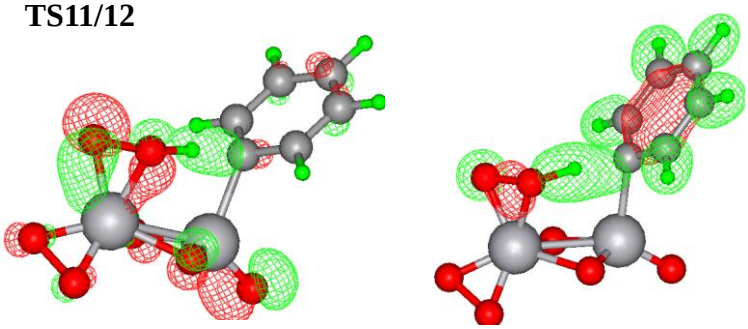


Fig. S5 The optimized structures involved in hydroxylation of benzene with $V(O_2)_2(\mu\text{-}O)_2VO(CH_3CN)$ as catalyst and selected parameters. The bond lengthens are in angstrom.

TS11/12



TS12/13

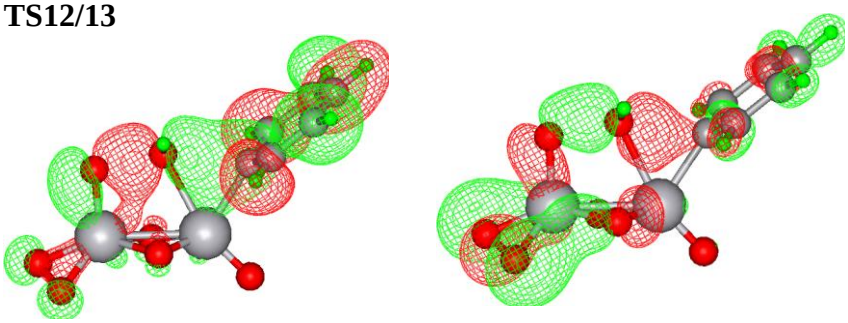


Fig. S6 The selected molecular orbitals of the C-H bond activation and hydroxyl transfer transition states with $V(O_2)_2(\mu\text{-}O)_2VO(CH_3CN)$ as the catalyst(Cutoff=0.025).

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Table S1 The predicted NICS(0) values of phenyl ring of phenyl or benzene in these intermediates

species	NICS(0)	species	NICS(0)
IM1	-7.41	**IM9**	-10.21
IM2	-9.89	**IM10**	-10.23
IM3	-9.85	**IM11**	-6.65
IM5	-6.52	**IM12**	-10.20
IM6	-9.79	**IM13**	-9.99
IM7	-9.84	**Ph**	-8.43

Table S2 The NPA charges on vanadium atom and V1-V2 bond lengths [BD(V1-V2)] in all stationary points

species	V_{NPA}	species	$V1_{NPA}$	$V2_{NPA}$	BD(V1-V2)	species	$V1_{NPA}$	$V2_{NPA}$	BD(V1-V2)
CA1	1.37	**CA2**	1.44	1.40	2.691	**TS9/10**	1.42	1.40	2.694
IM1	1.44	**IM5**	1.49	1.40	2.697	**IM10**	1.49	1.39	2.689
TS1/2	1.32	**TS5/6**	1.42	1.42	2.660	**CA3**	1.48	1.43	2.652
IM2	1.37	**IM6**	1.41	1.42	2.664	**IM11**	1.47	1.40	2.690
TS2/3	1.39	**TS6/7**	1.41	1.47	2.648	**TS11/12**	1.45	1.42	2.623
IM3	1.46	**IM7**	1.48	1.46	2.655	**IM12**	1.46	1.42	2.658
		IM8	1.44	1.46	2.674	**TS12/13**	1.43	1.47	2.604
		TS5/9	1.38	1.40	2.696	**IM13**	1.49	1.46	2.608
		IM9	1.45	1.40	2.700	**IM14**	1.48	1.46	2.652

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Table S3 The free energies in the gas phase (G, Hartree, 298.15 K, 1 atm), the solvation free energies (ΔG^{sol}, Kcal/mol, 298.15 K, 1 atm) for all stationary points

species	G	ΔG^{sol}	species	G	ΔG^{sol}
CA1	-1700.664281	-20.00	**TS6/7**	-2722.144872	2.68
IM1	-1800.105062	-17.64	**IM7**	-2722.31673	6.28
TS1/2	-1800.044578	-17.56	**IM8**	-2547.609433	2.83
IM2	-1800.0782	-19.37	**TS5/9**	-2722.153834	6.16
TS2/3	-1800.01994	-18.71	**IM9**	-2722.191644	4.00
IM3	-1800.207102	-18.11	**TS9/10**	-2722.12412	1.18
IM4	-1625.502191	-19.24	**IM10**	-2722.299177	-0.85
CA2	-2622.764539	3.3	**CA3**	-2547.590926	1.52
IM5	-2722.204041	4.45	**IM11**	-2647.043019	0.46
TS5/6	-2722.162839	6.73	**TS11/12**	-2647.001787	6.02
IM6	-2722.188765	5.28	**IM12**	-2647.039649	4.74
Ph	-232.244611	1.55	**TS12/13**	-2646.99282	3.45
PhOH	-307.488298	-0.63	**IM13**	-2647.147405	5.28
CH_3CN	-132.776221	-0.68	**IM14**	-2472.439565	0.76

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2. Cartesian coordinates

CA1

Zero-point correction= 0.198340 (Hartree/Particle)
Thermal correction to Energy= 0.221851
Thermal correction to Enthalpy= 0.222795
Thermal correction to Gibbs Free Energy= 0.138518
Sum of electronic and zero-point Energies= -1700.604460
Sum of electronic and thermal Energies= -1700.580949
Sum of electronic and thermal Enthalpies= -1700.580005
Sum of electronic and thermal Free Energies= -1700.664281

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
7	0	0.003254	-1.361474	1.185713
6	0	0.004072	-2.268738	1.885683
23	0	-0.001875	-0.010895	-0.802159
6	0	0.011531	-3.431652	2.756987
7	0	0.001382	1.508077	0.798398
7	0	-2.122886	0.221855	-0.449863
8	0	0.694160	-1.508658	-1.595158
8	0	-0.005127	1.112971	-1.896800
8	0	-0.700710	-1.508997	-1.592039
7	0	2.120373	0.223435	-0.459847
1	0	0.795559	-4.119324	2.442896
1	0	0.192152	-3.129518	3.787420
1	0	-0.948480	-3.942810	2.698684
6	0	0.002380	2.393376	1.522907
6	0	-3.263664	0.281513	-0.505727
6	0	3.261250	0.284318	-0.511550
6	0	0.001603	3.522008	2.436645
6	0	-4.711168	0.348387	-0.589848
6	0	4.708468	0.354399	-0.598426
1	0	0.819802	3.423741	3.148674
1	0	0.125350	4.447401	1.875689
1	0	-0.941131	3.557447	2.980537
1	0	-5.088346	-0.548430	-1.079502
1	0	-5.141105	0.419914	0.408111
1	0	-5.004782	1.221763	-1.170574
1	0	5.086278	-0.542095	-1.088390
1	0	4.998508	1.227711	-1.180969
1	0	5.141039	0.427325	0.398223

IM1

Zero-point correction= 0.252641 (Hartree/Particle)

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Thermal correction to Energy=	0.277514
Thermal correction to Enthalpy=	0.278458
Thermal correction to Gibbs Free Energy=	0.191378
Sum of electronic and zero-point Energies=	-1800.043798
Sum of electronic and thermal Energies=	-1800.018926
Sum of electronic and thermal Enthalpies=	-1800.017982
Sum of electronic and thermal Free Energies=	-1800.105062

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
7	0	-0.907074	1.690065	0.611383
6	0	-1.078469	2.747944	1.017612
23	0	-0.766092	-0.256635	-0.768534
6	0	-1.300032	4.095079	1.514922
7	0	0.189594	-0.862530	1.042441
8	0	-1.919378	0.708226	-1.819904
8	0	-0.457761	-1.643670	-1.427344
8	0	-0.569161	0.934375	-2.103840
7	0	-2.585589	-0.891860	0.079133
6	0	2.313254	-0.042856	-1.629442
1	0	-2.059592	4.587376	0.909126
1	0	-1.634562	4.062007	2.550657
1	0	-0.375366	4.667553	1.457162
6	0	0.797365	-1.271780	1.921528
6	0	-3.619341	-1.288853	0.365528
6	0	2.398286	1.140586	-0.893418
6	0	3.013288	-1.176176	-1.211939
1	0	1.746745	-0.068500	-2.549616
6	0	1.552551	-1.799075	3.040578
6	0	-4.933095	-1.793472	0.714491
6	0	3.189222	1.192808	0.252551
6	0	3.804150	-1.120371	-0.072521
1	0	1.873736	2.021711	-1.234676
1	0	2.951343	-2.087945	-1.789031
1	0	0.869765	-2.187956	3.795205
1	0	2.201749	-2.601317	2.693254
1	0	2.161764	-1.008843	3.475987
1	0	-5.689187	-1.274519	0.126423
1	0	-4.982513	-2.860377	0.500061
1	0	-5.125683	-1.629586	1.773864
6	0	3.894035	0.065883	0.659179
1	0	3.276487	2.115962	0.809201
1	0	4.374300	-1.987607	0.233039
1	0	4.535735	0.115159	1.529210

TS1/2

Zero-point correction=	0.247985 (Hartree/Particle)
Thermal correction to Energy=	0.272021
Thermal correction to Enthalpy=	0.272965
Thermal correction to Gibbs Free Energy=	0.188804

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Sum of electronic and zero-point Energies= -1799.985398
Sum of electronic and thermal Energies= -1799.961362
Sum of electronic and thermal Enthalpies= -1799.960417
Sum of electronic and thermal Free Energies= -1800.044578

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7	0	-0.937748	1.580286	0.772165
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23	0	-0.433427	-0.210286	-0.765786
6	0	-1.618042	3.822704	1.897313
7	0	-0.123222	-1.186263	1.132939
8	0	-1.276815	0.832837	-2.059217
8	0	-0.223326	-1.521477	-1.589362
8	0	0.038336	1.338179	-1.882772
7	0	-2.485793	-0.702753	-0.268759
6	0	1.748608	0.041534	-0.623155
1	0	-2.575076	3.715234	2.405537
1	0	-0.861734	4.120002	2.622301
1	0	-1.704510	4.596198	1.135381
6	0	0.130650	-1.782094	2.075958
6	0	-3.592767	-0.992104	-0.282830
6	0	2.305669	1.163741	0.010727
6	0	2.580776	-1.051259	-0.914721
1	0	0.950121	0.613064	-1.778241
6	0	0.473853	-2.538196	3.265809
6	0	-4.996451	-1.358994	-0.313911
6	0	3.654494	1.191791	0.344438
6	0	3.928541	-1.017924	-0.584863
1	0	1.690150	2.026306	0.223162
1	0	2.171759	-1.915889	-1.417778
1	0	-0.085570	-2.161834	4.120990
1	0	0.233142	-3.589701	3.114633
1	0	1.540668	-2.441284	3.463724
1	0	-5.562746	-0.590952	-0.839168
1	0	-5.113358	-2.307580	-0.836491
1	0	-5.379794	-1.458304	0.700529
6	0	4.464346	0.099630	0.050879
1	0	4.074790	2.066186	0.822397
1	0	4.563831	-1.857769	-0.831446
1	0	5.515136	0.123248	0.305629

IM2

Zero-point correction= 0.253354 (Hartree/Particle)
Thermal correction to Energy= 0.277859
Thermal correction to Enthalpy= 0.278803
Thermal correction to Gibbs Free Energy= 0.193982
Sum of electronic and zero-point Energies= -1800.018827
Sum of electronic and thermal Energies= -1799.994323
Sum of electronic and thermal Enthalpies= -1799.993379

Sum of electronic and thermal Free Energies= -1800.078200

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
7	0	-0.751635	1.509329	0.916719
6	0	-0.978490	2.405621	1.594152
23	0	-0.385556	-0.129868	-0.819106
6	0	-1.253856	3.550655	2.445678
7	0	-0.210442	-1.367242	0.933369
8	0	-1.286944	1.162774	-1.848035
8	0	-0.284001	-1.329118	-1.813274
8	0	0.102553	1.446545	-2.055003
7	0	-2.501004	-0.535927	-0.312556
6	0	1.673282	-0.030062	-0.424812
1	0	-1.978378	3.280352	3.212350
1	0	-0.334827	3.882579	2.926725
1	0	-1.656538	4.366115	1.846534
6	0	-0.023824	-2.084660	1.804544
6	0	-3.625380	-0.749644	-0.324690
6	0	2.268617	1.140913	0.046078
6	0	2.478039	-1.143180	-0.681575
1	0	0.294568	1.079789	-2.936218
6	0	0.251906	-2.993217	2.901481
6	0	-5.051376	-1.021401	-0.349118
6	0	3.642921	1.193601	0.267541
6	0	3.851315	-1.086168	-0.462512
1	0	1.680055	2.028635	0.225660
1	0	2.042373	-2.052918	-1.070475
1	0	-0.174528	-2.603354	3.824572
1	0	-0.181957	-3.969821	2.691128
1	0	1.329797	-3.098474	3.020892
1	0	-5.577585	-0.175501	-0.789396
1	0	-5.243388	-1.910769	-0.947932
1	0	-5.418190	-1.184860	0.663094
6	0	4.436298	0.080321	0.017993
1	0	4.091452	2.110682	0.626047
1	0	4.463223	-1.951893	-0.678995
1	0	5.503695	0.125004	0.184687

TS2/3

Zero-point correction= 0.250652 (Hartree/Particle)
Thermal correction to Energy= 0.274928
Thermal correction to Enthalpy= 0.275872
Thermal correction to Gibbs Free Energy= 0.192036
Sum of electronic and zero-point Energies= -1799.961324
Sum of electronic and thermal Energies= -1799.937049
Sum of electronic and thermal Enthalpies= -1799.936104
Sum of electronic and thermal Free Energies= -1800.019940

Atomic	Atomic	Coordinates (Angstroms)

Number	Type	X	Y	Z
7	0	-0.177352	-1.003907	1.346741
6	0	0.028921	-1.463369	2.374087
23	0	-0.421021	-0.379772	-0.711364
6	0	0.301262	-2.050052	3.673352
7	0	-0.810245	1.751431	0.562892
7	0	-2.474027	-0.756591	-0.235842
8	0	-1.374983	0.612770	-1.957508
8	0	-0.223850	-1.832161	-1.266814
6	0	1.807138	0.070648	-0.576823
1	0	1.257527	-1.687275	4.047875
1	0	-0.484967	-1.779367	4.376579
1	0	0.342192	-3.134761	3.582724
6	0	-1.301688	2.742871	0.867133
6	0	-3.589982	-1.000329	-0.303389
6	0	2.324911	1.158539	0.141290
6	0	2.661669	-0.928267	-1.068898
8	0	0.554525	0.547542	-1.978275
6	0	-1.931093	4.001200	1.232798
6	0	-5.003447	-1.305177	-0.417679
6	0	3.669355	1.169445	0.480312
6	0	4.002643	-0.907614	-0.719766
1	0	1.681355	1.962711	0.466305
1	0	2.268046	-1.713433	-1.696559
1	0	0.419450	1.501499	-1.860416
1	0	-2.572921	3.858643	2.100900
1	0	-1.170690	4.742615	1.473917
1	0	-2.531648	4.365662	0.400396
1	0	-5.415726	-0.781710	-1.279739
1	0	-5.137828	-2.377375	-0.554047
1	0	-5.530625	-0.989086	0.481216
6	0	4.506184	0.136793	0.055117
1	0	4.071182	1.986402	1.064030
1	0	4.661251	-1.690584	-1.069423
1	0	5.557484	0.160963	0.306641

IM3

Zero-point correction=	0.253755 (Hartree/Particle)
Thermal correction to Energy=	0.278756
Thermal correction to Enthalpy=	0.279700
Thermal correction to Gibbs Free Energy=	0.189972
Sum of electronic and zero-point Energies=	-1800.143319
Sum of electronic and thermal Energies=	-1800.118318
Sum of electronic and thermal Enthalpies=	-1800.117374
Sum of electronic and thermal Free Energies=	-1800.207102

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
7	0	-1.616558	1.721275	0.155337

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6	0	-2.010966	2.781127	0.341749
23	0	-0.870260	-0.340950	-0.809122
6	0	-2.512829	4.126347	0.568426
7	0	-0.099441	-0.473086	1.383666
8	0	-1.385924	0.211140	-2.209971
8	0	-0.288468	-1.791912	-1.088588
8	0	0.929196	0.765346	-1.061059
7	0	-2.732759	-1.034285	-0.089203
1	0	-3.166014	4.418243	-0.252679
1	0	-3.073247	4.163699	1.501309
1	0	-1.681134	4.827016	0.625798
6	0	0.431107	-0.740042	2.363352
6	0	-3.744569	-1.518524	0.134059
6	0	2.253781	0.372240	-0.712372
1	0	0.896336	1.037509	-1.986509
6	0	1.117466	-1.081865	3.596562
6	0	-5.026525	-2.139704	0.404690
6	0	2.967923	1.210069	0.126099
6	0	2.776370	-0.811255	-1.204060
1	0	0.624285	-0.608367	4.444037
1	0	1.110622	-2.162072	3.734636
1	0	2.149359	-0.737156	3.544087
1	0	-5.729416	-1.883829	-0.387207
1	0	-4.907066	-3.221797	0.441073
1	0	-5.416330	-1.788135	1.358933
6	0	4.264058	0.847908	0.481062
6	0	4.074783	-1.157899	-0.844490
1	0	2.519407	2.127945	0.477661
1	0	2.175795	-1.450370	-1.834448
6	0	4.816719	-0.332814	-0.004896
1	0	4.842678	1.494864	1.125491
1	0	4.503661	-2.075288	-1.222090
1	0	5.825996	-0.607868	0.266968

IM4

Zero-point correction= 0.194497 (Hartree/Particle)
Thermal correction to Energy= 0.216573
Thermal correction to Enthalpy= 0.217517
Thermal correction to Gibbs Free Energy= 0.136681
Sum of electronic and zero-point Energies= -1625.444375
Sum of electronic and thermal Energies= -1625.422299
Sum of electronic and thermal Enthalpies= -1625.421355
Sum of electronic and thermal Free Energies= -1625.502191

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
7	0	0.000479	-1.485403	0.962455
6	0	0.001222	-2.397546	1.656148
23	0	-0.000125	0.001199	-0.900689
6	0	0.001832	-3.560073	2.528777

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7	0	0.000147	1.474411	0.976024
7	0	-2.102189	-0.000872	-0.593867
8	0	-0.000360	-1.264326	-1.859694
8	0	-0.000367	1.278415	-1.844373
7	0	2.102054	-0.000591	-0.594732
1	0	0.928452	-4.117440	2.399658
1	0	-0.085268	-3.248637	3.568475
1	0	-0.836400	-4.208731	2.278580
6	0	-0.000635	2.391204	1.663609
6	0	-3.244007	-0.001408	-0.657717
6	0	3.243891	-0.000138	-0.658239
6	0	-0.001625	3.560873	2.526590
6	0	-4.691298	-0.002098	-0.754140
6	0	4.691200	0.000535	-0.754402
1	0	0.923749	3.601351	3.099193
1	0	-0.085537	4.462873	1.922084
1	0	-0.842981	3.514437	3.216334
1	0	-5.015439	-0.847798	-1.359307
1	0	-5.131457	-0.081129	0.238809
1	0	-5.026355	0.921845	-1.223674
1	0	5.018329	-0.862960	-1.332192
1	0	5.023290	0.910150	-1.253134
1	0	5.131386	-0.045170	0.240627

CA2

Zero-point correction= 0.074738 (Hartree/Particle)
Thermal correction to Energy= 0.090060
Thermal correction to Enthalpy= 0.091005
Thermal correction to Gibbs Free Energy= 0.030528
Sum of electronic and zero-point Energies= -2622.720329
Sum of electronic and thermal Energies= -2622.705006
Sum of electronic and thermal Enthalpies= -2622.704062
Sum of electronic and thermal Free Energies= -2622.764539

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
23	0	-0.873442	-1.077256	-0.032328
8	0	0.280682	-0.451277	-1.198626
8	0	-0.006690	-0.651552	1.289714
8	0	-2.439883	-2.025891	-0.118421
7	0	-2.045848	0.642101	-0.063442
8	0	-1.240121	-2.803428	-0.103397
23	0	1.457465	0.268400	-0.007805
6	0	-2.354867	1.742162	-0.026042
8	0	1.753915	2.009144	-0.490454
8	0	3.163873	-0.161750	-0.437628
8	0	0.847496	1.827741	0.608878
8	0	2.588171	-0.957362	0.600828
6	0	-2.702572	3.145950	0.030197
1	0	-3.443119	3.315587	0.810215

1	0	-1.798298	3.711999	0.253914
1	0	-3.105082	3.467709	-0.929067

IM5

Zero-point correction= 0.129148 (Hartree/Particle)
Thermal correction to Energy= 0.145691
Thermal correction to Enthalpy= 0.146635
Thermal correction to Gibbs Free Energy= 0.084064
Sum of electronic and zero-point Energies= -2722.158957
Sum of electronic and thermal Energies= -2722.142414
Sum of electronic and thermal Enthalpies= -2722.141470
Sum of electronic and thermal Free Energies= -2722.204041

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
23	0	-0.455264	1.226321	0.104944
8	0	0.269667	0.127616	-1.049341
8	0	0.625898	0.938707	1.298581
8	0	-1.713903	2.567285	0.066130
8	0	-0.399598	2.926545	-0.375296
23	0	1.739659	-0.331838	-0.059858
6	0	-2.307694	-0.112149	0.913242
8	0	2.928881	0.986668	-0.128084
8	0	1.482279	-1.640462	1.110968
8	0	1.937960	-2.154507	-0.154274
8	0	3.264671	-0.095641	-0.994629
6	0	-1.614594	-1.293496	1.231538
6	0	-3.007472	-0.020835	-0.308343
1	0	-2.446626	0.651426	1.670279
6	0	-1.597934	-2.350541	0.333780
6	0	-2.986883	-1.086334	-1.195947
1	0	-1.081646	-1.367307	2.167138
1	0	-3.554143	0.879802	-0.543382
6	0	-2.286695	-2.246034	-0.871320
1	0	-1.036100	-3.242954	0.564906
1	0	-3.513800	-1.015723	-2.136670
1	0	-2.267967	-3.071725	-1.569382

TS5/6

Zero-point correction= 0.124394 (Hartree/Particle)
Thermal correction to Energy= 0.139830
Thermal correction to Enthalpy= 0.140774
Thermal correction to Gibbs Free Energy= 0.081389
Sum of electronic and zero-point Energies= -2722.119834
Sum of electronic and thermal Energies= -2722.104398
Sum of electronic and thermal Enthalpies= -2722.103454
Sum of electronic and thermal Free Energies= -2722.162839

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Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
23	0	-0.003390	1.310050	-0.117327
8	0	1.054575	0.332160	-1.225171
8	0	0.930678	0.886445	1.186534
8	0	-1.470048	2.408749	-0.164795
8	0	-0.211644	3.054109	-0.336525
23	0	1.899558	-0.542992	0.040502
6	0	-1.480374	-0.267327	0.102373
8	0	3.475665	0.151482	0.464441
8	0	0.628477	-1.684200	0.857830
8	0	1.297199	-2.269682	-0.270528
8	0	3.580394	-0.994834	-0.383910
6	0	-1.976128	-0.815098	-1.102603
6	0	-2.359915	-0.201198	1.205778
1	0	-0.388077	-1.073802	0.494229
6	0	-3.272135	-1.300308	-1.189020
6	0	-3.653639	-0.686578	1.121616
1	0	-1.325412	-0.878634	-1.965372
1	0	-2.009030	0.224102	2.137395
6	0	-4.108973	-1.231643	-0.078288
1	0	-3.631983	-1.729501	-2.114051
1	0	-4.310937	-0.639605	1.979002
1	0	-5.121822	-1.605822	-0.146373

IM6

Zero-point correction=	0.130034 (Hartree/Particle)
Thermal correction to Energy=	0.146226
Thermal correction to Enthalpy=	0.147170
Thermal correction to Gibbs Free Energy=	0.085198
Sum of electronic and zero-point Energies=	-2722.143928
Sum of electronic and thermal Energies=	-2722.127736
Sum of electronic and thermal Enthalpies=	-2722.126792
Sum of electronic and thermal Free Energies=	-2722.188765

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
23	0	0.178214	1.207681	-0.052136
8	0	-0.808974	0.249053	1.191075
8	0	-0.827382	0.512205	-1.238280
8	0	1.328851	2.627532	-0.282048
23	0	-1.920113	-0.432600	0.042895
6	0	1.875594	0.100934	-0.133690
8	0	-0.000925	2.963786	0.101857
8	0	-1.780665	-2.402070	0.770921
8	0	-3.619125	-0.361786	0.562338
6	0	1.890273	-1.141054	-0.783562
6	0	2.996138	0.493964	0.604194
8	0	-3.311806	0.558816	-0.471046

8	0	-1.449731	-2.071408	-0.607740
6	0	2.999029	-1.974903	-0.677205
6	0	4.096722	-0.348944	0.720531
1	0	1.050501	-1.453965	-1.387479
1	0	3.011036	1.462676	1.085967
1	0	-0.903329	-2.528967	1.171660
6	0	4.099392	-1.583241	0.079372
1	0	3.005823	-2.926492	-1.192783
1	0	4.954457	-0.036350	1.301368
1	0	4.960366	-2.233333	0.159353

TS6/7

Zero-point correction= 0.127357 (Hartree/Particle)
Thermal correction to Energy= 0.143189
Thermal correction to Enthalpy= 0.144133
Thermal correction to Gibbs Free Energy= 0.083613
Sum of electronic and zero-point Energies= -2722.101127
Sum of electronic and thermal Energies= -2722.085296
Sum of electronic and thermal Enthalpies= -2722.084351
Sum of electronic and thermal Free Energies= -2722.144872

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-4.011530	-0.800668	-1.081312
6	0	-4.644491	-0.686413	0.155279
6	0	-2.644722	-0.582559	-1.182758
1	0	-4.581400	-1.072884	-1.959225
6	0	-3.915071	-0.357015	1.294740
6	0	-1.919513	-0.205106	-0.049248
1	0	-5.707660	-0.868232	0.233095
1	0	-2.146854	-0.695776	-2.136559
6	0	-2.545854	-0.134651	1.200916
1	0	-4.410105	-0.275984	2.252928
23	0	-0.046996	0.780125	-0.153075
1	0	-1.984604	0.130310	2.089086
8	0	1.226143	0.441318	-1.229536
8	0	1.273365	0.405041	1.214807
8	0	-0.803438	2.303371	-0.685285
23	0	2.283624	-0.445506	0.124840
8	0	3.970814	-0.641875	0.594568
8	0	1.506037	-2.003982	-0.084849
8	0	-0.104642	-1.378620	-0.112709
1	0	-0.354765	-1.780110	0.735062
8	0	-0.180136	2.425568	0.588432
8	0	3.840612	0.132292	-0.609267

IM7

Zero-point correction= 0.131679 (Hartree/Particle)

Thermal correction to Energy= 0.147479
Thermal correction to Enthalpy= 0.148424
Thermal correction to Gibbs Free Energy= 0.086730
Sum of electronic and zero-point Energies= -2722.271782
Sum of electronic and thermal Energies= -2722.255981
Sum of electronic and thermal Enthalpies= -2722.255037
Sum of electronic and thermal Free Energies= -2722.316730

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
23	0	0.429558	1.269028	0.068282
8	0	1.727208	0.942252	-1.027281
8	0	0.908680	0.104693	1.154766
8	0	-0.970260	2.442511	0.145302
23	0	2.236433	-0.659068	-0.189711
8	0	-0.835593	-0.025778	-0.955435
8	0	0.261638	2.890356	0.732980
8	0	3.930214	-1.168877	-0.134674
6	0	-2.097498	-0.411204	-0.451371
8	0	3.378717	-1.003564	1.178830
8	0	1.297048	-1.801071	-0.797390
1	0	-0.270059	-0.824206	-1.081329
6	0	-2.225726	-1.607370	0.236076
6	0	-3.167923	0.435659	-0.679554
6	0	-3.484698	-1.970045	0.700751
6	0	-4.416906	0.062889	-0.196956
1	0	-1.359710	-2.231996	0.407379
1	0	-3.020428	1.358876	-1.219411
6	0	-4.578119	-1.137312	0.487752
1	0	-3.605035	-2.901510	1.235686
1	0	-5.265076	0.712082	-0.362577
1	0	-5.553470	-1.422204	0.856166

IM8

Zero-point correction= 0.072028 (Hartree/Particle)
Thermal correction to Energy= 0.086125
Thermal correction to Enthalpy= 0.087069
Thermal correction to Gibbs Free Energy= 0.029870
Sum of electronic and zero-point Energies= -2547.567275
Sum of electronic and thermal Energies= -2547.553178
Sum of electronic and thermal Enthalpies= -2547.552234
Sum of electronic and thermal Free Energies= -2547.609433

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
23	0	-0.872146	-0.982400	-0.027455
8	0	0.195237	-0.501567	-1.284506
8	0	0.158950	-0.534976	1.199517
8	0	-2.497692	-1.829141	0.026494

7	0	-1.898736	0.834088	-0.016750
8	0	-1.347736	-2.683373	0.000865
23	0	1.479217	0.286860	-0.123774
6	0	-1.998082	1.972677	0.029178
8	0	3.197133	0.015622	-0.478063
8	0	1.200314	1.834142	0.037191
8	0	2.830684	-0.489091	0.816395
6	0	-2.062384	3.416854	0.092114
1	0	-1.039730	3.789737	0.157584
1	0	-2.539700	3.810257	-0.803918
1	0	-2.624373	3.728689	0.970966

TS5/9

Zero-point correction= 0.124035 (Hartree/Particle)
Thermal correction to Energy= 0.140212
Thermal correction to Enthalpy= 0.141156
Thermal correction to Gibbs Free Energy= 0.078785
Sum of electronic and zero-point Energies= -2722.108584
Sum of electronic and thermal Energies= -2722.092406
Sum of electronic and thermal Enthalpies= -2722.091462
Sum of electronic and thermal Free Energies= -2722.153834

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
23	0	-0.048505	1.196392	-0.049439
8	0	0.857880	0.221966	-1.166507
8	0	0.745689	0.745832	1.284846
8	0	-1.350706	2.713902	-0.009941
8	0	-0.003078	2.947647	-0.487268
6	0	-1.942987	0.243239	-0.150392
23	0	1.937714	-0.621661	0.060965
1	0	-1.843875	1.653661	-0.392410
6	0	-2.703912	0.114154	1.026025
6	0	-2.203217	-0.621484	-1.229817
8	0	3.325448	0.393341	0.487318
8	0	1.859738	-2.421055	-0.201432
8	0	1.050605	-1.923692	0.869898
8	0	3.665767	-0.590627	-0.493020
6	0	-3.701906	-0.844740	1.116696
6	0	-3.208029	-1.571517	-1.136971
1	0	-2.515866	0.773390	1.863346
1	0	-1.615840	-0.549430	-2.134654
6	0	-3.951362	-1.685190	0.035806
1	0	-4.282052	-0.938653	2.024105
1	0	-3.408357	-2.228527	-1.971889
1	0	-4.728059	-2.434548	0.107177

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IM9

Zero-point correction= 0.128975 (Hartree/Particle)
Thermal correction to Energy= 0.145937
Thermal correction to Enthalpy= 0.146881
Thermal correction to Gibbs Free Energy= 0.082507
Sum of electronic and zero-point Energies= -2722.145176
Sum of electronic and thermal Energies= -2722.128214
Sum of electronic and thermal Enthalpies= -2722.127270
Sum of electronic and thermal Free Energies= -2722.191644

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
23	0	-0.165729	0.917716	0.237017
8	0	0.900125	0.486149	-1.062703
8	0	0.664068	0.152810	1.398884
8	0	-0.981995	2.849148	-0.653418
23	0	2.089271	-0.527095	-0.106329
6	0	-1.892724	-0.072694	0.108419
8	0	-0.408666	2.660088	0.677238
8	0	2.336015	-2.133663	-0.921893
8	0	3.792221	-0.035256	-0.503389
6	0	-2.356361	-0.923916	1.119476
6	0	-2.672089	0.116157	-1.042220
8	0	3.271219	0.511113	0.711291
8	0	1.439252	-2.149370	0.193648
1	0	-1.922925	2.956055	-0.446213
6	0	-3.587661	-1.553966	0.989803
6	0	-3.899304	-0.524153	-1.170554
1	0	-1.754485	-1.096430	2.000493
1	0	-2.319519	0.744058	-1.851373
6	0	-4.357878	-1.353927	-0.152316
1	0	-3.942073	-2.207969	1.774983
1	0	-4.491508	-0.381312	-2.064329
1	0	-5.312768	-1.851866	-0.252305

TS9/10

Zero-point correction= 0.126019 (Hartree/Particle)
Thermal correction to Energy= 0.142576
Thermal correction to Enthalpy= 0.143521
Thermal correction to Gibbs Free Energy= 0.080362
Sum of electronic and zero-point Energies= -2722.078463
Sum of electronic and thermal Energies= -2722.061906
Sum of electronic and thermal Enthalpies= -2722.060962
Sum of electronic and thermal Free Energies= -2722.124120

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
23	0	-0.004376	1.256483	-0.007942

8	0	-0.866463	0.302604	1.177672
8	0	-0.820811	0.691969	-1.301664
8	0	-0.279429	2.990916	0.312243
8	0	1.515951	2.302751	-0.249313
23	0	-1.910220	-0.646270	0.009930
1	0	1.858202	2.686122	0.572367
8	0	-3.359219	0.268435	-0.450784
8	0	-0.970297	-1.946153	-0.748084
8	0	-1.726068	-2.426705	0.371030
8	0	-3.633712	-0.689905	0.575100
6	0	1.891021	0.227624	0.024184
6	0	2.454208	-0.222881	-1.185863
6	0	2.473764	-0.139710	1.253999
6	0	3.469101	-1.164395	-1.158803
6	0	3.490558	-1.075653	1.270942
1	0	2.061433	0.131013	-2.128697
1	0	2.078549	0.246293	2.185062
6	0	3.985955	-1.587489	0.065747
1	0	3.871341	-1.557096	-2.082257
1	0	3.903443	-1.413167	2.211629
1	0	4.795461	-2.304342	0.085327

IM10

Zero-point correction= 0.130720 (Hartree/Particle)
Thermal correction to Energy= 0.147193
Thermal correction to Enthalpy= 0.148137
Thermal correction to Gibbs Free Energy= 0.084766
Sum of electronic and zero-point Energies= -2722.253223
Sum of electronic and thermal Energies= -2722.236750
Sum of electronic and thermal Enthalpies= -2722.235806
Sum of electronic and thermal Free Energies= -2722.299177

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
23	0	0.392583	1.445051	-0.043632
8	0	1.324539	0.498396	-1.203043
8	0	0.954089	0.637567	1.280339
8	0	-1.620974	1.427941	-0.240314
23	0	2.088329	-0.642157	-0.013636
8	0	0.687408	2.999684	-0.003980
8	0	1.787582	-2.342708	-0.625566
8	0	3.864706	-0.830473	-0.316139
6	0	-2.604493	0.408999	-0.104004
8	0	3.530236	0.076014	0.736410
8	0	0.941279	-1.929323	0.460155
1	0	-2.024695	2.303488	-0.260584
6	0	-3.938491	0.771084	-0.070114
6	0	-2.173120	-0.899876	-0.022355
6	0	-4.889463	-0.236007	0.052628
6	0	-3.140808	-1.891396	0.101087

1	0	-4.237080	1.809832	-0.137110
1	0	-1.122271	-1.158174	-0.041455
6	0	-4.492243	-1.565509	0.137617
1	0	-5.937668	0.025185	0.081467
1	0	-2.824314	-2.922213	0.169717
1	0	-5.234159	-2.345229	0.233089

CA3

Zero-point correction= 0.071155 (Hartree/Particle)
Thermal correction to Energy= 0.085574
Thermal correction to Enthalpy= 0.086518
Thermal correction to Gibbs Free Energy= 0.028480
Sum of electronic and zero-point Energies= -2547.548252
Sum of electronic and thermal Energies= -2547.533832
Sum of electronic and thermal Enthalpies= -2547.532888
Sum of electronic and thermal Free Energies= -2547.590926

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
23	0	-0.681420	1.387686	-0.009945
8	0	0.243258	0.722934	1.260384
8	0	0.292035	0.703495	-1.227006
8	0	-0.804010	2.961348	-0.032869
7	0	-2.432208	0.290830	-0.033776
23	0	1.235089	-0.443712	0.053241
6	0	-2.863539	-0.771341	-0.015361
8	0	0.078382	-1.818784	0.431189
8	0	2.853597	-0.479071	0.735617
8	0	0.970603	-2.043966	-0.679736
8	0	2.856624	0.089138	-0.592045
6	0	-3.347907	-2.131171	0.015882
1	0	-3.857881	-2.368001	-0.916716
1	0	-2.476399	-2.777641	0.136030
1	0	-4.029880	-2.267229	0.853905

IM11

Zero-point correction= 0.126322 (Hartree/Particle)
Thermal correction to Energy= 0.141771
Thermal correction to Enthalpy= 0.142716
Thermal correction to Gibbs Free Energy= 0.081628
Sum of electronic and zero-point Energies= -2646.998324
Sum of electronic and thermal Energies= -2646.982875
Sum of electronic and thermal Enthalpies= -2646.981931
Sum of electronic and thermal Free Energies= -2647.043019

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

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23	0	0.549692	-1.130054	0.073100
8	0	-0.374733	-0.223187	-1.128239
8	0	-0.629545	-1.045420	1.229029
8	0	0.897778	-2.626830	-0.305636
23	0	-1.767636	0.229019	-0.059084
6	0	2.488909	-0.242351	1.030003
8	0	-1.897096	2.062541	-0.143780
8	0	-3.362520	0.055310	-0.892948
6	0	1.843973	0.991035	1.234809
6	0	3.163221	-0.490072	-0.182370
1	0	2.532354	-0.972477	1.830766
8	0	-3.018272	-1.035776	-0.036465
8	0	-1.320789	1.539228	1.066746
6	0	1.869594	1.959634	0.236162
6	0	3.184364	0.489325	-1.169018
1	0	1.306582	1.173019	2.152979
1	0	3.653256	-1.439602	-0.338409
6	0	2.546539	1.710294	-0.953188
1	0	1.337392	2.887794	0.379108
1	0	3.689710	0.299211	-2.104754
1	0	2.555218	2.461745	-1.730099

TS11/12

Zero-point correction= 0.121446 (Hartree/Particle)
Thermal correction to Energy= 0.135976
Thermal correction to Enthalpy= 0.136920
Thermal correction to Gibbs Free Energy= 0.079121
Sum of electronic and zero-point Energies= -2646.959461
Sum of electronic and thermal Energies= -2646.944931
Sum of electronic and thermal Enthalpies= -2646.943987
Sum of electronic and thermal Free Energies= -2647.001787

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
23	0	-0.090867	1.265469	-0.200656
8	0	1.118574	0.419084	-1.279578
8	0	0.928316	1.067972	1.114652
8	0	-0.597665	2.736894	-0.445058
23	0	1.923633	-0.396486	0.046113
6	0	-1.613295	-0.180815	0.096311
8	0	1.330690	-2.136638	-0.231748
8	0	3.620443	-0.855419	-0.303592
6	0	-2.216432	-0.653860	-1.091168
6	0	-2.440991	0.016036	1.223684
1	0	-0.442867	-0.950315	0.432750
8	0	3.484122	0.315294	0.507508
8	0	0.586263	-1.510562	0.826128
6	0	-3.572598	-0.936352	-1.141467
6	0	-3.797919	-0.261091	1.172421
1	0	-1.605545	-0.814825	-1.971180

1	0	-2.004314	0.379897	2.145097
6	0	-4.360690	-0.736617	-0.010070
1	0	-4.017527	-1.312081	-2.052557
1	0	-4.418118	-0.111959	2.045522
1	0	-5.419635	-0.954121	-0.049914

IM12

Zero-point correction= 0.127099 (Hartree/Particle)
Thermal correction to Energy= 0.142274
Thermal correction to Enthalpy= 0.143218
Thermal correction to Gibbs Free Energy= 0.083193
Sum of electronic and zero-point Energies= -2646.995743
Sum of electronic and thermal Energies= -2646.980567
Sum of electronic and thermal Enthalpies= -2646.979623
Sum of electronic and thermal Free Energies= -2647.039649

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
23	0	-0.278681	-1.103022	-0.007928
8	0	0.896705	-0.342013	1.199064
8	0	0.805523	-0.540531	-1.243393
8	0	-0.465128	-2.662263	0.063224
23	0	2.015836	0.238926	-0.004854
6	0	-2.081720	-0.246051	-0.075227
8	0	2.142233	2.190257	0.793883
8	0	3.730030	-0.001438	0.413425
6	0	-2.143023	1.112779	-0.426053
6	0	-3.261290	-0.898733	0.310654
8	0	3.283814	-0.861374	-0.622750
8	0	1.643275	1.945350	-0.553939
6	0	-3.350256	1.799873	-0.383855
6	0	-4.466362	-0.208308	0.357051
1	0	-1.250677	1.633333	-0.753043
1	0	-3.234209	-1.948248	0.570770
1	0	1.327440	2.375254	1.289739
6	0	-4.510272	1.139167	0.010272
1	0	-3.389189	2.844561	-0.662930
1	0	-5.371362	-0.720162	0.656277
1	0	-5.450643	1.673215	0.039986

TS12/13

Zero-point correction= 0.124190 (Hartree/Particle)
Thermal correction to Energy= 0.139116
Thermal correction to Enthalpy= 0.140060
Thermal correction to Gibbs Free Energy= 0.081448
Sum of electronic and zero-point Energies= -2646.950079
Sum of electronic and thermal Energies= -2646.935153
Sum of electronic and thermal Enthalpies= -2646.934208

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Sum of electronic and thermal Free Energies= -2646.992820

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-4.005751	-0.563949	-1.109541
6	0	-4.663838	-0.493134	0.116518
6	0	-2.634728	-0.355897	-1.170088
1	0	-4.558073	-0.797737	-2.009462
6	0	-3.956107	-0.215216	1.284614
6	0	-1.926310	-0.024131	-0.009210
1	0	-5.729596	-0.670366	0.164736
1	0	-2.118109	-0.441156	-2.117732
6	0	-2.585275	-0.002094	1.228313
1	0	-4.472407	-0.168585	2.233855
23	0	-0.035754	0.926279	-0.143824
1	0	-2.039481	0.221236	2.137215
8	0	1.295849	0.462229	-1.311816
8	0	1.094786	0.658263	1.134280
8	0	-0.431622	2.445061	-0.253858
23	0	2.231951	-0.349697	-0.060682
8	0	3.959429	-0.552594	-0.347219
8	0	1.484961	-1.891586	0.148795
8	0	-0.178306	-1.334007	-0.024307
1	0	-0.411086	-1.635046	0.867532
8	0	3.705936	0.232234	0.827107

IM13

Zero-point correction= 0.128002 (Hartree/Particle)
Thermal correction to Energy= 0.142804
Thermal correction to Enthalpy= 0.143748
Thermal correction to Gibbs Free Energy= 0.083933
Sum of electronic and zero-point Energies= -2647.103335
Sum of electronic and thermal Energies= -2647.088533
Sum of electronic and thermal Enthalpies= -2647.087589
Sum of electronic and thermal Free Energies= -2647.147405

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
23	0	0.430688	1.312243	-0.084493
8	0	1.811278	0.951831	-1.093858
8	0	1.036451	0.433590	1.209039
8	0	0.033888	2.810897	0.227365
23	0	2.252278	-0.552723	-0.084978
8	0	-0.897456	-0.017208	-0.808652
8	0	3.904285	-1.185372	-0.038041
6	0	-2.209943	-0.268831	-0.359484
8	0	3.436246	-0.821349	1.267633
8	0	1.183012	-1.674986	-0.528161
1	0	-0.332548	-0.845434	-0.820002

6	0	-2.656273	-1.575090	-0.256578
6	0	-3.011591	0.818557	-0.060092
6	0	-3.964615	-1.792802	0.160614
6	0	-4.316346	0.581253	0.355951
1	0	-1.997047	-2.400319	-0.488896
1	0	-2.619882	1.823645	-0.138971
6	0	-4.795363	-0.719960	0.464309
1	0	-4.329659	-2.806289	0.248675
1	0	-4.955271	1.418830	0.597296
1	0	-5.810665	-0.897380	0.788829

IM14

Zero-point correction= 0.068935 (Hartree/Particle)
Thermal correction to Energy= 0.081929
Thermal correction to Enthalpy= 0.082873
Thermal correction to Gibbs Free Energy= 0.028511
Sum of electronic and zero-point Energies= -2472.399141
Sum of electronic and thermal Energies= -2472.386148
Sum of electronic and thermal Enthalpies= -2472.385203
Sum of electronic and thermal Free Energies= -2472.439565

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
23	0	0.753851	1.285929	-0.025405
8	0	-0.256347	0.657029	-1.286044
8	0	-0.203027	0.660194	1.203232
7	0	2.392110	0.017562	-0.012597
8	0	0.964349	2.849398	0.031284
23	0	-1.237529	-0.462048	-0.130500
6	0	2.569910	-1.115725	0.036244
8	0	-2.963185	-0.714110	-0.465939
8	0	-0.492323	-1.861753	-0.007295
8	0	-2.748662	-0.138000	0.833725
6	0	2.721476	-2.549399	0.103932
1	0	3.287607	-2.826049	0.992048
1	0	1.710050	-2.960794	0.156861
1	0	3.227388	-2.916674	-0.787672

Ph

Zero-point correction= 0.100348 (Hartree/Particle)
Thermal correction to Energy= 0.104734
Thermal correction to Enthalpy= 0.105678
Thermal correction to Gibbs Free Energy= 0.072897
Sum of electronic and zero-point Energies= -232.217161
Sum of electronic and thermal Energies= -232.212774
Sum of electronic and thermal Enthalpies= -232.211830
Sum of electronic and thermal Free Energies= -232.244611

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Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	0.000000	0.695477	-1.204531
6	0	0.000000	-0.695477	-1.204531
6	0	0.000000	1.390968	-0.000013
6	0	0.000000	-1.390968	-0.000013
6	0	0.000000	0.695451	1.204552
1	0	0.000000	-1.236322	-2.141449
1	0	0.000000	2.472780	0.000025
6	0	0.000000	-0.695451	1.204552
1	0	0.000000	-2.472780	0.000025
1	0	0.000000	1.236349	2.141440
1	0	0.000000	-1.236349	2.141440
1	0	0.000000	1.236322	-2.141449

PhOH

Zero-point correction= 0.104530 (Hartree/Particle)
Thermal correction to Energy= 0.110039
Thermal correction to Enthalpy= 0.110984
Thermal correction to Gibbs Free Energy= 0.075555
Sum of electronic and zero-point Energies= -307.459324
Sum of electronic and thermal Energies= -307.453814
Sum of electronic and thermal Enthalpies= -307.452870
Sum of electronic and thermal Free Energies= -307.488298

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	0.066006	-0.128810	-0.044631
6	0	0.026894	-0.042051	1.342774
6	0	1.293544	-0.130607	-0.703734
1	0	-0.853512	-0.195034	-0.614488
6	0	2.477578	-0.045906	0.026923
6	0	1.202773	0.042673	2.078134
8	0	1.398656	-0.213334	-2.064285
1	0	-0.930378	-0.041396	1.846754
6	0	2.425080	0.040198	1.410692
1	0	3.419330	-0.048837	-0.503493
1	0	1.168968	0.109673	3.156390
1	0	0.517722	-0.266378	-2.445836
1	0	3.347492	0.105808	1.972176

CH_3CN

Zero-point correction= 0.045231 (Hartree/Particle)
Thermal correction to Energy= 0.048852
Thermal correction to Enthalpy= 0.049796
Thermal correction to Gibbs Free Energy= 0.021210
Sum of electronic and zero-point Energies= -132.752201

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Sum of electronic and thermal Energies= -132.748579
Sum of electronic and thermal Enthalpies= -132.747635
Sum of electronic and thermal Free Energies= -132.776221

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-0.000030	-1.176128	0.000000
6	0	0.000000	0.282026	0.000000
7	0	0.000042	1.431331	0.000000
1	0	1.022155	-1.551573	0.000000
1	0	-0.511134	-1.551566	0.885243
1	0	-0.511134	-1.551566	-0.885243