Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Mechanistic explorations on the decarboxylative allylation of amino esters via dual photoredox and palladium catalysis

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Computational Details

All of the calculations were performed with Gaussian 09 package. The M06-L functional with a mixed basis set of SDD for Pd and Ir and 6-31G(d) for other atoms was used for geometry optimizations and frequency calculations. Frequency outcomes were scrutinized to confirm stationary points as minima (no imaginary frequencies) or transition states (one imaginary frequency). Single-point energies were then calculated using the def2-TZVP basis set. The solvation effects were taken into consideration using the SMD model with CH_3CN as the solvent.

It should be emphasized that we have adopt the approximate approach proposed by Goddard Iii et al.[1] to correct free energies in the relevant figures. According to this approach, a correction of 1.89 kcal/mol applies to per component change for a reaction at 298.15K and 1 mol/L (i.e., a reaction from m- to n-components has an additional correction of (n – m) × 1.89 kcal/mol).

Activation barriers of Single Electron Transfer Processes

The SET processes can be described on the basis of the Marcus theory, [2,3] where the Gibbs free energy of activation ($\Delta G^{\neq}$), is related to the Gibbs free energy of electron transfer (ΔG) and the reorganization energy (λ) according to S1.

$$\Delta G^{\neq} = \frac{(\Delta G+\lambda)^2}{4\lambda} \quad \text{(S1)}$$

The reorganization energy λ including internal reorganization energy (λ_{int}) and external reorganization energy (λ_{ext}). Here, we used DFT calculation and continuum solvation models to estimate the reorganization energy of by the Buda method[4] where internal reorganization energy and external reorganization energy are not considered separately but as a parameter. Thus, the reorganization energy λ can be expressed as the sum of donor (λ_D) and acceptor (λ_A) reorganization energies, as expressed in S2.

$$\lambda = \lambda_i + \lambda_e = \lambda_D + \lambda_A \quad \text{(S2)}$$

$$\lambda_D = E(D^+ / D) - E(D^+ / D^+) \quad \text{(S3)}$$

$$\lambda_A = E(A^- / A) - E(A^- / A^-) \quad \text{(S4)}$$

Where D and A represent the cationic donor and the anionic acceptor, respectively (S6 and S7). $E(D^+ / D)$ and $E(D^+ / D^+)$ separately represent the energies of cationic donor at the optimized neutral and cationic geometries. $E(A^- / A)$ and $E(A^- / A^-)$ separately represent the energies of anionic acceptor at the optimized neutral and anionic geometries.

The reorganization energy calculation method discussed above is for self-exchange reaction. For cross reaction, such as $B + C = B^+ + C^-$, the reorganization energy λ is:

$$\lambda = \frac{1}{2}(\lambda_B + \lambda_C) \quad \text{(S5)}$$

Where λ_B and λ_C correspond to the reorganization energies of the two self-exchange reactions of B and C, respectively.

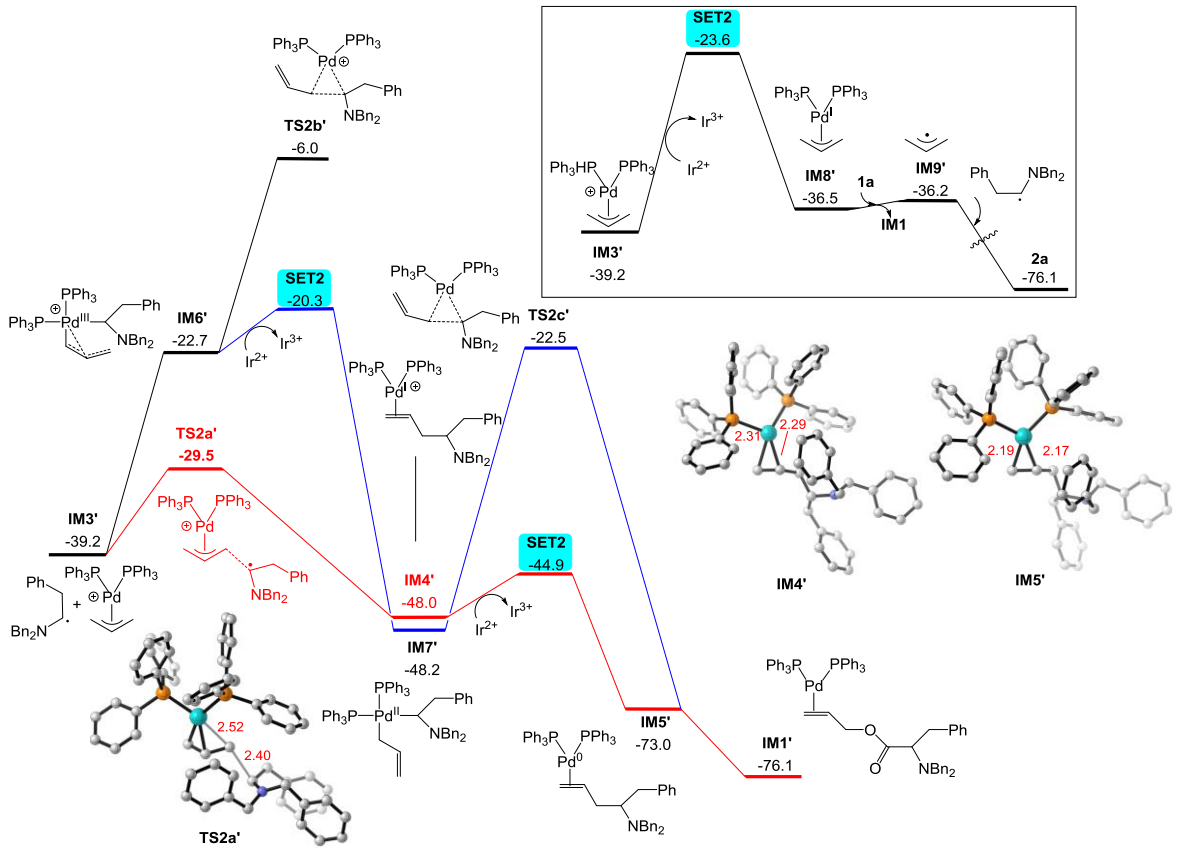

Fig. S1. Free energy profiles for the allylation of N,N-dibenzyl phenyalanine via inner-sphere pathway, outer-sphere pathway and radical coupling pathway.

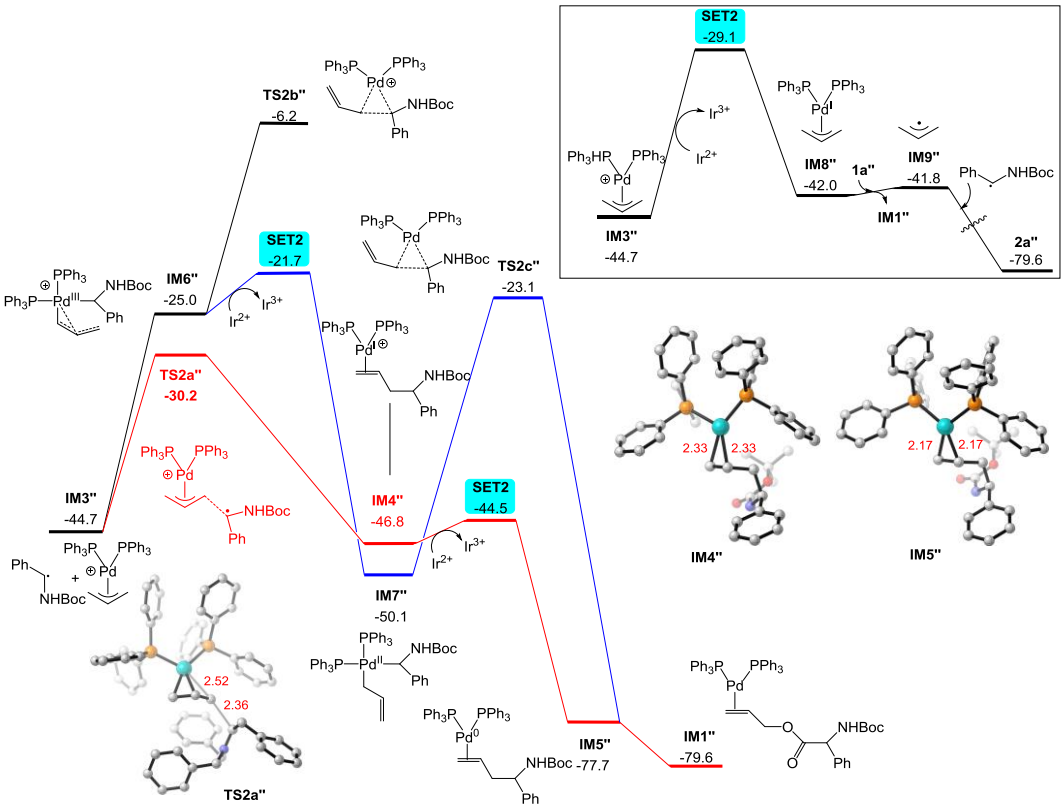

Fig. S2. Free energy profiles for the allylation of N-Boc phenylglycine via inner-sphere pathway, outer-sphere pathway, and radical coupling pathway.

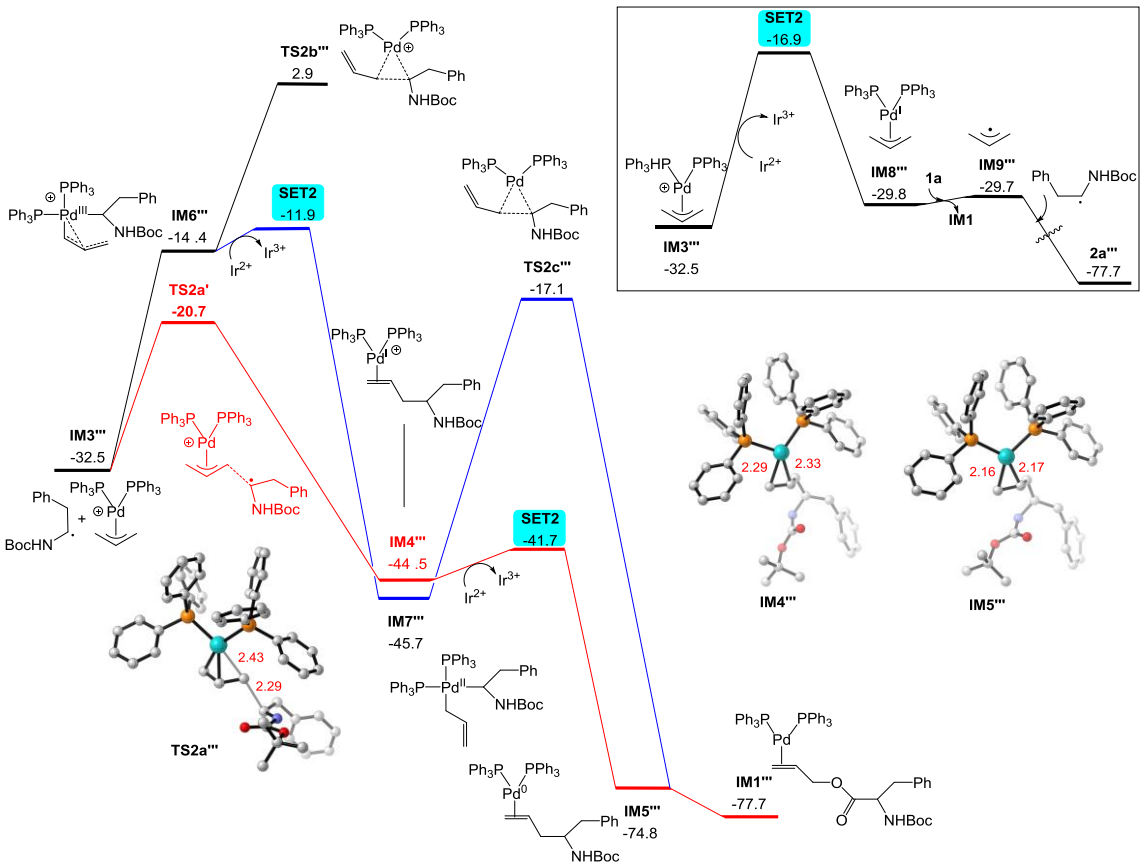

Fig. S3. Free energy profiles for the allylation of N-Boc phenylalanine via inner-sphere pathway, outer-sphere pathway and radical coupling pathway.

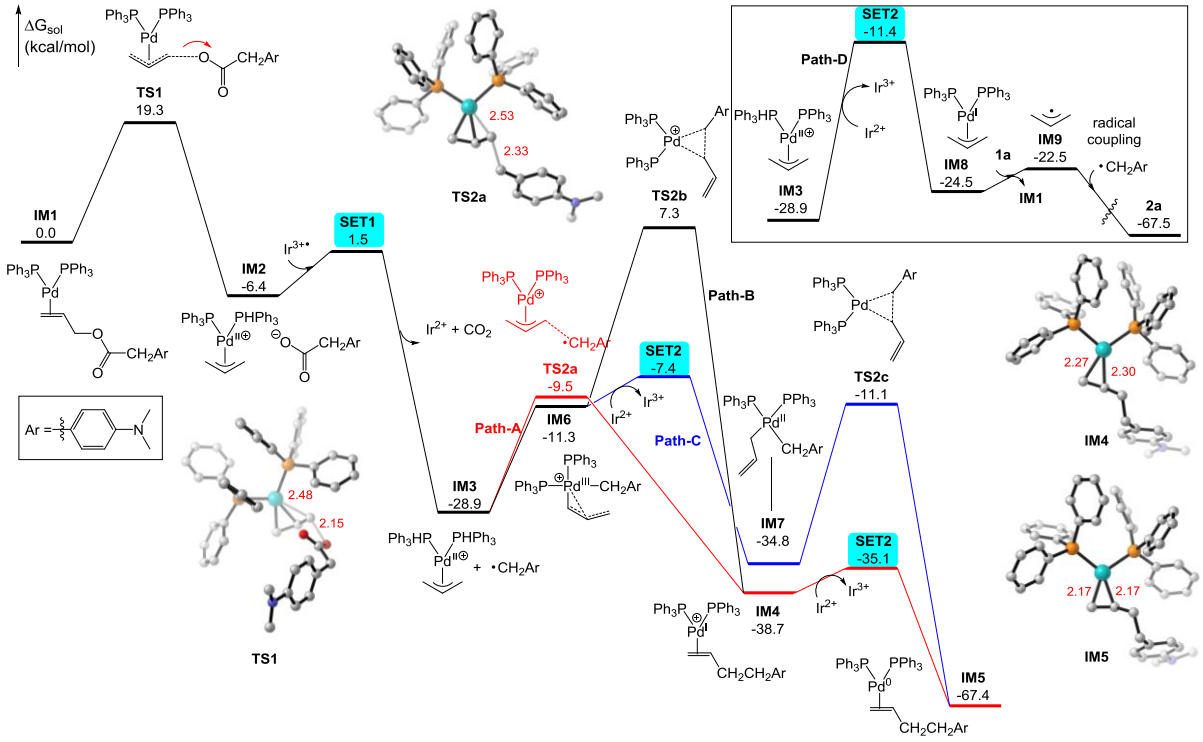

Fig. S4. Free energy profiles for the decarboxylative allylation of amino esters with other DFT functional and basis sets. (PBE0-D3(BJ)) functional with a mixed basis set of SDD for Pd and Ir and 6-311++G(d,p) for other atoms)

REFERENCES

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Energies and Cartesian Coordinates for the Optimized Structures

IM1

SCF energy in MeCN: -2912.025618 a.u.

Free energy in MeCN: -2911.286045 a.u.

C	-1.957715	-0.433096	-1.208768
H	-1.976667	0.188966	-0.303842
H	-1.909756	-1.479160	-0.883642
C	-0.849251	-0.054649	-2.126578
H	-0.681179	-0.741749	-2.960423
C	-0.428211	1.286020	-2.258888
H	-0.926588	2.074900	-1.690100
P	1.538155	-1.781884	0.032175
C	2.157578	-3.030915	-1.156867
C	2.064925	-2.745690	-2.523875
C	2.724026	-4.249644	-0.756396
C	2.518854	-3.659099	-3.472814
H	1.635938	-1.788791	-2.830803
C	3.174562	-5.162640	-1.703987
H	2.815089	-4.477563	0.306184
C	3.071820	-4.869062	-3.063407
H	2.443819	-3.422197	-4.532789
H	3.609035	-6.107392	-1.380932
H	3.429756	-5.583936	-3.802519
C	0.041436	-2.537700	0.768387
C	-0.744339	-1.727236	1.603713
C	-0.421180	-3.816070	0.443350
C	-1.955546	-2.186719	2.105682
H	-0.412536	-0.709344	1.824963
C	-1.642031	-4.270793	0.939339
H	0.162930	-4.456109	-0.215988
C	-2.410913	-3.459540	1.767632
H	-2.568040	-1.534895	2.724891
H	-1.996512	-5.263440	0.665064
H	-3.374493	-3.807624	2.134707
Pd	0.979954	0.272580	-1.002290
O	-3.237852	-0.248209	-1.895498
C	-4.317764	-0.480428	-1.130111
O	-4.268217	-0.789208	0.042873
C	2.785359	-1.914052	1.376587
C	2.440472	-1.921040	2.732640
C	4.145615	-1.901245	1.033544
C	3.428431	-1.924343	3.714269
H	1.392557	-1.929867	3.029353
C	5.130768	-1.897966	2.014627
H	4.437252	-1.910161	-0.015927
C	4.774945	-1.912177	3.361815
H	3.138472	-1.931565	4.764121
H	6.179790	-1.887039	1.721175
H	5.544061	-1.911461	4.132988
P	2.561614	1.772680	-0.160267
C	2.375104	3.575483	-0.461789
C	2.045933	3.980200	-1.762460
C	2.545272	4.552109	0.526141
C	1.903329	5.327857	-2.071711
H	1.892737	3.221734	-2.531739
C	2.391422	5.901954	0.217278
H	2.794281	4.255013	1.545059
C	2.072782	6.292821	-1.080242
H	1.647405	5.626007	-3.087165
H	2.522673	6.651595	0.996165
H	1.949964	7.348188	-1.318253
C	2.574371	1.689946	1.670757
C	3.713099	1.524809	2.463755
C	1.320323	1.764755	2.298559
C	3.601442	1.454104	3.851284
H	4.693880	1.427451	2.000597
C	1.212071	1.702089	3.682564
H	0.423307	1.874821	1.684358
C	2.356439	1.549874	4.464722
H	4.497795	1.311354	4.453718
H	0.231593	1.769042	4.152007
H	2.274185	1.492882	5.548940
C	4.302206	1.497362	-0.665442
C	5.342265	2.372676	-0.326239
C	4.595083	0.368442	-1.437505
C	6.648630	2.102099	-0.720110
H	5.122510	3.273845	0.248281
C	5.901712	0.098192	-1.836294
H	3.776816	-0.298852	-1.721507
C	6.930879	0.961348	-1.471032
H	7.450367	2.786008	-0.445506
H	6.113548	-0.786484	-2.435220
H	7.953854	0.753169	-1.780571
H	0.038518	1.623003	-3.185132

C	-5.586583	-0.351135	-1.950825
H	-5.413567	0.369392	-2.758555
H	-5.711741	-1.324010	-2.454165
C	-6.812440	0.002011	-1.160790
C	-7.249929	-0.784929	-0.091238
C	-7.574573	1.125540	-1.481128
C	-8.385601	-0.458812	0.634478
H	-6.679800	-1.668109	0.188797
C	-8.718511	1.465931	-0.769541
H	-7.270140	1.755880	-2.318028
C	-9.142447	0.688119	0.323511
H	-8.685035	-1.106170	1.454599
H	-9.278777	2.348026	-1.067841
N	-10.255242	1.043496	1.075631
C	-10.784819	0.092559	2.021814
H	-11.644083	0.536242	2.531894
H	-11.109720	-0.853974	1.554594
H	-10.037693	-0.153271	2.787233
C	-11.150304	2.047990	0.556303
H	-11.970917	2.196069	1.263243
H	-10.636354	3.011367	0.442219
H	-11.581673	1.780628	-0.424469

1a

SCF energy in MeCN: -710.976398 a.u.

Free energy in MeCN: -710.742974 a.u.

C	-3.062221	0.063590	-0.095300
C	-2.285458	-1.053669	0.271594
C	-0.950190	-0.914892	0.617857
C	-0.323086	0.334347	0.626667
C	-1.095262	1.441334	0.276000
C	-2.434790	1.323309	-0.071433
H	-2.727848	-2.046064	0.287939
H	-0.378075	-1.802624	0.880624
H	-0.640345	2.433083	0.281449
H	-2.991170	2.220380	-0.328044
N	-4.390094	-0.074725	-0.475693
C	-5.205918	1.110404	-0.579998
H	-6.217027	0.824467	-0.881297
H	-5.273228	1.676058	0.366024
H	-4.813192	1.790091	-1.347262
C	-5.054684	-1.331536	-0.228732
H	-6.085842	-1.267428	-0.585881
H	-4.566391	-2.147174	-0.776913
H	-5.074825	-1.609760	0.839596
C	1.111275	0.499192	1.032581
C	2.104097	-0.306615	0.225435
H	1.412374	1.552975	1.004507
H	1.262642	0.188389	2.079621
O	1.877844	-1.328471	-0.382930
O	3.332728	0.253566	0.311652
C	4.374985	-0.483003	-0.362101
H	4.195065	-0.456696	-1.444201
H	4.304764	-1.534528	-0.050299
C	5.678072	0.126306	0.004552
H	5.862439	0.242871	1.074090
C	6.604817	0.487998	-0.879816
H	6.440535	0.386648	-1.952345
H	7.566383	0.891052	-0.571366

2a

SCF energy in MeCN: -522.35349 a.u.

Free energy in MeCN: -522.129713 a.u.

C	-1.099068	-1.057211	0.173688
C	0.272270	-0.825895	0.204722
C	0.807137	0.460859	0.136952
C	-0.105767	1.515467	0.028512
C	-1.475730	1.308850	-0.003848
C	-2.011875	0.007906	0.081785
H	-1.456853	-2.082396	0.217646
H	0.934519	-1.688184	0.273716
H	0.270762	2.537563	-0.040329
H	-2.134526	2.168177	-0.098586
N	-3.384563	-0.209491	0.083885
C	-3.866757	-1.557167	-0.096869
H	-4.959785	-1.552813	-0.078723
H	-3.536940	-2.013393	-1.047006
H	-3.526728	-2.206386	0.720150
C	-4.253250	0.873917	-0.307915
H	-5.290967	0.532148	-0.273426
H	-4.162650	1.719133	0.386249
H	-4.046369	1.250893	-1.325021
C	2.285748	0.751035	0.165685
H	2.556022	1.365330	-0.707402
H	2.517432	1.386921	1.036033
C	3.200831	-0.470605	0.199821
H	3.008147	-1.109841	-0.674107

H	2.951047	-1.076310	1.086285
C	4.644720	-0.094593	0.243843
H	4.948606	0.523305	1.094414
C	5.556483	-0.433190	-0.666142
H	5.296063	-1.042170	-1.531960
H	6.595707	-0.121776	-0.586535

Benzyl radical

SCF energy in MeCN: -404.978152 a.u.

Free energy in MeCN: -404.825194 a.u.

C	0.599132	-0.000014	-0.063029
C	-0.135998	1.208387	-0.035180
C	-1.513332	1.205100	-0.003704
C	-2.270907	-0.000013	0.010195
C	-1.513331	-1.205118	-0.003483
C	-0.135991	-1.208414	-0.034952
H	0.386496	2.161686	-0.035239
H	-2.046273	2.155906	0.017520
H	-2.046258	-2.155925	0.017998
H	0.386510	-2.161706	-0.034767
N	1.981698	0.000018	-0.127483
C	2.696184	-1.239298	0.060264
H	3.768485	-1.054201	-0.040482
H	2.515273	-1.694548	1.048868
H	2.414132	-1.975015	-0.703763
C	2.696092	1.239336	0.060706
H	3.768451	1.054214	-0.039353
H	2.414526	1.975104	-0.703458
H	2.514564	1.694525	1.049216
C	-3.668766	0.000001	0.043209
H	-4.233123	0.929500	0.055685
H	-4.233158	-0.929465	0.055997

Allyl radical

SCF energy in MeCN: -117.283633 a.u.

Free energy in MeCN: -117.242817 a.u.

C	1.226662	0.195377	-0.000006
H	1.293646	1.282485	-0.000003
H	2.161278	-0.359098	0.000166
C	-0.000001	-0.442670	-0.000045
H	-0.000030	-1.535291	-0.000019
C	-1.226653	0.195382	0.000011
H	-1.293686	1.282489	-0.000036
H	-2.161253	-0.359119	0.000128

CO_2

SCF energy in MeCN: -188.653132 a.u.

Free energy in MeCN: -188.661954

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.168679
O	0.000000	0.000000	-1.168679

TS1

SCF energy in MeCN: -2912.00249 a.u.

Free energy in MeCN: -2911.263517 a.u.

C	-0.311124	-1.863225	-2.314904
H	-0.818353	-1.561582	-1.405972
H	0.037811	-2.890832	-2.371915
C	0.126344	-0.904852	-3.244788
H	0.728573	-1.218897	-4.098180
C	-0.147426	0.468754	-3.034251
H	-1.061757	0.747105	-2.503219
P	2.261535	-1.495293	0.152022
C	3.943314	-1.999522	-0.355211
C	4.341440	-1.731779	-1.670234
C	4.843722	-2.634325	0.511936
C	5.610273	-2.095708	-2.114503
H	3.640110	-1.227847	-2.340478
C	6.110657	-2.996874	0.067658
H	4.548496	-2.837066	1.541756
C	6.495047	-2.728118	-1.245882
H	5.908131	-1.880867	-3.139190
H	6.802550	-3.489599	0.748669
H	7.488519	-3.010987	-1.590031
C	1.325830	-3.049482	0.394002
C	-0.053795	-2.938658	0.622874
C	1.889911	-4.322552	0.261626
C	-0.850584	-4.072859	0.720756
H	-0.529464	-1.957890	0.676134
C	1.087978	-5.457860	0.360497
H	2.955439	-4.433286	0.065038
C	-0.280127	-5.337079	0.589723
H	-1.922943	-3.952964	0.866776
H	1.537754	-6.442957	0.247235

H	-0.903674	-6.227394	0.647918	C	5.107496	2.714991	0.181794
Pd	1.175127	-0.078227	-1.432130	H	3.853120	1.162896	-0.653732
O	-2.352296	-2.459483	-2.658908	C	5.135271	3.953134	0.816709
C	-3.024921	-2.099545	-1.637528	H	3.963731	5.595669	1.579183
O	-2.621668	-1.471731	-0.632350	H	6.036126	2.197789	-0.055332
C	2.514848	-0.876264	1.862942	H	6.087856	4.409105	1.081760
C	1.549317	-1.067331	2.858289	H	0.202964	1.210229	-3.752584
C	3.644290	-0.104252	2.166759	C	-4.494869	-2.575710	-1.661706
C	1.714735	-0.507172	4.121097	H	-4.811562	-2.681048	-2.705763
H	0.660580	-1.660338	2.651652	H	-4.473525	-3.597854	-1.250318
C	3.799525	0.469730	3.424559	C	-5.446772	-1.718958	-0.888442
H	4.419685	0.038742	1.416513	C	-5.378265	-1.619684	0.504874
C	2.834471	0.268320	4.408096	C	-6.432621	-0.965065	-1.525130
H	0.952155	-0.670317	4.881018	C	-6.239245	-0.805923	1.226752
H	4.683421	1.071090	3.633945	H	-4.621538	-2.194502	1.037782
H	2.955561	0.713057	5.394526	C	-7.306222	-0.142653	-0.821997
P	1.120586	1.974609	-0.339416	H	-6.526418	-1.023926	-2.610536
C	0.229384	3.327507	-1.193055	C	-7.218220	-0.029330	0.576556
C	0.924495	4.137972	-2.102108	H	-6.147712	-0.776842	2.309732
C	-1.155551	3.486161	-1.067799	H	-8.062302	0.411205	-1.372353
C	0.250158	5.090501	-2.857467	N	-8.056113	0.827160	1.291907
H	2.002927	4.023108	-2.215867	C	-8.136360	0.664506	2.722684
C	-1.827371	4.439078	-1.828992	H	-8.836092	1.400686	3.128428
H	-1.715928	2.863539	-0.371165	H	-8.473203	-0.341592	3.032306
C	-1.128792	5.243387	-2.724390	H	-7.160650	0.846357	3.190881
H	0.805129	5.716425	-3.554586	C	-9.221323	1.352953	0.624398
H	-2.904360	4.550519	-1.717799	H	-9.772125	1.995930	1.316860
H	-1.656215	5.987789	-3.318203	H	-8.931818	1.968937	-0.236371
C	0.135670	1.684527	1.174130	H	-9.908316	0.568613	0.257786
C	0.385841	2.275128	2.415530				
C	-0.944063	0.794423	1.046030	**IM2**			
C	-0.439827	1.993808	3.501910	SCF energy in MeCN: -2911.286045 a.u.			
H	1.241274	2.936949	2.544766	Free energy in MeCN: -2911.296328 a.u.			
C	-1.769916	0.520708	2.131703				
H	-1.155482	0.298765	0.094557	C	2.036967	-1.502320	-3.057732
C	-1.518035	1.122973	3.362937	H	1.161087	-1.414034	-3.702005
H	-0.227701	2.450670	4.467987	H	2.404519	-2.504226	-2.834215
H	-2.603702	-0.166394	1.994600	C	2.894159	-0.385240	-2.953405
H	-2.156920	0.907629	4.218274	H	3.916339	-0.482345	-2.581399
C	2.683642	2.782364	0.143072	C	2.286423	0.881816	-3.071117
C	2.724390	4.043166	0.755319	H	1.385985	0.983124	-3.680331
C	3.886727	2.135264	-0.154741	P	0.645966	-1.924156	0.031250
C	3.942649	4.619171	1.098223	C	1.925535	-3.183667	0.418131
H	1.794691	4.577964	0.951262	C	3.219580	-3.032141	-0.090917

C	1.641628	-4.298864	1.217565	H	4.501804	5.019360	-1.902946
C	4.210711	-3.969612	0.191980	H	0.304503	5.521993	-2.687032
H	3.441681	-2.160209	-0.709873	H	2.656956	6.262571	-3.015404
C	2.628572	-5.236898	1.497587	C	0.045544	2.103160	1.183283
H	0.640228	-4.430070	1.627269	C	0.163055	2.445066	2.535830
C	3.914999	-5.074481	0.984527	C	-1.221692	2.143016	0.578137
H	5.212777	-3.837558	-0.212564	C	-0.950702	2.867989	3.256022
H	2.393238	-6.099667	2.118331	H	1.122553	2.369328	3.043041
H	4.685482	-5.811886	1.203216	C	-2.325375	2.587409	1.301217
C	-0.752270	-2.898675	-0.640577	H	-1.351943	1.770450	-0.441388
C	-0.974226	-2.897996	-2.020809	C	-2.193758	2.958502	2.636628
C	-1.612605	-3.635054	0.186353	H	-0.840845	3.122853	4.309737
C	-2.022881	-3.632733	-2.568511	H	-3.298820	2.613653	0.814124
H	-0.366314	-2.270791	-2.667386	H	-3.065383	3.291546	3.199913
C	-2.659881	-4.367688	-0.363179	C	2.877900	1.494358	1.329192
H	-1.482591	-3.610837	1.268328	C	3.365726	2.590676	2.056716
C	-2.864807	-4.371442	-1.742159	C	3.470630	0.244396	1.526362
H	-2.191348	-3.597404	-3.643623	C	4.409171	2.429808	2.962158
H	-3.324473	-4.931215	0.289945	H	2.925964	3.576611	1.905170
H	-3.692761	-4.936021	-2.167860	C	4.511082	0.079106	2.437014
Pd	1.387558	-0.202508	-1.401232	H	3.110409	-0.605284	0.945625
O	-0.738567	-0.329771	-4.043729	C	4.981587	1.172777	3.157196
C	-1.393215	0.095859	-3.070938	H	4.778234	3.289678	3.518788
O	-0.950654	0.365529	-1.907390	H	4.953566	-0.906973	2.575238
C	0.031345	-1.435500	1.677491	H	5.797416	1.050545	3.867825
C	-1.251642	-0.876211	1.760922	H	2.854749	1.788653	-2.869766
C	0.821049	-1.506613	2.830559	C	-2.909304	0.324189	-3.286910
C	-1.746085	-0.431797	2.980429	H	-3.021903	1.224466	-3.908283
H	-1.859315	-0.777650	0.860340	H	-3.266557	-0.504524	-3.915264
C	0.326621	-1.046076	4.048896	C	-3.725793	0.448752	-2.037099
H	1.822465	-1.934276	2.780769	C	-3.744110	-0.584589	-1.093210
C	-0.958140	-0.516052	4.127323	C	-4.493939	1.574293	-1.743770
H	-2.741315	0.009903	3.024558	C	-4.460651	-0.493652	0.090036
H	0.950069	-1.106482	4.939549	H	-3.164064	-1.487286	-1.285493
H	-1.342282	-0.154810	5.080270	C	-5.226158	1.687130	-0.562691
P	1.487615	1.636301	0.146592	H	-4.529160	2.396534	-2.460672
C	1.862847	3.193031	-0.752199	C	-5.196950	0.665549	0.402274
C	3.185942	3.607549	-0.956444	H	-4.428975	-1.330719	0.785364
C	0.832768	3.892352	-1.392596	H	-5.812051	2.587313	-0.393156
C	3.467795	4.708461	-1.760968	N	-5.828476	0.805753	1.640473
H	4.004951	3.062777	-0.487971	C	-6.123752	-0.392019	2.392301
C	1.118743	4.990015	-2.198316	H	-6.661042	-0.117864	3.304670
H	-0.200800	3.572831	-1.267435	H	-6.739712	-1.117064	1.831764
C	2.435426	5.404113	-2.383980	H	-5.202488	-0.904736	2.697473

C	-6.711823	1.929506	1.827913
H	-7.093523	1.919093	2.852973
H	-6.167112	2.872743	1.688369
H	-7.574782	1.937384	1.137022

carboxylate anion

SCF energy in MeCN: -593.635425 a.u.

Free energy in MeCN: -593.47927 a.u.

O	-4.469788	0.460955	-0.678452
C	-3.516042	-0.215891	-0.245123
O	-3.223916	-1.423933	-0.408327
C	-2.538008	0.572741	0.734382
H	-2.795672	1.640469	0.730446
H	-2.779970	0.187817	1.738271
C	-1.084163	0.389730	0.470134
C	-0.490451	-0.883128	0.464836
C	-0.239237	1.467951	0.191316
C	0.861558	-1.059132	0.202846
H	-1.140118	-1.739397	0.631128
C	1.119025	1.308446	-0.074414
H	-0.658907	2.476349	0.187586
C	1.701556	0.032054	-0.083715
H	1.265865	-2.069728	0.218469
H	1.720401	2.192816	-0.275955
N	3.070802	-0.155322	-0.390653
C	3.670069	-1.390794	0.049115
H	4.733340	-1.387695	-0.216113
H	3.583126	-1.565734	1.139807
H	3.209071	-2.247244	-0.457101
C	3.921168	1.002299	-0.285110
H	4.950719	0.715285	-0.527141
H	3.616137	1.771224	-1.005544
H	3.917180	1.471267	0.719357

Π-allylpalladium cation

SCF energy in MeCN: -2318.239469 a.u.

Free energy in MeCN: -2317.687917 a.u.

C	-1.094812	0.380844	-3.451671
H	-1.074205	1.471393	-3.489250
H	-2.074600	-0.075146	-3.575499
C	0.072289	-0.342004	-3.751955
H	-0.007578	-1.403281	-3.995510
C	1.328601	0.184072	-3.391015
H	1.502098	1.261964	-3.414522
P	-1.788444	0.006602	-0.122304
C	-3.151372	-0.918282	-0.909700
C	-2.834656	-2.013498	-1.724945
C	-4.494332	-0.611755	-0.668354
C	-3.842022	-2.794905	-2.281468
H	-1.785457	-2.248632	-1.923595
C	-5.500852	-1.386570	-1.238412
H	-4.756481	0.239033	-0.040563
C	-5.177772	-2.478908	-2.039700
H	-3.585314	-3.646218	-2.908503
H	-6.543118	-1.135958	-1.052723
H	-5.967675	-3.082760	-2.481224
C	-2.447055	1.668609	0.224819
C	-2.205668	2.695502	-0.696790
C	-3.219791	1.941887	1.361211
C	-2.728191	3.968096	-0.494018
H	-1.593451	2.491576	-1.576770
C	-3.738565	3.217566	1.564417
H	-3.410469	1.155548	2.090847
C	-3.494959	4.230461	0.639234
H	-2.535445	4.755912	-1.219371
H	-4.337458	3.420354	2.449784
H	-3.903452	5.225632	0.801710
Pd	0.078397	0.046128	-1.600603
C	-1.632961	-0.792258	1.512223
C	-0.998266	-0.117532	2.565006
C	-2.070549	-2.107781	1.712739
C	-0.794838	-0.753832	3.785324
H	-0.686056	0.918675	2.440748
C	-1.870708	-2.735819	2.938493
H	-2.577276	-2.644850	0.912242
C	-1.225687	-2.064661	3.973946
H	-0.305489	-0.215181	4.594801
H	-2.225934	-3.754233	3.084300
H	-1.069235	-2.558205	4.930927
P	1.877801	-0.007993	-0.078783
C	3.508609	0.374145	-0.802800
C	4.223244	-0.639250	-1.457173
C	4.020486	1.676029	-0.791472
C	5.433792	-0.353968	-2.078449
H	3.836185	-1.658972	-1.467542
C	5.232481	1.956381	-1.418013

H	3.480560	2.471334	-0.278665
C	5.939885	0.944842	-2.061103
H	5.985610	-1.149342	-2.575024
H	5.627270	2.970094	-1.395381
H	6.888040	1.166150	-2.546515
C	1.642526	1.268977	1.201121
C	2.127586	1.143860	2.507048
C	0.910462	2.411107	0.850156
C	1.874897	2.141257	3.443857
H	2.675213	0.251761	2.805925
C	0.654089	3.405633	1.789222
H	0.517173	2.507666	-0.164740
C	1.134822	3.268584	3.089866
H	2.251216	2.033359	4.459378
H	0.071437	4.280108	1.505729
H	0.932511	4.040165	3.829713
C	2.122082	-1.608762	0.744274
C	3.276916	-1.883798	1.493165
C	1.147814	-2.602562	0.602761
C	3.426390	-3.116915	2.117548
H	4.067529	-1.137096	1.569693
C	1.301192	-3.836533	1.227566
H	0.265874	-2.403766	-0.007770
C	2.436406	-4.091229	1.990597
H	4.323380	-3.323129	2.697568
H	0.535059	-4.600670	1.111314
H	2.560537	-5.056632	2.476783
H	2.223298	-0.429873	-3.469554

IM4

SCF energy in MeCN: -2723.251845 a.u.

Free energy in MeCN: -2722.520969 a.u.

Pd	-0.243666	0.588049	-0.446489
P	-2.410270	1.366771	0.020861
P	-0.327172	-1.699084	0.076057
C	-3.666107	0.158578	-0.507430
C	-4.823002	-0.120955	0.229634
C	-3.401893	-0.575317	-1.671883
C	-5.692700	-1.122038	-0.195407
H	-5.030787	0.425202	1.149392
C	-4.272309	-1.573587	-2.094818
H	-2.489046	-0.372812	-2.236039
C	-5.417016	-1.852923	-1.350432
H	-6.587529	-1.338925	0.385153
H	-4.041476	-2.146789	-2.991178
H	-6.094590	-2.642774	-1.668563
C	-2.730122	1.697659	1.778162
C	-3.747918	2.570253	2.191072
C	-1.973330	1.021692	2.743145
C	-4.004451	2.751280	3.545999
H	-4.336866	3.108433	1.448608
C	-2.239970	1.199140	4.096922
H	-1.172504	0.351501	2.427226
C	-3.254146	2.064146	4.499146
H	-4.794727	3.430621	3.859105
H	-1.649770	0.662110	4.837120
H	-3.458908	2.208899	5.558088
C	-2.815333	2.913743	-0.843279
C	-3.486728	2.906895	-2.072612
C	-2.332705	4.129637	-0.333791
C	-3.679253	4.094413	-2.771904
H	-3.873349	1.972061	-2.476412
C	-2.531936	5.312726	-1.034588
H	-1.811024	4.147008	0.624189
C	-3.201958	5.297321	-2.257435
H	-4.213293	4.079716	-3.719941
H	-2.163925	6.251230	-0.625131
H	-3.355771	6.224417	-2.805672
C	-1.211843	-2.250545	1.564472
C	-0.566894	-2.374258	2.801215
C	-2.605077	-2.401931	1.499238
C	-1.305719	-2.642757	3.950480
H	0.515634	-2.268479	2.865096
C	-3.336315	-2.670560	2.650510
H	-3.116489	-2.321999	0.539904
C	-2.689614	-2.785016	3.879605
H	-0.794820	-2.747912	4.905857
H	-4.416357	-2.789344	2.583028
H	-3.262787	-2.993817	4.780555
C	-0.868943	-2.802929	-1.265144
C	-0.647939	-2.387618	-2.585818
C	-1.456415	-4.051246	-1.030717
C	-1.011946	-3.202228	-3.652200
H	-0.192251	-1.411250	-2.770129
C	-1.827640	-4.861604	-2.100707
H	-1.624439	-4.390292	-0.009522
C	-1.608219	-4.439299	-3.409574

H	-0.835016	-2.871049	-4.673638
H	-2.285525	-5.829955	-1.909343
H	-1.899090	-5.075255	-4.243210
C	1.437931	-2.098610	0.325460
C	2.043962	-3.214880	-0.261955
C	2.229790	-1.192513	1.051799
C	3.414254	-3.420797	-0.119980
H	1.446838	-3.921483	-0.836215
C	3.595878	-1.403590	1.193913
H	1.765185	-0.305498	1.490894
C	4.189327	-2.518194	0.602404
H	3.876730	-4.291984	-0.579917
H	4.203182	-0.689778	1.748083
H	5.262087	-2.675113	0.698324
C	6.805728	0.964361	0.308699
C	6.582521	-0.012837	-0.685332
C	5.573514	0.148024	-1.621494
C	4.749518	1.279317	-1.637870
C	4.979060	2.249457	-0.654907
C	5.973645	2.106223	0.299632
H	7.210601	-0.898427	-0.734407
H	5.427872	-0.628227	-2.374556
H	4.371046	3.155631	-0.646937
H	6.119959	2.895504	1.031802
N	7.793945	0.810602	1.254611
C	8.084611	1.888288	2.171849
H	8.902225	1.589709	2.830495
H	7.215953	2.124648	2.801620
H	8.383799	2.809449	1.648997
C	8.691271	-0.317807	1.176473
H	9.397069	-0.275953	2.008078
H	9.266346	-0.330692	0.237787
H	8.144254	-1.268618	1.249058
C	3.653031	1.421813	-2.644543
C	2.285608	0.851560	-2.169636
H	2.450371	-0.189658	-1.848529
C	1.699773	1.664182	-1.060766
H	2.276986	1.689175	-0.131424
C	0.643948	2.540267	-1.195947
H	0.164555	2.703643	-2.163594
H	0.436516	3.288389	-0.432543
H	1.593219	0.831433	-3.023473
H	3.506749	2.476046	-2.916606
H	3.920209	0.889866	-3.566994

IM5

SCF energy in MeCN: -2723.402061 a.u.

Free energy in MeCN: -2722.671256 a.u.

Pd	0.331379	-0.800175	-0.360185
P	2.622453	-1.124300	0.038460
P	-0.167224	1.467639	-0.024474
C	3.715384	0.277789	-0.422388
C	4.766488	0.732250	0.381044
C	3.427892	0.964651	-1.610007
C	5.500903	1.857399	0.012646
H	5.001951	0.214064	1.310423
C	4.163098	2.086262	-1.980183
H	2.599310	0.624598	-2.233758
C	5.197698	2.540423	-1.162773
H	6.310969	2.205883	0.652391
H	3.914179	2.616209	-2.898765
H	5.765540	3.426472	-1.442018
C	3.049603	-1.377714	1.805476
C	4.067625	-2.235558	2.239481
C	2.341126	-0.633399	2.758521
C	4.370916	-2.341201	3.594630
H	4.630408	-2.820718	1.512318
C	2.654961	-0.729862	4.110129
H	1.539727	0.030505	2.431384
C	3.669271	-1.586668	4.531885
H	5.164274	-3.013390	3.918706
H	2.098000	-0.136020	4.833593
H	3.911470	-1.668788	5.590415
C	3.449939	-2.550747	-0.767199
C	4.627748	-2.450450	-1.515269
C	2.848206	-3.809526	-0.623642
C	5.187997	-3.581877	-2.106066
H	5.114185	-1.483103	-1.636274
C	3.417865	-4.939426	-1.197539
H	1.921876	-3.892332	-0.053625
C	4.588990	-4.827611	-1.946083
H	6.102918	-3.487367	-2.689291
H	2.941816	-5.910259	-1.069221
H	5.030613	-5.710318	-2.405826
C	0.607241	2.328837	1.397932
C	-0.049810	2.456699	2.627929
C	1.959306	2.699445	1.318770

C	0.626209	2.936419	3.747373
H	-1.100377	2.179863	2.712046
C	2.629043	3.184042	2.436406
H	2.490996	2.605757	0.371169
C	1.967536	3.299257	3.657577
H	0.096905	3.031158	4.694707
H	3.677475	3.466993	2.351395
H	2.495280	3.670991	4.534421
C	0.267292	2.529524	-1.453177
C	0.253226	1.934871	-2.721694
C	0.590523	3.887623	-1.349193
C	0.552826	2.677801	-3.859346
H	0.020002	0.869856	-2.798085
C	0.899092	4.629383	-2.486408
H	0.605242	4.365162	-0.369545
C	0.879286	4.027721	-3.742770
H	0.538597	2.200443	-4.838048
H	1.152880	5.684120	-2.390577
H	1.121512	4.609955	-4.630375
C	-1.957171	1.817878	0.211288
C	-2.615803	2.900077	-0.381655
C	-2.701070	0.924290	0.996602
C	-3.982834	3.087259	-0.187712
H	-2.060338	3.599484	-1.005155
C	-4.062158	1.119792	1.201890
H	-2.198209	0.060306	1.435569
C	-4.705872	2.202393	0.605627
H	-4.483819	3.929828	-0.662408
H	-4.630069	0.409115	1.802480
H	-5.776862	2.344885	0.746072
C	-6.611414	-1.442093	0.257169
C	-6.430357	-0.489485	-0.762338
C	-5.420936	-0.637230	-1.704098
C	-4.549186	-1.728029	-1.691296
C	-4.730979	-2.670632	-0.675663
C	-5.725959	-2.535840	0.284382
H	-7.073653	0.385017	-0.818573
H	-5.299074	0.134094	-2.467091
H	-4.062965	-3.532097	-0.626857
H	-5.813269	-3.294495	1.057695
N	-7.631891	-1.312318	1.199634
C	-7.552025	-2.114810	2.397374
H	-8.405628	-1.883483	3.040160
H	-6.624796	-1.944626	2.974874
H	-7.602888	-3.183262	2.155835
C	-8.276402	-0.027861	1.326108
H	-9.039951	-0.085352	2.106727
H	-8.781456	0.250003	0.393184
H	-7.576697	0.788846	1.586204
C	-3.418906	-1.833439	-2.673547
C	-2.149592	-1.091038	-2.209146
H	-2.406442	-0.029109	-2.057768
C	-1.562342	-1.675997	-0.952945
H	-2.228072	-1.637187	-0.085455
C	-0.573020	-2.675016	-0.968659
H	-0.143129	-3.015611	-1.914261
H	-0.499548	-3.390593	-0.148502
H	-1.402929	-1.126817	-3.017715
H	-3.162564	-2.889721	-2.842191
H	-3.730765	-1.424248	-3.645766

IM6

SCF energy in MeCN: -2723.215546 a.u.

Free energy in MeCN: -2722.484727 a.u.

Pd	-0.047629	0.053601	-1.364937
P	-1.345270	1.553832	0.010366
P	-0.184329	-1.983652	0.094761
C	-0.830474	1.663667	1.760542
C	-1.690740	2.050656	2.794318
C	0.491151	1.321194	2.069506
C	-1.233387	2.087197	4.108144
H	-2.728889	2.298296	2.578999
C	0.949175	1.358935	3.383345
H	1.155512	0.988973	1.273020
C	0.084295	1.740549	4.406412
H	-1.912406	2.380830	4.906633
H	1.976839	1.070325	3.603988
H	0.431350	1.762473	5.437541
C	-3.116700	1.105865	0.004456
C	-4.104373	2.009855	0.423958
C	-3.508309	-0.159640	-0.444839
C	-5.443648	1.635706	0.429582
H	-3.824781	3.019600	0.724509
C	-4.848636	-0.534186	-0.436504
H	-2.749698	-0.852243	-0.810129
C	-5.817308	0.360704	0.007879
H	-6.200106	2.345804	0.757602
H	-5.134803	-1.526739	-0.781157

H	-6.866192	0.071887	0.012811
C	-1.398696	3.299232	-0.527828
C	-0.772474	4.328249	0.182784
C	-2.026883	3.596136	-1.746974
C	-0.779947	5.630958	-0.314193
H	-0.287488	4.116562	1.136030
C	-2.036372	4.896310	-2.236045
H	-2.514265	2.799297	-2.312109
C	-1.409337	5.916949	-1.521312
H	-0.295073	6.424940	0.250184
H	-2.533861	5.115220	-3.178892
H	-1.415004	6.934520	-1.906263
C	-1.551910	-2.282015	1.288066
C	-2.564371	-3.227862	1.085717
C	-1.610686	-1.475344	2.434365
C	-3.617592	-3.342836	1.989568
H	-2.529201	-3.902739	0.234888
C	-2.665880	-1.590450	3.332119
H	-0.807993	-0.772894	2.645840
C	-3.679695	-2.518437	3.108500
H	-4.388133	-4.092249	1.818888
H	-2.684953	-0.958291	4.218000
H	-4.505223	-2.609618	3.811422
C	1.294738	-2.013672	1.169479
C	2.426726	-1.273918	0.808720
C	1.333811	-2.800877	2.328244
C	3.575230	-1.314541	1.596449
H	2.399877	-0.653082	-0.091507
C	2.478672	-2.832297	3.117474
H	0.461624	-3.387285	2.613745
C	3.600180	-2.088929	2.753782
H	4.450824	-0.736412	1.304814
H	2.496155	-3.443318	4.017533
H	4.494648	-2.116451	3.373344
C	-0.062023	-3.537194	-0.863709
C	1.096652	-4.324134	-0.857425
C	-1.111422	-3.898212	-1.723505
C	1.193814	-5.443202	-1.681358
H	1.929812	-4.063012	-0.207213
C	-1.015668	-5.019777	-2.538866
H	-2.020589	-3.296859	-1.752632
C	0.141790	-5.794670	-2.521758
H	2.100112	-6.045043	-1.661796
H	-1.844660	-5.285683	-3.191581
H	0.222416	-6.669207	-3.163604
C	4.663042	1.397185	-0.332561
C	3.608381	2.202693	0.170177
C	2.419280	2.310279	-0.513380
C	2.176116	1.613572	-1.724558
C	3.240105	0.812321	-2.214813
C	4.442394	0.708443	-1.554118
H	3.739120	2.762341	1.092674
H	1.633823	2.959551	-0.121839
H	3.107182	0.276341	-3.153724
H	5.227343	0.090758	-1.981089
N	5.846430	1.281221	0.340263
C	6.926880	0.490312	-0.213768
H	7.794504	0.555775	0.444020
H	6.647776	-0.568929	-0.307368
H	7.224146	0.855270	-1.205481
C	6.031827	1.957789	1.607757
H	7.014572	1.707142	2.009482
H	5.975196	3.049311	1.498534
H	5.272657	1.647414	2.340336
C	0.916345	1.724608	-2.409369
C	0.478508	-1.146275	-3.117031
H	1.181998	-0.580756	-3.728623
C	-0.916258	-0.984862	-3.405869
H	-1.583810	-1.770485	-3.048572
C	-1.504446	0.075792	-4.045273
H	-0.920917	0.891371	-4.468981
H	-2.583587	0.127048	-4.168389
H	0.827792	-2.145252	-2.855155
H	0.929363	1.461194	-3.467862
H	0.335628	2.626474	-2.210233

IM7

SCF energy in MeCN: -2723.358017 a.u.

Free energy in MeCN: -2722.624973 a.u.

Pd	0.005734	0.098531	-1.353279
P	0.639966	-1.876749	-0.161449
P	1.059740	1.698138	0.150943
C	0.169123	-1.808506	1.610989
C	0.857778	-2.461534	2.639672
C	-0.945400	-1.024833	1.938157
C	0.443298	-2.326871	3.961528
H	1.743283	-3.053490	2.413557

C	-1.366153	-0.897207	3.259109	C	-1.149266	3.412883	3.200444
H	-1.480438	-0.498416	1.148811	H	0.941429	3.114958	2.780975
C	-0.667930	-1.544793	4.275586	C	-2.457572	3.221976	2.760004
H	0.996168	-2.830604	4.753389	H	-3.709633	2.435093	1.181373
H	-2.233685	-0.278332	3.487377	H	-0.959457	3.902319	4.154526
H	-0.984361	-1.439198	5.312236	H	-3.293505	3.559094	3.371544
C	2.442922	-2.223795	-0.175546	C	1.751383	3.183643	-0.674924
C	2.972219	-3.456649	0.235013	C	1.575050	4.486735	-0.203103
C	3.319103	-1.243148	-0.649618	C	2.510305	2.978532	-1.834021
C	4.344196	-3.680300	0.212070	C	2.153239	5.561350	-0.874907
H	2.299646	-4.253813	0.553127	H	0.974204	4.666113	0.687900
C	4.692768	-1.467546	-0.676437	C	3.093861	4.050380	-2.500567
H	2.906552	-0.301453	-1.014444	H	2.618002	1.963577	-2.223789
C	5.208309	-2.682346	-0.236573	C	2.914402	5.346021	-2.020705
H	4.740770	-4.640827	0.537169	H	2.004035	6.573192	-0.501338
H	5.359262	-0.688293	-1.043913	H	3.674122	3.874920	-3.404955
H	6.282315	-2.860403	-0.257053	H	3.360338	6.188680	-2.546228
C	-0.002374	-3.512191	-0.686837	C	-5.023461	0.123478	-0.111161
C	-0.839757	-4.306790	0.102293	C	-4.190752	-0.959954	0.231552
C	0.344582	-3.959707	-1.969771	C	-3.118072	-1.315736	-0.571227
C	-1.310221	-5.528311	-0.377377	C	-2.772522	-0.609622	-1.738244
H	-1.124238	-3.973458	1.100380	C	-3.643946	0.436687	-2.093068
C	-0.119357	-5.180969	-2.442620	C	-4.728190	0.804605	-1.307101
H	0.983430	-3.338359	-2.599494	H	-4.381935	-1.536629	1.134395
C	-0.948936	-5.969565	-1.645982	H	-2.495889	-2.162340	-0.271557
H	-1.959565	-6.137805	0.248952	H	-3.463440	0.985156	-3.017614
H	0.161512	-5.515891	-3.439721	H	-5.350360	1.634475	-1.633850
H	-1.317117	-6.923818	-2.018364	N	-6.106076	0.486898	0.692056
C	2.397180	1.327852	1.358395	C	-6.778375	1.729899	0.405785
C	3.736396	1.607194	1.049173	H	-7.604037	1.861479	1.110608
C	2.121011	0.624442	2.539707	H	-6.119998	2.616577	0.473992
C	4.764994	1.182012	1.882875	H	-7.205718	1.714703	-0.604235
H	3.980898	2.161728	0.143540	C	-6.107985	0.039461	2.064214
C	3.153015	0.193195	3.367269	H	-6.978199	0.458066	2.577510
H	1.089988	0.416900	2.822304	H	-6.187067	-1.053199	2.123827
C	4.479185	0.462901	3.039924	H	-5.198648	0.338520	2.619261
H	5.797040	1.412362	1.622010	C	-1.534259	-0.907509	-2.475441
H	2.910912	-0.356739	4.275927	C	-0.500113	1.738843	-2.675043
H	5.284984	0.122312	3.687940	H	-1.591856	1.765048	-2.756989
C	-0.303934	2.335744	1.198116	C	0.150834	1.526178	-3.968269
C	-1.624890	2.155013	0.761411	H	1.239757	1.653082	-3.985617
C	-0.079339	2.975397	2.424500	C	-0.445473	1.179013	-5.122593
C	-2.692657	2.596198	1.538075	H	-1.527575	1.058953	-5.189434
H	-1.817420	1.641607	-0.184790	H	0.119374	1.008333	-6.036792

H	-0.162689	2.666159	-2.197137
H	-1.507974	-0.505536	-3.492867
H	-1.295353	-1.976816	-2.486764

IM8

SCF energy in MeCN: -2318.330913 a.u.

Free energy in MeCN: -2317.788177 a.u.

C	-0.814797	-3.182969	1.573804
H	-1.528069	-3.577072	0.847029
H	-1.197453	-3.098252	2.590407
C	0.571456	-3.411161	1.379217
H	1.234638	-3.327796	2.243577
C	1.155810	-3.729658	0.147707
H	0.539151	-3.938847	-0.725625
P	-1.916408	-0.149437	0.086686
C	-2.522152	1.076638	1.307786
C	-1.712756	1.425583	2.393538
C	-3.786138	1.669679	1.182610
C	-2.148386	2.365847	3.325383
H	-0.737345	0.944863	2.498802
C	-4.221465	2.606022	2.112900
H	-4.428970	1.389485	0.347041
C	-3.400599	2.957566	3.184600
H	-1.507987	2.632188	4.164795
H	-5.204669	3.061423	2.005480
H	-3.743485	3.688962	3.914877
C	-3.439547	-1.139105	-0.176810
C	-3.889675	-1.897495	0.915350
C	-4.151879	-1.206841	-1.379075
C	-5.021319	-2.695485	0.809964
H	-3.338926	-1.854377	1.856062
C	-5.281521	-2.016764	-1.485310
H	-3.831238	-0.617764	-2.237194
C	-5.719638	-2.762439	-0.395243
H	-5.356319	-3.273539	1.669770
H	-5.825920	-2.056491	-2.427890
H	-6.602484	-3.393497	-0.481898
Pd	-0.000854	-1.319661	0.717562
C	-1.765571	0.811407	-1.464958
C	-1.339919	0.116169	-2.608625
C	-1.964475	2.194395	-1.560129
C	-1.161255	0.774935	-3.817956
H	-1.138914	-0.954936	-2.538626
C	-1.756764	2.858532	-2.768010
H	-2.281478	2.759661	-0.683531
C	-1.366767	2.151732	-3.900894
H	-0.835533	0.215555	-4.693178
H	-1.910741	3.935386	-2.822027
H	-1.209126	2.671802	-4.844637
P	1.884475	-0.028047	0.153421
C	3.494070	-0.798182	0.585405
C	3.589978	-1.444166	1.824910
C	4.617840	-0.768722	-0.247694
C	4.780196	-2.040447	2.226920
H	2.710260	-1.477767	2.470965
C	5.806285	-1.377476	0.149395
H	4.562799	-0.268324	-1.214345
C	5.890967	-2.012817	1.385726
H	4.838498	-2.537710	3.193910
H	6.671884	-1.352287	-0.510877
H	6.820359	-2.490229	1.692046
C	2.047587	0.213279	-1.657209
C	2.211601	1.459347	-2.268632
C	1.987364	-0.934539	-2.462575
C	2.316816	1.555119	-3.655119
H	2.257945	2.362374	-1.661557
C	2.111549	-0.838022	-3.843403
H	1.843719	-1.909359	-1.989614
C	2.274397	0.410203	-4.444364
H	2.437276	2.533554	-4.118202
H	2.074301	-1.738809	-4.454470
H	2.362821	0.488700	-5.526979
C	2.056212	1.663608	0.829228
C	3.202686	2.124940	1.487531
C	0.957579	2.527036	0.709201
C	3.243417	3.414587	2.012002
H	4.069908	1.474328	1.590702
C	1.003727	3.817475	1.222199
H	0.057824	2.177435	0.200839
C	2.148175	4.264638	1.880661
H	4.141328	3.757467	2.524156
H	0.135745	4.468242	1.119169
H	2.185165	5.271872	2.292423
H	2.234777	-3.814275	0.038954

TS2a

SCF energy in MeCN: -2723.211991 a.u.

Free energy in MeCN: -2722.48362 a.u.

C	-0.295564	2.847496	-0.457084
H	0.001118	3.062922	-1.486531
H	0.041015	3.580799	0.273090
C	-1.476885	2.106386	-0.220178
H	-1.967731	2.172352	0.752723
C	-1.988873	1.193311	-1.158082
H	-1.521732	1.089515	-2.136952
P	2.593404	1.165607	0.164762
C	2.940561	2.769271	0.966735
C	2.110469	3.186006	2.016618
C	4.033129	3.563554	0.604927
C	2.378622	4.366246	2.702372
H	1.247575	2.575071	2.294215
C	4.290057	4.752277	1.282944
H	4.683782	3.255921	-0.212711
C	3.468952	5.152289	2.333557
H	1.732317	4.676841	3.521061
H	5.139069	5.366297	0.989631
H	3.674712	6.080375	2.863011
C	3.455838	1.230125	-1.441641
C	2.730554	1.605721	-2.579568
C	4.820422	0.940568	-1.570474
C	3.353454	1.695261	-3.820115
H	1.662991	1.815047	-2.483741
C	5.441246	1.025260	-2.813595
H	5.396465	0.643174	-0.694910
C	4.710613	1.402160	-3.938236
H	2.778654	1.988861	-4.696252
H	6.501566	0.797299	-2.902460
H	5.199311	1.467882	-4.908301
Pd	0.285503	0.781054	-0.124231
C	3.557782	-0.022654	1.160260
C	3.895816	-1.267742	0.609789
C	3.860805	0.231598	2.504247
C	4.517066	-2.236667	1.390157
H	3.686399	-1.472992	-0.439580
C	4.482564	-0.742594	3.280261
H	3.618517	1.197611	2.945618
C	4.806897	-1.979292	2.728674
H	4.776201	-3.196381	0.945874
H	4.721252	-0.528641	4.320505
H	5.292148	-2.738932	3.338244
P	0.076937	-1.592202	-0.024230
C	-1.563132	-2.149709	-0.616543
C	-2.660248	-2.082906	0.255633
C	-1.781149	-2.480786	-1.957827
C	-3.945022	-2.343137	-0.207237
H	-2.504205	-1.823705	1.303662
C	-3.070791	-2.739654	-2.418099
H	-0.939615	-2.543624	-2.647390
C	-4.153800	-2.669745	-1.546989
H	-4.788270	-2.285540	0.479196
H	-3.225699	-3.005990	-3.462133
H	-5.160577	-2.872506	-1.909018
C	1.263713	-2.398410	-1.152956
C	1.861235	-3.637416	-0.900410
C	1.633511	-1.684860	-2.301057
C	2.814182	-4.145710	-1.779806
H	1.605144	-4.193323	0.000816
C	2.579774	-2.196733	-3.182884
H	1.190037	-0.703345	-2.485515
C	3.176137	-3.427876	-2.918477
H	3.281327	-5.106414	-1.570549
H	2.859477	-1.628040	-4.067688
H	3.926211	-3.827295	-3.598053
C	0.251302	-2.420368	1.585986
C	-0.233808	-3.719328	1.798889
C	0.889004	-1.749017	2.634675
C	-0.067107	-4.335110	3.034502
H	-0.751825	-4.243036	0.995235
C	1.059633	-2.370535	3.868731
H	1.254549	-0.733191	2.479802
C	0.582549	-3.662459	4.068979
H	-0.447762	-5.342340	3.192098
H	1.562642	-1.839780	4.674709
H	0.709974	-4.146396	5.035334
H	-2.671435	0.404138	-0.860382
C	-3.812334	2.233656	-2.165479
C	-4.927941	1.878863	-1.379651
C	-5.338050	2.651708	-0.262583
C	-5.665192	0.693906	-1.635898
C	-6.405130	2.285046	0.524698
H	-4.795709	3.568737	-0.030891
C	-6.734988	0.316657	-0.857691
H	-5.373442	0.068388	-2.479938
C	-7.142843	1.104084	0.249553

H	-6.686838	2.919154	1.360630
H	-7.274729	-0.593260	-1.107832
N	-8.207751	0.737906	1.025138
C	-8.630168	1.577034	2.126203
H	-9.485887	1.115654	2.621372
H	-7.831879	1.696768	2.871213
H	-8.931609	2.576779	1.783706
C	-8.967261	-0.450569	0.702560
H	-9.771383	-0.572271	1.429741
H	-9.417819	-0.387012	-0.297732
H	-8.340000	-1.352303	0.738165
H	-3.377677	3.226976	-2.078234
H	-3.644228	1.723586	-3.112523

TS2b

SCF energy in MeCN: -2723.197429 a.u.

Free energy in MeCN: -2722.470427 a.u.

Pd	-0.035463	-0.214562	-1.047093
P	1.058648	1.354999	0.316387
P	-2.148492	-0.612981	0.021683
C	0.722019	1.441108	2.104193
C	0.309871	2.618980	2.740411
C	0.826947	0.261624	2.853704
C	-0.002508	2.607629	4.097361
H	0.216361	3.543679	2.172108
C	0.522790	0.256327	4.210511
H	1.142755	-0.661106	2.361956
C	0.098959	1.429042	4.832807
H	-0.326824	3.526802	4.582067
H	0.601641	-0.668808	4.778793
H	-0.151989	1.424220	5.891385
C	0.679776	3.030289	-0.304880
C	1.608231	4.077569	-0.227960
C	-0.590598	3.282226	-0.840406
C	1.267370	5.348859	-0.679672
H	2.598930	3.896320	0.187893
C	-0.930591	4.556574	-1.283175
H	-1.315590	2.469642	-0.909320
C	-0.000370	5.590450	-1.206382
H	1.995401	6.155222	-0.617596
H	-1.922521	4.736908	-1.693295
H	-0.261262	6.586129	-1.559650
C	2.879564	1.255854	0.181835
C	3.718904	1.004250	1.271169
C	3.446824	1.413866	-1.091819
C	5.099259	0.927544	1.090535
H	3.301302	0.887595	2.269697
C	4.823176	1.352937	-1.266559
H	2.796404	1.584308	-1.952846
C	5.655000	1.108005	-0.173187
H	5.742834	0.741713	1.948739
H	5.249759	1.493421	-2.258257
H	6.734169	1.061643	-0.307418
C	-3.112849	0.908125	0.298755
C	-4.047405	1.396455	-0.622215
C	-2.768053	1.701738	1.404294
C	-4.623254	2.651964	-0.438282
H	-4.345539	0.790012	-1.476150
C	-3.346074	2.952665	1.582917
H	-2.044546	1.333476	2.131392
C	-4.271922	3.434612	0.659142
H	-5.357874	3.014892	-1.154499
H	-3.068068	3.551895	2.448552
H	-4.723633	4.414718	0.797334
C	-2.076963	-1.397657	1.667274
C	-1.008133	-2.250358	1.960795
C	-3.110027	-1.254485	2.603526
C	-0.970277	-2.954491	3.160029
H	-0.194228	-2.347695	1.242927
C	-3.064789	-1.949925	3.807809
H	-3.955165	-0.603383	2.383830
C	-1.998326	-2.803435	4.087228
H	-0.131140	-3.616171	3.373445
H	-3.871251	-1.830966	4.528572
H	-1.972166	-3.351050	5.027418
C	-3.200805	-1.754802	-0.945730
C	-3.708321	-2.941664	-0.397610
C	-3.441873	-1.486195	-2.303169
C	-4.451050	-3.819269	-1.182947
H	-3.529128	-3.181124	0.648734
C	-4.195419	-2.358446	-3.080197
H	-3.030275	-0.586645	-2.758213
C	-4.700609	-3.530739	-2.521541
H	-4.840709	-4.734071	-0.740795
H	-4.382421	-2.125380	-4.126650
H	-5.283930	-4.218403	-3.129997
C	3.194373	-2.908164	-0.260008

C	1.865377	-3.382278	-0.116148	H	2.756480	-0.311470	5.098170
C	0.865533	-2.959867	-0.968972	H	0.072204	-3.284379	3.531472
C	1.121971	-2.062326	-2.034807	H	1.146311	-2.165042	5.479790
C	2.457941	-1.617288	-2.185933	C	3.359940	0.970965	0.311796
C	3.462023	-2.020738	-1.330540	C	4.748781	0.813385	0.249333
H	1.621347	-4.100520	0.662548	C	2.837303	2.248064	0.552987
H	-0.144823	-3.356294	-0.850562	C	5.591577	1.909886	0.417116
H	2.692307	-0.934338	-3.003520	H	5.174576	-0.173018	0.067455
H	4.466061	-1.635531	-1.483694	C	3.678486	3.338015	0.745870
N	4.180986	-3.302734	0.600250	H	1.754788	2.381713	0.574950
C	5.556668	-2.928899	0.344320	C	5.060593	3.172510	0.670319
H	6.191024	-3.331697	1.135716	H	6.670542	1.774420	0.356507
H	5.915745	-3.322646	-0.617684	H	3.251386	4.321058	0.939776
H	5.677623	-1.837803	0.334113	H	5.723001	4.026327	0.804895
C	3.886508	-4.248468	1.654102	C	3.200542	-1.720339	-0.643964
H	4.779680	-4.399663	2.262463	C	3.568942	-2.917721	-0.020657
H	3.091075	-3.871886	2.312598	C	3.542819	-1.531118	-1.993141
H	3.569437	-5.226069	1.261398	C	4.252237	-3.903575	-0.731371
C	0.066560	-1.642145	-2.952898	H	3.320473	-3.082533	1.027264
C	-0.668435	0.355754	-3.346484	C	4.238037	-2.508155	-2.694641
H	-1.125765	-0.128834	-4.209209	H	3.253304	-0.597908	-2.483342
C	0.484930	1.199278	-3.608134	C	4.588423	-3.704117	-2.066780
H	0.652391	2.018051	-2.902652	H	4.529183	-4.831336	-0.232083
C	1.350086	1.043021	-4.630595	H	4.500664	-2.341257	-3.738432
H	1.229874	0.254212	-5.373982	H	5.120508	-4.476969	-2.618733
H	2.191185	1.717328	-4.772985	C	-1.034104	2.586648	1.383021
H	-1.440737	0.829450	-2.731479	C	-1.557498	3.874596	1.539232
H	-0.855706	-2.227501	-2.930894	C	-0.125844	2.110211	2.338721
H	0.437999	-1.485955	-3.963637	C	-1.159156	4.672530	2.610606
				H	-2.284315	4.257474	0.823471
TS2c				C	0.262560	2.901350	3.413155
SCF energy in MeCN: -2723.31607 a.u.				H	0.283965	1.103233	2.228453
Free energy in MeCN: -2722.588875 a.u.				C	-0.248028	4.191356	3.547397
Pd	0.175801	0.153702	-1.002640	H	-1.570615	5.675600	2.715736
P	2.171104	-0.412030	0.123951	H	0.973863	2.508649	4.139043
P	-1.486469	1.400088	0.046489	H	0.060368	4.819048	4.382003
C	1.972228	-0.997867	1.852811	C	-2.702382	0.393199	0.989519
C	2.582098	-0.387685	2.955551	C	-2.304509	-0.887589	1.381595
C	1.064563	-2.043740	2.083338	C	-3.941269	0.880870	1.424116
C	2.280668	-0.804499	4.251240	C	-3.116382	-1.663451	2.205070
H	3.287322	0.429135	2.802600	H	-1.347214	-1.269723	1.020275
C	0.780649	-2.471027	3.374606	C	-4.765425	0.095970	2.224356
H	0.564254	-2.511242	1.231224	H	-4.258719	1.884096	1.136048
C	1.382033	-1.845148	4.466207	C	-4.350289	-1.174898	2.624282

H	-2.787354	-2.658657	2.505901
H	-5.728849	0.483015	2.553231
H	-4.991702	-1.781403	3.262707
C	-2.497227	2.379420	-1.117599
C	-3.676815	1.861682	-1.673867
C	-1.963555	3.554602	-1.672934
C	-4.307963	2.505769	-2.733857
H	-4.098926	0.938929	-1.274605
C	-2.598823	4.200063	-2.728356
H	-1.033080	3.962756	-1.274885
C	-3.774881	3.678431	-3.264271
H	-5.225644	2.088707	-3.146729
H	-2.168749	5.112687	-3.138299
H	-4.269713	4.180732	-4.093405
C	-2.501367	-3.461612	-0.665564
C	-1.102906	-3.646587	-0.642357
C	-0.260353	-2.823653	-1.376965
C	-0.762052	-1.787601	-2.194408
C	-2.165358	-1.617395	-2.210389
C	-3.012680	-2.420642	-1.473198
H	-0.664759	-4.442973	-0.044816
H	0.817045	-3.001033	-1.354970
H	-2.583867	-0.819762	-2.827186
H	-4.083191	-2.231849	-1.507035
N	-3.343337	-4.262259	0.079119
C	-4.757276	-3.978225	0.111679
H	-5.249812	-4.684142	0.784927
H	-4.966007	-2.957478	0.471186
H	-5.214600	-4.087659	-0.882910
C	-2.783903	-5.241564	0.972919
H	-3.590469	-5.746137	1.510145
H	-2.208302	-6.007065	0.431374
H	-2.106115	-4.788929	1.718311
C	0.093962	-0.972567	-3.060302
C	0.460588	1.182392	-3.194081
H	0.805522	0.865919	-4.179866
C	1.445559	2.040016	-2.547990
H	1.098913	2.662872	-1.717901
C	2.744319	2.113779	-2.905572
H	3.137825	1.511266	-3.725914
H	3.451096	2.755624	-2.384971
H	-0.562480	1.566860	-3.238414
H	-0.410444	-0.733176	-3.995761
H	1.097156	-1.369901	-3.233112

Ir^{III}

SCF energy in MeCN: -1557.653878 a.u.

Free energy in MeCN: -1557.23251 a.u.

Ir	0.067384	-0.030941	0.002917
C	1.778346	0.215271	1.041953
C	2.633512	1.234303	0.544136
C	2.174359	-0.454010	2.205647
C	3.826398	1.560682	1.206218
C	3.360240	-0.122320	2.858765
H	1.555667	-1.255502	2.610008
C	4.188178	0.886294	2.362806
H	4.476662	2.345014	0.819768
H	3.646386	-0.660241	3.761488
H	5.113601	1.138334	2.875154
C	2.186189	1.895595	-0.669228
C	2.883048	2.882556	-1.376342
C	2.353323	3.417737	-2.538128
H	3.849899	3.216123	-1.009510
C	0.460690	1.990927	-2.262446
C	1.115425	2.963900	-2.995384
H	2.899967	4.179769	-3.088673
H	-0.499449	1.586403	-2.575841
H	0.665287	3.351688	-3.904324
C	-2.823160	0.870412	-0.566746
C	-2.225803	-0.843706	-2.027915
C	-4.101270	0.921056	-1.128437
C	-3.477257	-0.839989	-2.627651
H	-1.436382	-1.526598	-2.341522
C	-4.431883	0.061299	-2.166949
H	-4.840259	1.623231	-0.753347
H	-3.693098	-1.532534	-3.436255
H	-5.425007	0.093850	-2.608099
C	-2.393566	1.743636	0.539842
C	-3.208407	2.736418	1.088678
C	-2.732938	3.519171	2.131836
H	-4.209341	2.903536	0.701348
C	-0.683350	2.297141	2.022232
C	-1.445272	3.297083	2.610198
H	-3.361073	4.294353	2.563760
H	0.331638	2.074851	2.351161
H	-1.031785	3.886795	3.423385
C	-0.225688	-2.880572	0.673700
C	-1.339897	-1.548810	2.257989
C	-0.615806	-4.027482	1.375389

C	-1.743022	-2.653499	2.986105
H	-1.587707	-0.535903	2.568987
C	-1.371006	-3.919009	2.530708
H	-0.309145	-5.003873	1.010411
H	-2.328141	-2.521508	3.891302
H	-1.664432	-4.811699	3.078166
C	0.581641	-2.846589	-0.533413
C	1.030749	-3.998718	-1.195228
C	0.900876	-1.553172	-1.024956
C	1.803874	-3.887826	-2.341112
H	0.777551	-4.988358	-0.815724
C	1.691894	-1.471922	-2.177113
C	2.135054	-2.621986	-2.828201
H	2.152853	-4.781546	-2.852776
H	1.975828	-0.497029	-2.575067
H	2.750630	-2.531638	-3.722122
N	-0.605840	-1.649629	1.135083
N	-1.898989	-0.011138	-1.027013
N	-1.139857	1.534564	1.016371
N	0.971608	1.467871	-1.132729

***Ir^{III}**

SCF energy in MeCN: -1557.573039 a.u.

Free energy in MeCN: -1557.155987 a.u.

Ir	-0.007026	0.160201	0.005597
C	-1.169529	1.434384	1.007065
C	-2.464691	1.630856	0.423693
C	-0.876536	2.092552	2.216272
C	-3.399726	2.458219	1.051994
C	-1.813675	2.912851	2.827877
H	0.102991	1.960686	2.675850
C	-3.077954	3.090649	2.247206
H	-4.384980	2.614848	0.615723
H	-1.571351	3.420940	3.759225
H	-3.812703	3.728521	2.733576
C	-2.709360	0.944481	-0.831864
C	-3.877859	1.011782	-1.597295
C	-3.973515	0.306957	-2.785885
H	-4.708703	1.621778	-1.252627
C	-1.751223	-0.501530	-2.420256
C	-2.890478	-0.467949	-3.206920
H	-4.881544	0.357845	-3.381416
H	-0.874171	-1.082276	-2.697942
H	-2.923460	-1.040867	-4.128623
C	0.545991	-2.807569	-0.558791
C	1.855265	-1.471841	-1.990661
C	1.026958	-3.959111	-1.221639
C	2.368283	-2.568939	-2.648105
H	2.146465	-0.460227	-2.271502
C	1.927971	-3.849428	-2.253618
H	0.663946	-4.937734	-0.918501
H	3.090147	-2.433583	-3.447545
H	2.288337	-4.739959	-2.762987
C	-0.379897	-2.842259	0.532958
C	-0.793903	-4.029178	1.178172
C	-1.705893	-3.987293	2.205425
H	-0.372012	-4.980270	0.863947
C	-1.773944	-1.606086	1.974297
C	-2.224617	-2.740811	2.613612
H	-2.015545	-4.904319	2.700925
H	-2.125506	-0.616945	2.266286
H	-2.957181	-2.659003	3.410581
C	2.658800	1.066030	0.831769
C	1.775849	-0.417775	2.428444
C	3.831465	1.179123	1.585146
C	2.919836	-0.337662	3.204643
H	0.925272	-1.033024	2.713728
C	3.967531	0.478739	2.772298
H	4.633578	1.822300	1.232737
H	2.983762	-0.907315	4.126742
H	4.879017	0.565676	3.358361
C	2.372812	1.750593	-0.415325
C	3.264315	2.624911	-1.043713
C	1.080548	1.505528	-0.987534
C	2.900001	3.261171	-2.224391
H	4.247898	2.816808	-0.618103
C	0.742978	2.170685	-2.181087
C	1.635535	3.040964	-2.790356
H	3.600736	3.936640	-2.710088
H	-0.236621	2.005451	-2.629483
H	1.358671	3.554812	-3.708751
N	1.642776	0.261602	1.277238
N	0.965891	-1.559036	-0.978789
N	-0.875229	-1.626855	0.967340
N	-1.656884	0.183646	-1.268886

Ir^{II}

SCF energy in MeCN: -1557.753311 a.u.

Free energy in MeCN: -1557.337141 a.u.

N	-0.248299	-1.728153	-1.134373
N	0.608358	1.635544	1.130393
C	1.211706	-1.347007	1.020027
C	1.986915	-1.123940	2.167250
C	2.655952	-2.164496	2.806322
C	2.576767	-3.470142	2.314245
C	1.829103	-3.724257	1.174501
C	1.154946	-2.679166	0.525732
C	0.360984	-2.866123	-0.675860
C	0.195630	-4.065628	-1.377850
C	-0.577472	-4.105434	-2.525742
C	-1.190900	-2.934513	-2.972713
C	-1.001152	-1.770991	-2.247913
C	1.707687	0.611111	-1.028499
C	2.283010	0.048560	-2.177461
C	3.370147	0.643914	-2.811939
C	3.926117	1.825326	-2.313530
C	3.390669	2.401371	-1.171761
C	2.296937	1.804744	-0.527419
C	1.689301	2.343838	0.676441
C	2.119669	3.471117	1.385648
C	1.459128	3.871464	2.534664
C	0.357434	3.137391	2.975648
C	-0.033537	2.029334	2.244768
H	2.070019	-0.113327	2.571208
H	3.098444	-4.281275	2.818390
H	0.685126	-4.965162	-1.012952
H	-0.702346	-5.039269	-3.070202
H	-1.449223	-0.824233	-2.541496
H	1.873097	-0.876981	-2.585924
H	4.773726	2.288906	-2.814461
H	2.982286	4.026040	1.025298
H	1.798133	4.746851	3.084921
H	-0.881868	1.412744	2.533931
C	-2.897282	0.290541	0.572750
C	-4.143814	0.131921	1.231974
C	-4.265112	-0.695721	2.320015
C	-3.131496	-1.400679	2.788150
C	-1.936346	-1.210730	2.122601
N	-1.791878	-0.398532	1.061651
H	-5.010119	0.681299	0.870018
H	-3.184454	-2.072973	3.639266
H	-1.023146	-1.717902	2.438487
C	-2.689235	1.125358	-0.563829
C	-3.714289	1.859849	-1.213956
C	-1.140985	1.990310	-2.123214
C	-3.435371	2.647411	-2.302577
H	-4.734860	1.788984	-0.844412
H	-0.098611	2.002990	-2.446234
C	-2.106234	2.728010	-2.780234
H	-1.838205	3.346487	-3.631642
N	-1.392539	1.205152	-1.061701
Ir	0.082940	-0.019700	-0.004055
H	-0.194075	3.415136	3.869246
H	-5.227138	-0.804323	2.817549
H	-4.232905	3.202642	-2.792944
H	-1.809191	-2.918053	-3.865621
H	1.768511	-4.743087	0.790201
H	3.793542	0.183869	-3.704853
H	3.825893	3.322646	-0.783009
H	3.248219	-1.959656	3.698208

IM1'

SCF energy in MeCN: -3413.544595 a.u.

Free energy in MeCN: -3412.625188 a.u.

C	-1.160955	0.427161	0.273518
H	-0.968381	-0.533813	-0.221636
H	-1.176710	1.201087	-0.503639
C	-0.191075	0.706983	1.368175
H	-0.239608	1.719847	1.778876
C	0.294383	-0.331377	2.195203
H	-0.036233	-1.360663	2.032518
P	2.339994	1.514084	-1.096637
C	2.464740	3.306659	-0.737629
C	2.018016	3.770255	0.504918
C	2.977721	4.228041	-1.661166
C	2.073460	5.126643	0.817328
H	1.630353	3.047212	1.225557
C	3.033458	5.582129	-1.348470
H	3.337416	3.876416	-2.628535
C	2.580749	6.033397	-0.109069
H	1.723285	5.474226	1.787748
H	3.432341	6.289258	-2.073950
H	2.627771	7.093503	0.134606
C	0.950996	1.382258	-2.281825

C	0.507828	0.090073	-2.605383	C	4.526193	-3.140552	-3.160812
C	0.241477	2.481293	-2.775543	H	6.550575	-2.440509	-2.928650
C	-0.613609	-0.097737	-3.403048	H	2.439608	-3.691452	-3.114467
H	1.041113	-0.772015	-2.196697	H	4.702838	-3.575112	-4.143459
C	-0.890322	2.289725	-3.566468	C	5.209668	-0.543616	1.595818
H	0.559805	3.492644	-2.526114	C	6.326327	-1.320288	1.931039
C	-1.321226	1.004646	-3.879151	C	5.283475	0.845472	1.743299
H	-0.959479	-1.105712	-3.624750	C	7.496572	-0.717208	2.379899
H	-1.443457	3.154188	-3.930549	H	6.272825	-2.406252	1.842512
H	-2.218492	0.858184	-4.477231	C	6.455248	1.450717	2.191540
Pd	1.821339	0.170924	0.781354	H	4.401758	1.446548	1.506795
O	-2.502046	0.362405	0.856513	C	7.563636	0.669691	2.507299
C	-3.474407	-0.068387	0.045153	H	8.358496	-1.330720	2.636977
O	-3.313405	-0.398880	-1.112801	H	6.498389	2.533178	2.302098
C	3.824076	1.258389	-2.147955	H	8.479321	1.139467	2.863018
C	3.780054	0.629632	-3.396429	H	0.606039	-0.113390	3.217761
C	5.069788	1.660817	-1.643039	C	-4.821099	-0.067400	0.766538
C	4.949998	0.420260	-4.123186	H	-5.259461	0.920192	0.546037
H	2.825386	0.305596	-3.809111	N	-5.688285	-1.041597	0.127141
C	6.235794	1.450980	-2.369150	C	-4.703738	-0.182001	2.305598
H	5.123669	2.159299	-0.675063	H	-3.905649	-0.886748	2.571690
C	6.179155	0.830879	-3.616396	H	-5.645158	-0.621738	2.669928
H	4.895620	-0.070025	-5.094516	C	-5.295511	-2.426232	0.351731
H	7.191018	1.777101	-1.959615	H	-4.196300	-2.456588	0.364521
H	7.090852	0.666080	-4.188872	H	-5.628779	-2.805153	1.340717
P	3.643116	-1.277980	0.989380	C	-7.100880	-0.825103	0.366855
C	3.505093	-2.768914	2.055169	H	-7.629155	-1.664933	-0.111339
C	2.906332	-2.616204	3.312694	H	-7.368926	-0.887239	1.445925
C	3.982672	-4.031590	1.684292	C	-5.802611	-3.327158	-0.741503
C	2.802164	-3.694255	4.184688	C	-5.546532	-2.993938	-2.076330
H	2.516128	-1.638075	3.597880	C	-6.512727	-4.492845	-0.455872
C	3.866983	-5.113401	2.553910	C	-5.987103	-3.822561	-3.101538
H	4.447004	-4.171089	0.708146	H	-4.994655	-2.076857	-2.284017
C	3.279565	-4.947448	3.805227	C	-6.955527	-5.323939	-1.483247
H	2.337133	-3.558853	5.159797	H	-6.722127	-4.748699	0.584001
H	4.239497	-6.090807	2.250664	C	-6.692432	-4.989995	-2.808232
H	3.189106	-5.794656	4.482987	H	-5.780282	-3.559106	-4.137954
C	4.074118	-2.013723	-0.632318	H	-7.512683	-6.229377	-1.247133
C	5.339820	-1.950082	-1.220969	H	-7.039192	-5.636053	-3.613410
C	3.032629	-2.639022	-1.335912	C	-7.612353	0.471608	-0.199819
C	5.561152	-2.509370	-2.478502	C	-8.666660	1.140994	0.425276
H	6.156688	-1.447870	-0.704961	C	-7.070578	1.009336	-1.371982
C	3.257425	-3.203726	-2.586002	C	-9.186196	2.314432	-0.114157
H	2.037390	-2.684833	-0.887372	H	-9.082942	0.733454	1.348187

C	-7.583298	2.187217	-1.906998
H	-6.231284	0.496052	-1.842993
C	-8.645099	2.840550	-1.284225
H	-10.009139	2.823354	0.385304
H	-7.150576	2.599071	-2.817711
H	-9.043586	3.762233	-1.705195
C	-4.489618	1.138970	2.988788
C	-3.307702	1.436303	3.670485
C	-5.492766	2.113534	2.934758
C	-3.133579	2.672601	4.286784
H	-2.511070	0.692734	3.697960
C	-5.321262	3.351207	3.546355
H	-6.420875	1.895606	2.399514
C	-4.139287	3.634417	4.227096
H	-2.204166	2.886640	4.813463
H	-6.113358	4.096621	3.491261
H	-4.002002	4.602275	4.706726

1a'

SCF energy in MeCN: -1212.499006 a.u.

Free energy in MeCN: -1212.085088 a.u.

C	-2.661766	-2.365188	-1.540554
C	-1.435390	-1.748896	-1.764474
C	-1.368885	-0.453834	-2.289314
C	-2.563889	0.201193	-2.593015
C	-3.795572	-0.415148	-2.379602
C	-3.848479	-1.699325	-1.847045
H	-2.691216	-3.370054	-1.120071
H	-0.515201	-2.272070	-1.500884
H	-2.526407	1.216590	-2.990401
H	-4.714946	0.116775	-2.619068
H	-4.808903	-2.180808	-1.670325
C	-0.047121	0.235736	-2.479949
H	0.525460	-0.236230	-3.292306
H	-0.201035	1.274355	-2.799406
C	0.835941	0.214863	-1.228513
C	1.985430	1.200305	-1.373942
O	1.893532	2.309837	-1.858247
O	3.104174	0.726381	-0.779127
C	4.211868	1.654714	-0.707722
H	4.723767	1.669499	-1.678425
H	3.799294	2.657954	-0.537407
C	5.110322	1.215765	0.388927
H	4.643863	1.115117	1.371586
C	6.412447	0.982883	0.237810
H	6.898139	1.074115	-0.733388
H	7.046893	0.702370	1.074812
N	0.081066	0.507669	-0.007906
C	-0.544171	1.823313	0.058334
C	0.773276	0.148111	1.227261
H	1.737309	0.680774	1.348332
H	0.125196	0.489312	2.047327
C	-1.746762	1.808237	0.966730
C	-2.655258	0.745966	0.901634
C	-1.992570	2.850621	1.860853
C	-3.791232	0.737755	1.702699
H	-2.453709	-0.075350	0.214672
C	-3.129786	2.843249	2.666566
H	-1.283122	3.676978	1.925778
C	-4.033488	1.787390	2.587861
H	-4.491886	-0.094046	1.632812
H	-3.305481	3.662129	3.362672
H	-4.921472	1.779793	3.217810
C	0.980446	-1.336182	1.338410
C	-0.134996	-2.180091	1.366362
C	2.255512	-1.899030	1.405657
C	0.021548	-3.557122	1.470615
H	-1.129536	-1.737047	1.296966
C	2.415694	-3.279693	1.514058
H	3.128227	-1.246475	1.359181
C	1.299774	-4.110645	1.547571
H	-0.855164	-4.203057	1.496750
H	3.416021	-3.706720	1.566248
H	1.423908	-5.189077	1.631384
H	0.163497	2.618061	0.368926
H	1.256644	-0.789299	-1.082644
H	-0.856605	2.093307	-0.959903

2a'

SCF energy in MeCN: -1023.874812 a.u.

Free energy in MeCN: -1023.470918 a.u.

C	2.616504	0.043957	3.538184
H	2.934195	-0.966547	3.279670
H	3.381984	0.708019	3.933461
C	1.351884	0.435311	3.376863
H	1.079108	1.457096	3.659505

C	0.248942	-0.428206	2.859149	C	-3.674581	2.576509	-1.490859
H	0.637776	-1.434532	2.651476	H	-2.318680	4.234658	-1.730252
H	-0.513896	-0.537570	3.648127	H	-4.858283	0.846772	-0.983512
C	-0.479320	0.064267	1.593203	H	-4.294022	2.852217	-2.342366
H	-1.275205	-0.671824	1.409242				
C	-1.165835	1.424754	1.823764	**IM4'**			
H	-1.742700	1.350145	2.759250	SCF energy in MeCN: -3224.77204 a.u.			
H	-0.408349	2.202452	1.999076	Free energy in MeCN: -3223.8616 a.u.			
N	0.399147	-0.019965	0.419876				
C	1.279631	1.119149	0.208764	C	-0.071843	-2.475900	0.599993
H	0.757824	1.967186	-0.281689	H	-0.115049	-2.603456	1.683757
H	1.598930	1.479749	1.196036	H	0.492013	-3.225903	0.048226
C	-0.253762	-0.425573	-0.823875	C	-0.959622	-1.635127	-0.030453
H	0.542700	-0.467700	-1.583409	H	-1.014473	-1.662751	-1.122763
H	-0.984751	0.320522	-1.192745	C	-2.026042	-0.855889	0.659448
C	2.499770	0.756008	-0.595468	H	-1.862518	-0.877133	1.747396
C	2.921202	1.555273	-1.658639	P	3.147491	-1.423781	-0.053769
C	3.243474	-0.384025	-0.274129	C	2.986850	-2.933783	-1.061830
C	4.066125	1.233208	-2.383597	C	2.065118	-2.937254	-2.120089
H	2.336468	2.437357	-1.923734	C	3.748464	-4.080408	-0.812613
C	4.387108	-0.708841	-0.995243	C	1.924646	-4.062141	-2.925450
H	2.899059	-1.014931	0.545457	H	1.446473	-2.051997	-2.298551
C	4.803005	0.099879	-2.052272	C	3.594863	-5.208399	-1.614371
H	4.377316	1.863854	-3.215105	H	4.459682	-4.094573	0.012202
H	4.958134	-1.598774	-0.734193	C	2.688312	-5.200595	-2.670983
H	5.695586	-0.158024	-2.619909	H	1.210815	-4.056311	-3.746951
C	-0.907305	-1.775485	-0.721439	H	4.187774	-6.097533	-1.410456
C	-2.190137	-1.992005	-1.227690	H	2.571315	-6.084506	-3.294389
C	-0.229706	-2.845408	-0.126063	C	3.943822	-1.948660	1.495790
C	-2.782511	-3.251074	-1.151073	C	3.128862	-2.327039	2.571274
H	-2.726818	-1.157947	-1.682620	C	5.336075	-2.023107	1.634512
C	-0.820838	-4.100807	-0.041620	C	3.692653	-2.774019	3.761329
H	0.768154	-2.670395	0.276745	H	2.044379	-2.259469	2.468005
C	-2.100523	-4.308084	-0.555354	C	5.897148	-2.463514	2.829785
H	-3.783634	-3.404134	-1.551705	H	5.981156	-1.737783	0.804698
H	-0.281930	-4.923809	0.425727	C	5.078800	-2.838445	3.892897
H	-2.564665	-5.290726	-0.487853	H	3.050742	-3.067848	4.589455
C	-2.064941	1.849895	0.696465	H	6.979335	-2.517929	2.928191
C	-1.775467	2.986391	-0.063074	H	5.521066	-3.183591	4.825194
C	-3.193027	1.094984	0.354443	Pd	0.992779	-0.466237	0.205870
C	-2.568111	3.348567	-1.148754	C	4.387694	-0.415386	-0.923056
H	-0.905270	3.589723	0.199345	C	5.041259	0.617850	-0.232877
C	-3.988694	1.451738	-0.729730	C	4.609786	-0.562906	-2.299269
H	-3.440372	0.204630	0.935093	C	5.891339	1.485834	-0.908869

H	4.896075	0.731418	0.841335	C	-4.090549	-2.006657	1.603554
C	5.465218	0.307128	-2.968476	H	-3.470072	-2.863442	1.909697
H	4.119605	-1.365818	-2.848457	H	-4.002193	-1.274778	2.419493
C	6.101946	1.336578	-2.278452	N	-4.345180	-0.499110	-0.340829
H	6.393199	2.279868	-0.358503	C	-4.601691	0.751569	0.339211
H	5.640260	0.174243	-4.034623	H	-4.574692	0.538556	1.420376
H	6.767703	2.016756	-2.805798	C	-4.313592	-0.484233	-1.799384
P	1.450062	1.822497	0.432005	C	-5.531756	-2.395571	1.436712
C	-0.069559	2.574975	1.112752	C	-6.519191	-1.791348	2.216982
C	-1.014112	3.174586	0.266425	C	-5.925169	-3.322148	0.464849
C	-0.374312	2.432128	2.473867	C	-7.866120	-2.094953	2.032697
C	-2.222107	3.639456	0.777395	H	-6.227660	-1.060574	2.973075
H	-0.794136	3.299534	-0.793464	C	-7.268622	-3.625588	0.273214
C	-1.588378	2.888305	2.976913	H	-5.168536	-3.808322	-0.153940
H	0.349402	1.973266	3.147541	C	-8.245223	-3.009780	1.055941
C	-2.516312	3.493836	2.131548	H	-8.619891	-1.605691	2.646963
H	-2.933819	4.122946	0.109040	H	-7.557150	-4.347693	-0.488764
H	-1.805060	2.780976	4.037983	H	-9.296498	-3.246821	0.904225
H	-3.465119	3.852858	2.526050	H	-3.799217	1.501142	0.183327
C	2.741812	2.114398	1.688708	C	-2.949094	-0.300879	-2.421945
C	3.641585	3.183472	1.615892	C	-2.389941	-1.307754	-3.215520
C	2.883468	1.173122	2.717920	C	-2.189840	0.851882	-2.182059
C	4.659847	3.306916	2.556761	C	-1.102004	-1.183603	-3.736958
H	3.567631	3.906345	0.805079	H	-2.975803	-2.204027	-3.423773
C	3.897690	1.302544	3.661858	C	-0.894642	0.968917	-2.674309
H	2.207467	0.315898	2.757329	H	-2.618121	1.666227	-1.595880
C	4.790985	2.368595	3.578624	C	-0.341557	-0.053027	-3.449364
H	5.358838	4.138296	2.486853	H	-0.694236	-1.972763	-4.367305
H	3.997140	0.562657	4.453837	H	-0.313864	1.870627	-2.479009
H	5.592276	2.466146	4.308193	H	0.668517	0.049661	-3.847095
C	1.894879	2.847658	-0.999395	H	-5.000428	0.307322	-2.126693
C	1.770942	4.245206	-0.982431	H	-4.743840	-1.433137	-2.157759
C	2.385813	2.219815	-2.149769	C	-5.934511	1.361378	-0.012031
C	2.139529	4.994200	-2.094917	C	-6.090988	2.748535	-0.003900
H	1.375526	4.745073	-0.097744	C	-7.040860	0.557443	-0.303107
C	2.757149	2.972356	-3.260014	C	-7.330130	3.327349	-0.262208
H	2.466367	1.132256	-2.173478	H	-5.228273	3.381025	0.214031
C	2.634276	4.358947	-3.233340	C	-8.279568	1.134324	-0.564278
H	2.037869	6.077250	-2.074252	H	-6.919424	-0.525444	-0.321211
H	3.139408	2.471677	-4.148047	C	-8.429235	2.519408	-0.542377
H	2.918051	4.948049	-4.102885	H	-7.436577	4.410582	-0.251439
H	-2.004679	0.201465	0.359977	H	-9.133353	0.495394	-0.784915
C	-3.462315	-1.429746	0.319746	H	-9.398965	2.968983	-0.746996
H	-3.332978	-2.262355	-0.389175				

IM5'

SCF energy in MeCN: -3224.918477 a.u.

Free energy in MeCN: -3224.006131 a.u.

C	0.111955	2.456685	0.147553
H	0.171994	2.858879	1.163558
H	-0.292267	3.148128	-0.592637
C	0.935356	1.385838	-0.229475
H	1.055687	1.221514	-1.302677
C	2.047505	0.818823	0.600656
H	1.832802	0.975556	1.670420
P	-3.320618	1.311585	-0.003710
C	-3.493513	2.734930	-1.151837
C	-2.602678	2.824994	-2.229737
C	-4.494102	3.702947	-1.017270
C	-2.719525	3.854429	-3.159862
H	-1.807950	2.078772	-2.326388
C	-4.600826	4.740479	-1.939013
H	-5.190421	3.644931	-0.180186
C	-3.716849	4.816148	-3.013118
H	-2.022487	3.912290	-3.994681
H	-5.378777	5.492885	-1.818889
H	-3.802473	5.628009	-3.733615
C	-4.028155	1.939557	1.566062
C	-3.130627	2.493967	2.489422
C	-5.387728	1.886719	1.896459
C	-3.580652	2.989742	3.708929
H	-2.068548	2.520344	2.234429
C	-5.835994	2.372862	3.122314
H	-6.099434	1.455573	1.192851
C	-4.935376	2.924944	4.030287
H	-2.871020	3.418889	4.414539
H	-6.895771	2.322437	3.367899
H	-5.288916	3.302683	4.988307
Pd	-1.067761	0.615653	0.079378
C	-4.616031	0.174740	-0.632670
C	-5.071163	-0.867575	0.189986
C	-5.043847	0.209002	-1.966546
C	-5.926172	-1.843673	-0.308889
H	-4.758532	-0.904589	1.233963
C	-5.897646	-0.772220	-2.463606
H	-4.707596	1.010772	-2.623917
C	-6.338261	-1.804117	-1.639707
H	-6.268276	-2.641787	0.349113
H	-6.221717	-0.726740	-3.502701
H	-7.002972	-2.572643	-2.030772
P	-1.111410	-1.710704	0.386707
C	0.400169	-2.567862	0.986696
C	1.229539	-3.335914	0.158187
C	0.830338	-2.310950	2.297176
C	2.432558	-3.852398	0.635246
H	0.932111	-3.541987	-0.869405
C	2.036474	-2.815763	2.768872
H	0.209880	-1.700074	2.954462
C	2.842453	-3.595579	1.940946
H	3.053536	-4.458646	-0.024426
H	2.346744	-2.602898	3.790784
H	3.788691	-3.990605	2.307684
C	-2.297244	-2.055065	1.758364
C	-3.088694	-3.205931	1.832834
C	-2.472425	-1.059559	2.731151
C	-4.037761	-3.351169	2.841389
H	-2.991827	-3.985076	1.078910
C	-3.415862	-1.205975	3.744264
H	-1.886139	-0.139817	2.657884
C	-4.207317	-2.351836	3.796949
H	-4.655866	-4.247511	2.873501
H	-3.547572	-0.411122	4.477154
H	-4.958762	-2.462697	4.576959
C	-1.717576	-2.776034	-0.975137
C	-1.621568	-4.175095	-0.992073
C	-2.329602	-2.132784	-2.057777
C	-2.133096	-4.907150	-2.059234
H	-1.131386	-4.692736	-0.167077
C	-2.849473	-2.864575	-3.121567
H	-2.381869	-1.041860	-2.057014
C	-2.751927	-4.253264	-3.123411
H	-2.049055	-5.992826	-2.060151
H	-3.330324	-2.346251	-3.949848
H	-3.151962	-4.828440	-3.956966
H	2.100376	-0.270442	0.464469
C	3.436251	1.438609	0.248473
H	3.275018	2.193997	-0.536868
C	4.011922	2.172466	1.470701
H	3.288884	2.956412	1.747109
H	4.041745	1.486667	2.331349
N	4.425941	0.518752	-0.311416
C	4.640418	-0.708817	0.425345

H	4.568029	-0.454662	1.496654	P	0.352769	-1.965602	-0.434057
C	4.455674	0.420321	-1.766930	P	2.383013	0.964064	-0.035499
C	5.378906	2.751981	1.245766	C	0.781343	-2.413933	1.278207
C	6.454909	2.383127	2.056347	C	1.181447	-3.702827	1.662713
C	5.619525	3.651257	0.200465	C	0.629622	-1.433038	2.264526
C	7.733296	2.890795	1.834204	C	1.476897	-3.976912	2.993338
H	6.288099	1.671511	2.866782	H	1.234988	-4.501077	0.922992
C	6.893918	4.156666	-0.030932	C	0.912690	-1.709701	3.599629
H	4.793716	3.956091	-0.444553	H	0.293881	-0.433865	1.977713
C	7.958306	3.777281	0.785668	C	1.351192	-2.979520	3.961821
H	8.556916	2.583834	2.477431	H	1.792700	-4.977965	3.280628
H	7.058413	4.853286	-0.851989	H	0.785708	-0.928831	4.348095
H	8.956262	4.173356	0.605150	H	1.578194	-3.202533	5.002484
H	3.856479	-1.476891	0.271321	C	1.762005	-2.302270	-1.554573
C	3.142423	0.147353	-2.464069	C	2.769753	-3.241352	-1.317404
C	2.603456	1.097625	-3.336472	C	1.771094	-1.588776	-2.762589
C	2.406113	-1.019684	-2.221279	C	3.755211	-3.468302	-2.274330
C	1.355088	0.910945	-3.928823	H	2.808640	-3.782209	-0.373814
H	3.168830	2.009807	-3.535539	C	2.754520	-1.821060	-3.719858
C	1.151357	-1.202282	-2.793541	H	0.992199	-0.842719	-2.949133
H	2.810890	-1.787430	-1.560345	C	3.749170	-2.765054	-3.476267
C	0.617054	-0.234605	-3.644797	H	4.540517	-4.194328	-2.071446
H	0.953644	1.668801	-4.600947	H	2.743077	-1.263444	-4.655282
H	0.580138	-2.107194	-2.582758	H	4.521346	-2.948931	-4.220571
H	-0.368017	-0.381486	-4.086830	C	-0.810330	-3.311133	-0.893090
H	5.193172	-0.354829	-2.017761	C	-1.667669	-3.875355	0.064223
H	4.863286	1.367184	-2.159283	C	-0.956960	-3.688114	-2.234589
C	5.992034	-1.321385	0.157348	C	-2.646915	-4.789257	-0.315833
C	6.135313	-2.707083	0.066220	H	-1.561780	-3.610175	1.116839
C	7.128215	-0.516586	0.018016	C	-1.937615	-4.599788	-2.610000
C	7.387154	-3.284248	-0.134615	H	-0.298119	-3.265681	-2.992974
H	5.247261	-3.336270	0.148974	C	-2.789567	-5.148625	-1.653805
C	8.378812	-1.090453	-0.183621	H	-3.297220	-5.226129	0.440191
H	7.010473	0.566128	0.058680	H	-2.034219	-4.885471	-3.655547
C	8.514169	-2.476290	-0.256320	H	-3.556784	-5.860825	-1.950124
H	7.480807	-4.367015	-0.205723	C	3.745804	-0.252065	0.186361
H	9.254393	-0.450328	-0.286207	C	4.729436	-0.445172	-0.791322
H	9.493655	-2.924236	-0.416446	C	3.795995	-1.036562	1.348635
				C	5.735750	-1.388637	-0.606297
IM6'				H	4.729372	0.152771	-1.699363
SCF energy in MeCN: -3224.735181 a.u.				C	4.797203	-1.985283	1.525356
Free energy in MeCN: -3223.82131 a.u.				H	3.064357	-0.889000	2.138795
				C	5.772127	-2.165983	0.547422
Pd	-0.009537	0.457602	-0.676291	H	6.496140	-1.514010	-1.375299

H	4.819079	-2.574333	2.440789
H	6.561421	-2.901916	0.688459
C	2.291150	1.787854	1.595190
C	1.069504	2.326950	2.017731
C	3.411551	1.915750	2.427620
C	0.966358	2.967252	3.250046
H	0.191757	2.239178	1.370320
C	3.303630	2.547630	3.662631
H	4.371411	1.512792	2.107375
C	2.080556	3.070515	4.078666
H	0.010322	3.384849	3.566539
H	4.179949	2.633534	4.301836
H	1.998464	3.563099	5.045610
C	3.140029	2.216962	-1.136322
C	3.571647	3.465362	-0.674588
C	3.250277	1.926584	-2.504293
C	4.109750	4.395460	-1.561289
H	3.486920	3.717129	0.381364
C	3.799108	2.852719	-3.384980
H	2.909108	0.958754	-2.877117
C	4.227556	4.091923	-2.914358
H	4.441328	5.362384	-1.188209
H	3.885411	2.608530	-4.442145
H	4.649186	4.820483	-3.603401
C	-2.211450	0.457068	-0.793567
C	-0.106454	2.529136	-1.343814
H	-1.016707	2.985278	-0.948661
C	-0.144129	2.142542	-2.728890
H	0.806947	1.856838	-3.187332
C	-1.254447	2.120163	-3.518164
H	-2.215189	2.475619	-3.142114
H	-1.218023	1.802362	-4.557212
H	0.796284	3.044686	-1.010369
H	-2.385782	1.420063	-1.276473
N	-2.645744	0.536201	0.530331
C	-3.619207	1.596723	0.888282
H	-3.761892	1.541927	1.973233
H	-4.580737	1.334127	0.411535
C	-2.773365	-0.692688	1.296146
H	-3.746218	-1.173499	1.081694
H	-2.005407	-1.378759	0.909750
C	-2.723615	-0.676926	-1.672304
H	-2.187321	-0.623405	-2.631632
H	-2.510894	-1.657133	-1.238770
C	-4.211736	-0.527856	-1.866638
C	-5.102299	-1.427642	-1.271871
C	-4.734916	0.546732	-2.595848
C	-6.478911	-1.252949	-1.392510
H	-4.704552	-2.286519	-0.727807
C	-6.109125	0.724857	-2.717816
H	-4.048861	1.242709	-3.082258
C	-6.985698	-0.171854	-2.108585
H	-7.158283	-1.967315	-0.931283
H	-6.498574	1.560901	-3.296283
H	-8.060682	-0.034060	-2.202748
C	-2.601985	-0.535195	2.783270
C	-3.177005	-1.477298	3.638546
C	-1.832049	0.491750	3.334683
C	-2.981775	-1.399682	5.014344
H	-3.786524	-2.279687	3.219955
C	-1.646601	0.581249	4.710869
H	-1.368867	1.219283	2.666883
C	-2.220070	-0.366642	5.555575
H	-3.436696	-2.141499	5.667548
H	-1.046522	1.391158	5.124277
H	-2.079734	-0.296971	6.632250
C	-3.193277	2.974912	0.480825
C	-2.290989	3.700630	1.263892
C	-3.663963	3.541508	-0.706806
C	-1.840277	4.951190	0.852256
H	-1.946740	3.276925	2.208750
C	-3.216687	4.793572	-1.122338
H	-4.385259	2.985400	-1.308877
C	-2.297050	5.495880	-0.347218
H	-1.134556	5.504773	1.469774
H	-3.587556	5.221380	-2.051786
H	-1.944260	6.472789	-0.671132

IM7'

SCF energy in MeCN: -3224.878774 a.u.

Free energy in MeCN: -3223.966569 a.u.

Pd	0.035644	0.474218	-0.681536
P	0.570282	-1.886853	-0.518506
P	2.317668	1.141398	-0.010737
C	1.009081	-2.386038	1.185696
C	1.479398	-3.658671	1.541836
C	0.784286	-1.446417	2.197606

C	1.770894	-3.954769	2.868945	C	0.646748	2.821786	3.343285
H	1.588945	-4.429872	0.779557	H	-0.021209	2.060863	1.433246
C	1.064647	-1.743964	3.528810	C	3.019901	2.733489	3.746922
H	0.388030	-0.464700	1.925445	H	4.219378	1.909299	2.162271
C	1.570997	-2.995665	3.863326	C	1.735108	3.057228	4.178856
H	2.141927	-4.943975	3.133010	H	-0.361517	3.075701	3.672405
H	0.874935	-0.994595	4.296514	H	3.876817	2.918977	4.392560
H	1.792942	-3.235973	4.901798	H	1.584516	3.493416	5.165102
C	2.028332	-2.136777	-1.606735	C	3.007045	2.474297	-1.067387
C	3.072115	-3.035346	-1.372793	C	3.517903	3.675868	-0.568384
C	2.035631	-1.385768	-2.791883	C	2.990539	2.271133	-2.453858
C	4.087034	-3.194917	-2.312512	C	4.012509	4.645972	-1.437048
H	3.111831	-3.600143	-0.443483	H	3.519520	3.863122	0.504552
C	3.050133	-1.547759	-3.731268	C	3.496698	3.235010	-3.319602
H	1.229173	-0.665301	-2.961842	H	2.566287	1.347093	-2.852075
C	4.076771	-2.458656	-3.494213	C	4.007499	4.427241	-2.811682
H	4.899970	-3.891280	-2.110593	H	4.399971	5.580610	-1.034871
H	3.039165	-0.957655	-4.646894	H	3.476075	3.061510	-4.394401
H	4.873220	-2.587663	-4.225474	H	4.391586	5.188779	-3.488107
C	-0.489675	-3.299983	-1.039990	C	-2.105232	0.396276	-0.782707
C	-1.316828	-3.956941	-0.117121	C	-0.322838	2.553501	-1.193338
C	-0.609837	-3.628319	-2.397078	H	-1.184268	2.934931	-0.631667
C	-2.243786	-4.904311	-0.543078	C	-0.545411	2.555051	-2.638147
H	-1.235912	-3.727050	0.945454	H	0.327909	2.313218	-3.256780
C	-1.534857	-4.576612	-2.819583	C	-1.709740	2.792594	-3.273127
H	0.020983	-3.128598	-3.132443	H	-2.600605	3.088948	-2.716785
C	-2.360618	-5.213333	-1.895606	H	-1.803081	2.729305	-4.355834
H	-2.877988	-5.401965	0.189683	H	0.571160	3.122782	-0.908092
H	-1.613299	-4.816602	-3.878603	H	-2.404024	1.369143	-1.183545
H	-3.089586	-5.949450	-2.229547	N	-2.606466	0.326145	0.577167
C	3.796605	0.070518	0.232214	C	-3.821892	1.104080	0.862176
C	4.771093	-0.072759	-0.764460	H	-4.084381	0.901305	1.911029
C	3.916130	-0.710443	1.391928	H	-4.677333	0.765601	0.247312
C	5.831602	-0.958272	-0.599895	C	-2.619489	-0.989166	1.174360
H	4.708398	0.518133	-1.677237	H	-3.480503	-1.609106	0.844882
C	4.971315	-1.602030	1.550021	H	-1.725531	-1.504187	0.790707
H	3.187393	-0.608971	2.192606	C	-2.591186	-0.681905	-1.756564
C	5.936318	-1.730190	0.554127	H	-2.035763	-0.537263	-2.696930
H	6.577760	-1.049448	-1.388427	H	-2.336733	-1.684443	-1.393729
H	5.036469	-2.194929	2.461687	C	-4.074018	-0.622533	-2.019202
H	6.765185	-2.425765	0.676910	C	-4.930771	-1.625018	-1.554637
C	2.123423	1.917875	1.642920	C	-4.635189	0.465534	-2.698518
C	0.836461	2.257408	2.083842	C	-6.308840	-1.534645	-1.737029
C	3.212763	2.170400	2.488865	H	-4.502399	-2.490561	-1.044486

C	-6.010072	0.557625	-2.888780
H	-3.970749	1.248510	-3.071115
C	-6.854690	-0.438271	-2.398782
H	-6.958873	-2.324491	-1.361922
H	-6.427415	1.411847	-3.421571
H	-7.931671	-0.362544	-2.540057
C	-2.552318	-0.994316	2.679548
C	-3.053857	-2.080598	3.400656
C	-1.930067	0.041115	3.382162
C	-2.931714	-2.135668	4.786409
H	-3.548784	-2.891755	2.862903
C	-1.817899	-0.001961	4.768198
H	-1.523128	0.875635	2.811154
C	-2.316551	-1.093476	5.476598
H	-3.328401	-2.991127	5.331459
H	-1.330639	0.817422	5.297299
H	-2.230817	-1.130642	6.561411
C	-3.609640	2.580550	0.678520
C	-2.762652	3.283665	1.540702
C	-4.218607	3.272509	-0.369274
C	-2.515743	4.638560	1.353959
H	-2.290062	2.746993	2.364566
C	-3.977615	4.632024	-0.560780
H	-4.877275	2.727209	-1.047710
C	-3.121849	5.316705	0.296549
H	-1.845930	5.168183	2.031041
H	-4.452494	5.154705	-1.389797
H	-2.925752	6.376518	0.142728

TS2a'

SCF energy in MeCN: -3224.744917 a.u.

Free energy in MeCN: -3223.832871 a.u.

C	0.361327	-2.739139	0.294170
H	0.308626	-2.907518	1.372367
H	0.864870	-3.520389	-0.272068
C	-0.598550	-1.920813	-0.329582
H	-0.691654	-1.964564	-1.415437
C	-1.339900	-0.940969	0.360226
H	-1.300999	-0.890420	1.448975
P	3.473287	-1.161188	0.208634
C	3.869202	-2.679105	-0.727906
C	3.095347	-3.009748	-1.847918
C	4.967763	-3.478723	-0.396014
C	3.420860	-4.117136	-2.626375
H	2.229619	-2.391309	-2.101668
C	5.284401	-4.591619	-1.168936
H	5.576164	-3.231779	0.473647
C	4.514745	-4.910163	-2.285538
H	2.815387	-4.365790	-3.496190
H	6.137489	-5.210955	-0.899548
H	4.765398	-5.780009	-2.889147
C	4.075201	-1.472975	1.902710
C	3.171678	-1.996837	2.836553
C	5.395496	-1.225389	2.299634
C	3.577317	-2.274676	4.137419
H	2.139275	-2.177146	2.530862
C	5.797267	-1.495009	3.605173
H	6.109527	-0.815484	1.586401
C	4.891796	-2.019579	4.524340
H	2.866629	-2.685647	4.851784
H	6.824952	-1.297012	3.903388
H	5.210408	-2.230380	5.543284
Pd	1.154762	-0.680808	0.132876
C	4.639561	0.061558	-0.482718
C	4.908095	1.238781	0.231521
C	5.172862	-0.085819	-1.770087
C	5.674075	2.250078	-0.337768
H	4.528373	1.356364	1.245987
C	5.948174	0.925563	-2.330742
H	4.986019	-0.996798	-2.338122
C	6.193285	2.098661	-1.622069
H	5.871684	3.156805	0.232176
H	6.364862	0.792697	-3.327701
H	6.794379	2.889953	-2.065646
P	1.089358	1.699421	0.197465
C	-0.573997	2.405207	0.508623
C	-1.374475	2.889036	-0.535287
C	-1.125152	2.326283	1.795433
C	-2.680987	3.306578	-0.291536
H	-0.967826	2.961558	-1.544048
C	-2.433527	2.734473	2.035057
H	-0.517941	1.953319	2.621330
C	-3.215893	3.230675	0.992797
H	-3.280391	3.701166	-1.111788
H	-2.838954	2.678752	3.044332
H	-4.236293	3.561183	1.183712
C	2.066025	2.283316	1.631321

C	2.749985	3.502726	1.673682	C	-2.209223	-2.140298	-3.523345
C	2.176028	1.406352	2.719235	C	-2.103366	0.091386	-2.639432
C	3.532000	3.829740	2.778166	C	-0.945999	-1.976788	-4.092235
H	2.706502	4.186072	0.827353	H	-2.739506	-3.085133	-3.646342
C	2.950490	1.737672	3.827046	C	-0.833392	0.250690	-3.183806
H	1.672228	0.437328	2.676090	H	-2.536862	0.909943	-2.064332
C	3.635631	2.949724	3.854219	C	-0.248255	-0.785324	-3.911482
H	4.071170	4.775300	2.794091	H	-0.502687	-2.789929	-4.664351
H	3.031468	1.040029	4.658609	H	-0.292947	1.186662	-3.038390
H	4.254942	3.207589	4.710810	H	0.744858	-0.657234	-4.340595
C	1.691221	2.592565	-1.269288	H	-4.944614	-0.810636	-2.709103
C	1.543859	3.978628	-1.432645	H	-4.408932	-2.390996	-2.159228
C	2.311111	1.851803	-2.282810	C	-6.352378	0.504524	-0.734803
C	2.027443	4.606415	-2.575437	C	-6.981529	1.751951	-0.772404
H	1.028054	4.562654	-0.669990	C	-7.129653	-0.650351	-0.800468
C	2.791015	2.481303	-3.427644	C	-8.365642	1.842821	-0.857527
H	2.401723	0.769526	-2.170158	H	-6.377399	2.660392	-0.729189
C	2.654619	3.859150	-3.571706	C	-8.516594	-0.560602	-0.889645
H	1.908774	5.681655	-2.692685	H	-6.648735	-1.626878	-0.750988
H	3.274126	1.893707	-4.206427	C	-9.138203	0.683688	-0.914312
H	3.028398	4.353189	-4.466468	H	-8.843955	2.820193	-0.883203
H	-1.731835	-0.069086	-0.153364	H	-9.112362	-1.470821	-0.928292
C	-3.657960	-1.541429	0.236200	H	-10.221828	0.753385	-0.981172
H	-3.405845	-2.564365	-0.043933				
C	-3.942171	-1.247644	1.681600	**TS2b'**			
H	-3.339986	-1.951588	2.271369	SCF energy in MeCN: -3224.730095 a.u.			
H	-3.572825	-0.244247	1.947375	Free energy in MeCN: -3223.817672 a.u.			
N	-4.254457	-0.844324	-0.763248				
C	-4.852970	0.466759	-0.565776	Pd	0.020004	0.209084	-0.206934
H	-4.572996	0.822101	0.433079	P	1.044783	-1.903563	-0.038523
C	-4.153637	-1.322212	-2.143057	P	1.954817	1.596758	-0.434394
C	-5.403204	-1.358938	2.057981	C	1.951496	-2.278234	1.494537
C	-6.118367	-0.240762	2.490279	C	2.582480	-3.517099	1.686442
C	-6.069118	-2.584189	1.953489	C	1.973777	-1.335153	2.526009
C	-7.472079	-0.335974	2.800983	C	3.262923	-3.781313	2.868936
H	-5.607713	0.721926	2.573488	H	2.525108	-4.280571	0.910540
C	-7.420167	-2.684973	2.267473	C	2.649386	-1.605199	3.713949
H	-5.520007	-3.468170	1.624697	H	1.450502	-0.384726	2.394547
C	-8.126084	-1.559135	2.688172	C	3.302364	-2.822647	3.881767
H	-8.017389	0.548284	3.125615	H	3.754893	-4.742053	3.006672
H	-7.924242	-3.646365	2.186104	H	2.655893	-0.863235	4.510559
H	-9.184728	-1.636230	2.927657	H	3.831455	-3.034544	4.808932
H	-4.388705	1.179522	-1.264687	C	2.211030	-2.051996	-1.438908
C	-2.799281	-1.113531	-2.781762	C	3.503257	-2.574219	-1.339571

C	1.751941	-1.609250	-2.689198	C	1.727867	1.995598	-3.189401
C	4.305492	-2.678886	-2.473335	C	1.220074	4.724367	-3.004975
H	3.899003	-2.880986	-0.373300	H	1.479249	4.493918	-0.884453
C	2.552768	-1.723587	-3.821393	C	1.486160	2.736618	-4.340367
H	0.755408	-1.163657	-2.768241	H	1.897590	0.920860	-3.262060
C	3.832478	-2.264344	-3.715046	C	1.225882	4.103137	-4.250002
H	5.313293	-3.079704	-2.379253	H	1.011304	5.789347	-2.927225
H	2.177805	-1.383879	-4.785749	H	1.487149	2.242412	-5.310380
H	4.463448	-2.350820	-4.597325	H	1.021080	4.680230	-5.149161
C	-0.006578	-3.400262	-0.220758	C	-2.842406	0.258750	-0.461478
C	-0.601279	-3.954894	0.924542	C	-1.565236	2.087849	-0.803310
C	-0.280990	-3.977782	-1.468118	C	-1.789487	2.223252	-2.231745
C	-1.435000	-5.063633	0.823697	H	-0.932259	1.998805	-2.875254
H	-0.393757	-3.522193	1.904347	C	-2.964741	2.522404	-2.817503
C	-1.108480	-5.093571	-1.562985	H	-3.841203	2.788363	-2.223712
H	0.173209	-3.571674	-2.370665	H	-3.072792	2.573743	-3.898194
C	-1.685878	-5.641542	-0.420269	H	-2.293301	2.587553	-0.160048
H	-1.877115	-5.487739	1.724095	H	-3.541929	0.989347	-0.866663
H	-1.297977	-5.538022	-2.537879	N	-3.161985	-0.101100	0.803812
H	-2.328595	-6.516249	-0.497204	C	-4.271951	0.561044	1.525193
C	3.634350	0.892226	-0.496856	H	-4.132175	0.326038	2.587338
C	4.422392	0.836181	-1.651699	H	-5.208398	0.078574	1.200509
C	4.139936	0.355435	0.697019	C	-2.603129	-1.260298	1.476598
C	5.686071	0.252815	-1.606383	H	-3.415166	-1.968812	1.711011
H	4.062319	1.262745	-2.585784	H	-1.947899	-1.786402	0.772539
C	5.395011	-0.237640	0.734832	C	-2.493289	-0.782939	-1.501895
H	3.551613	0.422704	1.609812	H	-2.135697	-0.249381	-2.391404
C	6.172826	-0.291518	-0.420981	H	-1.701568	-1.476108	-1.188560
H	6.293458	0.225208	-2.509351	C	-3.753348	-1.559888	-1.800494
H	5.766593	-0.649934	1.671754	C	-3.939110	-2.839294	-1.272463
H	7.160443	-0.748301	-0.394978	C	-4.778948	-0.973946	-2.548518
C	2.074705	2.808494	0.928694	C	-5.122653	-3.533504	-1.506549
C	0.958624	3.089715	1.725797	H	-3.139535	-3.298799	-0.688715
C	3.261211	3.524307	1.143645	C	-5.962210	-1.667186	-2.782703
C	1.021470	4.073882	2.709283	H	-4.634567	0.030940	-2.953132
H	0.032694	2.534094	1.573403	C	-6.136912	-2.948035	-2.260606
C	3.323696	4.500419	2.131970	H	-5.250753	-4.536105	-1.100763
H	4.136614	3.314788	0.529916	H	-6.750790	-1.208652	-3.376433
C	2.203678	4.779680	2.914026	H	-7.062714	-3.489515	-2.444738
H	0.142002	4.288007	3.315550	C	-1.836437	-0.902454	2.724540
H	4.250012	5.049127	2.289795	C	-1.682764	-1.830711	3.756585
H	2.255443	5.547180	3.683545	C	-1.256916	0.361569	2.860115
C	1.749842	2.618832	-1.930695	C	-0.955804	-1.504645	4.898470
C	1.483887	3.991612	-1.850562	H	-2.149330	-2.813372	3.669284

C	-0.540767	0.696226	4.007286
H	-1.398362	1.088868	2.057672
C	-0.387692	-0.238553	5.028337
H	-0.844682	-2.236497	5.696041
H	-0.099334	1.688230	4.101480
H	0.165488	0.021203	5.928976
C	-4.350279	2.046507	1.331837
C	-3.625971	2.911022	2.159971
C	-5.124248	2.588405	0.302133
C	-3.651779	4.284689	1.942350
H	-3.041086	2.499135	2.983788
C	-5.149278	3.963092	0.080663
H	-5.710030	1.922164	-0.334674
C	-4.405911	4.812476	0.895479
H	-3.087809	4.948146	2.595677
H	-5.753807	4.371114	-0.727151
H	-4.425299	5.886743	0.724497
H	-0.571060	2.445997	-0.509391

TS2c'

SCF energy in MeCN: -3224.830545 a.u.

Free energy in MeCN: -3223.920101 a.u.

Pd	0.090222	0.179599	-0.329450
P	0.416743	-2.122787	-0.363937
P	2.126875	1.366187	-0.180642
C	1.643146	-2.801363	0.822685
C	2.177946	-4.092070	0.690607
C	1.941203	-2.060463	1.967467
C	3.021936	-4.609762	1.664806
H	1.917332	-4.695884	-0.179494
C	2.761227	-2.594165	2.961142
H	1.516503	-1.058981	2.075408
C	3.310653	-3.861759	2.806996
H	3.440619	-5.608116	1.545487
H	2.976704	-2.003739	3.851247
H	3.961288	-4.273793	3.577413
C	1.120419	-2.420874	-2.031641
C	2.449709	-2.796609	-2.256391
C	0.328689	-2.082316	-3.143409
C	2.966940	-2.844119	-3.550048
H	3.095171	-3.030949	-1.412221
C	0.837840	-2.153623	-4.434897
H	-0.691069	-1.726050	-2.981452
C	2.164340	-2.532881	-4.642979
H	4.008706	-3.126133	-3.700633
H	0.203482	-1.890522	-5.280416
H	2.571431	-2.572655	-5.652048
C	-0.837882	-3.475055	-0.178796
C	-1.232356	-3.805484	1.129991
C	-1.505376	-4.096092	-1.242402
C	-2.246215	-4.727847	1.364658
H	-0.716046	-3.343512	1.974622
C	-2.521542	-5.019665	-1.006420
H	-1.219619	-3.870349	-2.268787
C	-2.897567	-5.341340	0.295041
H	-2.523615	-4.973620	2.389381
H	-3.018811	-5.495879	-1.850199
H	-3.692133	-6.063444	0.474752
C	3.623445	0.450013	0.358409
C	4.276334	-0.394137	-0.550309
C	4.042179	0.432960	1.696782
C	5.316567	-1.220000	-0.137530
H	3.964684	-0.407782	-1.594844
C	5.101448	-0.373058	2.101513
H	3.527598	1.051838	2.432756
C	5.741874	-1.206454	1.188604
H	5.802952	-1.872458	-0.862893
H	5.414823	-0.363196	3.144954
H	6.560903	-1.847463	1.510466
C	2.237084	2.939628	0.767796
C	1.043383	3.646893	0.960377
C	3.420401	3.474090	1.296126
C	1.026078	4.837806	1.680585
H	0.118900	3.242589	0.539034
C	3.403041	4.662184	2.021975
H	4.363879	2.950989	1.142696
C	2.204928	5.343469	2.223314
H	0.086583	5.369478	1.830887
H	4.331682	5.058828	2.429773
H	2.190730	6.267165	2.799405
C	2.616463	1.904529	-1.875611
C	3.368466	3.056290	-2.135669
C	2.205996	1.113466	-2.958858
C	3.705008	3.401971	-3.441551
H	3.689649	3.694617	-1.313094
C	2.554247	1.452862	-4.262833
H	1.598676	0.225543	-2.769537
C	3.303002	2.600605	-4.507872

H	4.285719	4.304544	-3.627058
H	2.228629	0.820076	-5.087529
H	3.567393	2.875279	-5.527790
C	-2.565732	0.591077	-0.345973
C	-1.199677	1.882219	-1.704801
C	-1.957027	1.623461	-2.904916
H	-1.494143	0.930983	-3.618860
C	-3.187588	2.100589	-3.191979
H	-3.679832	2.817866	-2.532430
H	-3.710559	1.837891	-4.109199
H	-0.121105	1.890604	-1.888762
N	-2.565072	0.659732	1.037807
C	-3.410521	1.643473	1.732843
H	-2.987723	1.763849	2.740861
H	-4.422424	1.211570	1.854751
C	-2.232545	-0.481405	1.863202
H	-3.145346	-0.849995	2.367765
H	-1.905446	-1.297148	1.207617
C	-2.962616	-0.698988	-1.036082
H	-2.808756	-0.549694	-2.112373
H	-2.345696	-1.547527	-0.734250
C	-4.409252	-0.999128	-0.731818
C	-4.744339	-2.076689	0.092998
C	-5.433526	-0.177086	-1.214116
C	-6.072600	-2.332694	0.424729
H	-3.949280	-2.726303	0.465379
C	-6.761281	-0.429958	-0.882638
H	-5.171098	0.664529	-1.860718
C	-7.084694	-1.507433	-0.058261
H	-6.316956	-3.182656	1.060994
H	-7.549419	0.213596	-1.272345
H	-8.123443	-1.704262	0.202194
C	-1.155933	-0.216707	2.887577
C	-0.952664	-1.139823	3.915764
C	-0.316937	0.897763	2.809118
C	0.080519	-0.968684	4.832408
H	-1.610600	-2.008155	3.991331
C	0.711243	1.081021	3.732727
H	-0.470203	1.615066	2.001680
C	0.916829	0.143141	4.742873
H	0.233870	-1.705673	5.619293
H	1.350505	1.961727	3.654879
H	1.721354	0.281837	5.464103
C	-3.503677	2.975846	1.052222
C	-2.500597	3.933474	1.223818
C	-4.577995	3.269502	0.208422
C	-2.555819	5.146779	0.544414
H	-1.670137	3.716676	1.898716
C	-4.639960	4.485176	-0.467589
H	-5.363317	2.523960	0.071927
C	-3.623047	5.422468	-0.307932
H	-1.763702	5.882909	0.675468
H	-5.480311	4.697311	-1.126660
H	-3.663072	6.369454	-0.842974
H	-1.509129	2.763314	-1.133337
H	-3.157452	1.411030	-0.748611

IM1''

SCF energy in MeCN: -3179.321517 a.u.

Free energy in MeCN: -3178.515335 a.u.

C	1.833268	0.137918	0.946011
H	1.706717	0.398967	-0.112229
H	1.914460	-0.953540	1.012450
C	0.751757	0.700877	1.796371
H	0.716025	0.325396	2.822643
C	0.192018	1.967470	1.518824
H	0.570035	2.558771	0.680473
P	-1.501593	-1.848746	0.480061
C	-1.850866	-2.749869	2.037918
C	-1.592274	-2.102046	3.251439
C	-2.364289	-4.053777	2.062467
C	-1.833626	-2.743714	4.464096
H	-1.206940	-1.080371	3.227825
C	-2.607901	-4.693016	3.273651
H	-2.578112	-4.565775	1.123890
C	-2.343248	-4.038631	4.476171
H	-1.629281	-2.227290	5.400541
H	-3.006165	-5.706472	3.280033
H	-2.537816	-4.539789	5.423068
C	0.014371	-2.638853	-0.179166
C	0.630162	-2.035221	-1.286747
C	0.635775	-3.739203	0.419539
C	1.830027	-2.526200	-1.788262
H	0.168507	-1.153422	-1.738838
C	1.843433	-4.224033	-0.078991
H	0.183119	-4.213251	1.289354
C	2.441947	-3.621421	-1.181151

H	2.308368	-2.031085	-2.631419	C	-6.960611	1.721180	0.693944
H	2.322158	-5.073884	0.405002	H	-5.690871	2.568060	-0.824912
H	3.390994	-3.994859	-1.560487	C	-5.884713	0.264742	2.288020
Pd	-1.151257	0.469014	0.787419	H	-3.760042	-0.031295	2.000044
O	3.125837	0.687908	1.375026	C	-7.032131	0.895376	1.815251
C	4.102207	0.610695	0.472527	H	-7.854491	2.225543	0.330054
O	4.012874	0.108769	-0.631166	H	-5.931174	-0.369260	3.172060
C	-2.826007	-2.501394	-0.615823	H	-7.983335	0.753221	2.325870
C	-2.581847	-2.978943	-1.907433	H	-0.251490	2.556585	2.322082
C	-4.152935	-2.445766	-0.162952	C	5.365013	1.314172	0.982496
C	-3.634665	-3.400965	-2.716487	H	5.556362	0.962700	2.002738
H	-1.561149	-3.030649	-2.284972	N	6.508212	0.950033	0.163207
C	-5.201927	-2.868335	-0.970762	H	6.564189	1.436296	-0.723940
H	-4.365523	-2.081773	0.841908	C	6.762054	-0.401934	0.072248
C	-4.945642	-3.351597	-2.252380	O	6.416008	-1.207691	0.917191
H	-3.423741	-3.771330	-3.719051	O	7.462065	-0.655544	-1.052216
H	-6.223228	-2.819013	-0.594489	C	7.658081	-2.051537	-1.461969
H	-5.765522	-3.683229	-2.887882	C	8.543726	-2.777289	-0.461922
P	-2.954407	1.468832	-0.309871	H	9.486912	-2.236046	-0.322460
C	-2.939814	3.281426	-0.613843	H	8.047320	-2.874789	0.505712
C	-2.620352	4.107925	0.471922	H	8.782607	-3.779149	-0.840102
C	-3.229688	3.871559	-1.848938	C	6.303095	-2.723763	-1.634627
C	-2.605555	5.490332	0.331640	H	5.795281	-2.848758	-0.675070
H	-2.376461	3.651423	1.432627	H	5.658322	-2.121231	-2.286153
C	-3.201882	5.257727	-1.991301	H	6.436438	-3.710348	-2.096044
H	-3.478483	3.245359	-2.705622	C	8.362369	-1.905752	-2.800432
C	-2.893213	6.069153	-0.903609	H	8.571013	-2.893450	-3.227144
H	-2.357307	6.118226	1.185723	H	7.740643	-1.347759	-3.509351
H	-3.425293	5.704309	-2.959217	H	9.312835	-1.372934	-2.684502
H	-2.871432	7.151613	-1.018060	C	5.180818	2.813361	0.981713
C	-3.152476	0.789683	-1.998474	C	5.718305	3.596181	2.003907
C	-4.350650	0.306871	-2.531007	C	4.500002	3.439249	-0.066635
C	-1.989513	0.720517	-2.782483	C	5.575139	4.980075	1.983029
C	-4.386884	-0.223573	-3.818942	H	6.252211	3.111736	2.820967
H	-5.259409	0.322024	-1.931252	C	4.355423	4.823044	-0.088795
C	-2.030195	0.203802	-4.072143	H	4.071954	2.831826	-0.866091
H	-1.045189	1.078953	-2.365368	C	4.892944	5.596510	0.936687
C	-3.232789	-0.270054	-4.594649	H	5.995726	5.579454	2.788825
H	-5.325485	-0.611191	-4.212681	H	3.817872	5.298179	-0.907563
H	-1.119589	0.163840	-4.668228	H	4.777741	6.678923	0.922521
H	-3.266132	-0.685557	-5.600671				
C	-4.588516	1.262126	0.495968	**1a''**			
C	-5.745928	1.909040	0.042754	SCF energy in MeCN: -978.270089 a.u.			
C	-4.669809	0.451271	1.633022	Free energy in MeCN: -977.970262 a.u.			

2a''

SCF energy in MeCN: -789.651315 a.u.

Free energy in MeCN: -789.361704 a.u.

C	1.273351	0.577113	0.913231
C	0.645318	1.663421	0.032147
O	1.206511	2.244956	-0.864481
O	-0.607932	1.935353	0.454201
C	-1.325618	2.855640	-0.393243
H	-0.700100	3.746535	-0.539652
H	-1.465092	2.386279	-1.376154
C	-2.616018	3.178499	0.265579
H	-2.547361	3.557068	1.287316
C	-3.801829	3.066052	-0.329334
H	-3.894347	2.684037	-1.345980
H	-4.724629	3.355807	0.167859
N	0.318404	-0.488280	1.196702
H	1.464862	1.061163	1.882367
H	0.059024	-0.659032	2.156802
C	-0.582042	-0.877137	0.245152
O	-0.499268	-0.566162	-0.933426
O	-1.534638	-1.640270	0.813341
C	-2.675637	-2.088313	-0.001065
C	-3.535233	-2.815990	1.018788
H	-4.429582	-3.224389	0.534920
H	-2.982043	-3.644291	1.474900
H	-3.855572	-2.136184	1.816149
C	-2.199433	-3.039317	-1.086239
H	-1.560035	-2.527533	-1.809022
H	-1.640785	-3.874492	-0.648153
H	-3.064909	-3.454190	-1.617015
C	-3.412865	-0.882183	-0.563980
H	-3.608964	-0.149102	0.227737
H	-2.838220	-0.392686	-1.353947
H	-4.376706	-1.201348	-0.978875
C	2.593141	0.078512	0.374040
C	3.729032	0.126947	1.181218
C	2.693302	-0.462493	-0.911246
C	4.950989	-0.359988	0.722887
H	3.657009	0.553462	2.183222
C	3.911689	-0.950710	-1.368104
H	1.809440	-0.491181	-1.544233
C	5.042829	-0.902721	-0.554279
H	5.829075	-0.314925	1.364883
H	3.981818	-1.367706	-2.371490
H	5.995046	-1.284349	-0.918937
C	0.077256	3.069180	-0.465689
H	-0.959678	2.828137	-0.226000
H	0.423135	4.058544	-0.173282
C	0.871541	2.197026	-1.089380
H	1.905834	2.477488	-1.300817
C	0.454785	0.812587	-1.467038
H	-0.622729	0.785194	-1.676794
H	0.970513	0.483627	-2.379852
C	0.721342	-0.243031	-0.359991
C	2.193552	-0.427741	-0.082464
C	2.928557	0.502803	0.660121
C	2.862347	-1.534285	-0.610026
C	4.292583	0.326134	0.872027
H	2.436044	1.385824	1.069190
C	4.227052	-1.712901	-0.403463
H	2.299370	-2.268685	-1.187132
C	4.946672	-0.782497	0.340642
H	4.846945	1.060034	1.454635
H	4.727648	-2.585347	-0.820296
H	0.317591	-1.194101	-0.727710
N	0.005351	0.067545	0.871103
H	0.451820	0.702177	1.518623
C	-1.359783	0.099686	0.984986
O	-1.944953	0.654923	1.898575
O	-1.928676	-0.590279	-0.031117
C	-3.391926	-0.623398	-0.150419
C	-3.927674	0.789247	-0.325957
H	-5.002875	0.752730	-0.538504
H	-3.770274	1.388004	0.574426
H	-3.436632	1.284265	-1.173440
C	-3.595608	-1.438300	-1.416880
H	-3.169585	-2.441696	-1.307105
H	-4.664827	-1.539946	-1.634260
H	-3.114697	-0.953253	-2.274428
C	-4.002648	-1.327705	1.050404
H	-3.858779	-0.747497	1.964093
H	-5.078071	-1.468072	0.886480
H	-3.550697	-2.317203	1.185269
H	6.013235	-0.921029	0.508281

IM4''

SCF energy in MeCN: -2990.549443 a.u.

Free energy in MeCN: -2989.749846 a.u.

C	1.559928	-1.459922	1.294288
H	1.738947	-2.096002	0.423903
H	1.168216	-1.957655	2.180601
C	2.098967	-0.197493	1.357062
H	2.083581	0.329113	2.315056
C	2.894158	0.416653	0.249289
H	2.511100	0.090717	-0.727985
P	-1.980245	-1.315755	0.902032
C	-1.795128	-2.204519	2.478404
C	-1.161106	-1.549227	3.543835
C	-2.292405	-3.499166	2.663919
C	-1.036653	-2.174673	4.779669
H	-0.758393	-0.543694	3.392613
C	-2.157670	-4.124623	3.900506
H	-2.783591	-4.017441	1.841121
C	-1.533308	-3.465099	4.956763
H	-0.545041	-1.659377	5.602075
H	-2.543645	-5.132416	4.038700
H	-1.428749	-3.959459	5.920229
C	-2.227217	-2.586955	-0.374818
C	-1.093768	-3.188665	-0.938069
C	-3.499322	-3.001535	-0.791557
C	-1.227153	-4.185797	-1.897869
H	-0.101334	-2.869739	-0.617215
C	-3.628234	-3.995156	-1.757804
H	-4.390839	-2.552789	-0.356738
C	-2.496067	-4.586495	-2.312853
H	-0.338920	-4.651167	-2.321026
H	-4.620253	-4.312268	-2.072910
H	-2.602742	-5.364075	-3.066346
Pd	-0.073683	0.034596	0.561393
C	-3.572927	-0.448380	1.031461
C	-4.142645	0.095043	-0.131063
C	-4.188552	-0.214636	2.267734
C	-5.300598	0.859318	-0.055777
H	-3.681346	-0.094184	-1.100432
C	-5.348576	0.552874	2.335982
H	-3.766511	-0.637069	3.178614
C	-5.903106	1.095159	1.179128
H	-5.733235	1.271600	-0.965851
H	-5.824079	0.721165	3.300351
H	-6.807630	1.696915	1.237860
P	-0.925881	1.838763	-0.652585
C	0.591554	2.732182	-1.123264
C	1.147809	3.640655	-0.207311
C	1.303906	2.409328	-2.285190
C	2.389958	4.212656	-0.453948
H	0.601948	3.898707	0.700570
C	2.552338	2.977462	-2.522134
H	0.873864	1.716808	-3.008884
C	3.099635	3.875603	-1.607349
H	2.807510	4.922598	0.257114
H	3.095841	2.723201	-3.430445
H	4.074183	4.320911	-1.797379
C	-1.686016	1.255584	-2.200296
C	-2.726256	1.920307	-2.858948
C	-1.235821	0.024235	-2.698809
C	-3.299165	1.359408	-3.997437
H	-3.108784	2.862336	-2.468172
C	-1.801863	-0.528153	-3.842107
H	-0.451866	-0.515668	-2.160876
C	-2.839243	0.139300	-4.490586
H	-4.113220	1.877213	-4.500544
H	-1.446715	-1.489617	-4.209891
H	-3.296613	-0.295233	-5.377155
C	-1.981685	3.117547	0.082906
C	-2.152557	4.362398	-0.542247
C	-2.594131	2.878222	1.317177
C	-2.948102	5.336235	0.050030
H	-1.645952	4.572156	-1.484855
C	-3.387402	3.857659	1.908088
H	-2.444952	1.919094	1.813709
C	-3.568108	5.083329	1.273586
H	-3.077365	6.299589	-0.438862
H	-3.861117	3.661448	2.868129
H	-4.185466	5.850290	1.736884
H	2.826431	1.511457	0.278821
C	4.412176	0.045272	0.275608
C	5.078619	0.560883	1.524874
C	4.983950	-0.122234	2.742130
C	5.757648	1.780571	1.491932
C	5.567709	0.396399	3.894233
H	4.443697	-1.068746	2.799565
C	6.339706	2.303089	2.643123

H	5.836390	2.319900	0.546861
C	6.248075	1.610157	3.847476
H	5.493361	-0.152120	4.831307
H	6.875993	3.248914	2.596818
H	4.844362	0.552803	-0.598790
N	4.623645	-1.381068	0.123923
H	4.889930	-1.925664	0.931469
C	4.206608	-2.139487	-0.936252
O	4.137805	-3.355057	-0.910794
O	3.897353	-1.337333	-1.982937
C	3.194422	-1.908909	-3.138873
C	1.884438	-2.523675	-2.669358
H	1.250374	-2.766868	-3.531391
H	2.050992	-3.435011	-2.087749
H	1.339175	-1.798441	-2.044955
C	2.918496	-0.684181	-3.993673
H	3.851152	-0.180757	-4.271056
H	2.393770	-0.970350	-4.912246
H	2.291019	0.030262	-3.445790
C	4.082813	-2.901399	-3.868179
H	4.293602	-3.775599	-3.249012
H	3.587991	-3.231178	-4.789526
H	5.031862	-2.430485	-4.147287
H	6.708809	2.013038	4.747017

IM5''

SCF energy in MeCN: -2990.702598 a.u.

Free energy in MeCN: -2989.903637 a.u.

C	1.311498	-1.336091	1.699816
H	1.479346	-2.209552	1.061974
H	1.027203	-1.577391	2.725249
C	1.932391	-0.108924	1.393681
H	2.068714	0.605621	2.211969
C	2.870858	0.070723	0.233809
H	2.487012	-0.445080	-0.657457
P	-2.237392	-1.127284	0.788158
C	-2.622467	-1.994638	2.359334
C	-2.009471	-1.538674	3.531731
C	-3.528597	-3.058410	2.436209
C	-2.302818	-2.126821	4.759284
H	-1.290689	-0.718551	3.464457
C	-3.811637	-3.654778	3.660931
H	-4.009918	-3.423476	1.528199
C	-3.202127	-3.187985	4.824306
H	-1.821149	-1.761833	5.665109
H	-4.511525	-4.487710	3.708540
H	-3.424430	-3.656731	5.781647
C	-2.400082	-2.462157	-0.460969
C	-1.260131	-3.230845	-0.731973
C	-3.589406	-2.760830	-1.137191
C	-1.311156	-4.278449	-1.646257
H	-0.328218	-2.996160	-0.213072
C	-3.633785	-3.796836	-2.066534
H	-4.488182	-2.178594	-0.937812
C	-2.496772	-4.558754	-2.322171
H	-0.419975	-4.874409	-1.835163
H	-4.565290	-4.013375	-2.587650
H	-2.534946	-5.372448	-3.044724
Pd	-0.159179	-0.012115	0.810266
C	-3.758392	-0.137686	0.520917
C	-3.979310	0.420835	-0.747976
C	-4.619541	0.216116	1.566422
C	-5.026634	1.308080	-0.963645
H	-3.321911	0.152417	-1.575240
C	-5.667434	1.109217	1.348430
H	-4.470786	-0.206092	2.559829
C	-5.872683	1.660767	0.086963
H	-5.172285	1.733062	-1.956094
H	-6.327463	1.373741	2.173756
H	-6.686280	2.365473	-0.077091
P	-0.414924	1.930077	-0.505433
C	1.155440	2.780113	-0.927675
C	1.800819	3.504637	0.087045
C	1.816882	2.597463	-2.146300
C	3.071596	4.028884	-0.112214
H	1.304883	3.637658	1.050030
C	3.096003	3.116852	-2.342156
H	1.334994	2.038255	-2.947906
C	3.727612	3.829994	-1.328095
H	3.562549	4.577622	0.690173
H	3.599070	2.960217	-3.295580
H	4.728987	4.229772	-1.480598
C	-1.037715	1.398920	-2.150911
C	-1.867604	2.172223	-2.968737
C	-0.701628	0.101783	-2.566063
C	-2.355152	1.655186	-4.167588
H	-2.159649	3.174136	-2.654526

C	-1.179653	-0.411876	-3.767069
H	-0.079706	-0.514731	-1.910868
C	-2.014380	0.365214	-4.569016
H	-3.010543	2.263510	-4.789450
H	-0.916149	-1.426938	-4.063722
H	-2.404136	-0.036400	-5.502878
C	-1.485750	3.348292	-0.056980
C	-1.329601	4.617302	-0.633224
C	-2.492817	3.156671	0.895183
C	-2.172501	5.664050	-0.275657
H	-0.536227	4.782002	-1.362989
C	-3.337539	4.204942	1.251281
H	-2.611986	2.174815	1.355435
C	-3.179546	5.458285	0.666366
H	-2.041529	6.644805	-0.730314
H	-4.118496	4.039516	1.991855
H	-3.836183	6.279810	0.948903
H	2.948570	1.131438	-0.031879
C	4.316113	-0.437620	0.465467
C	4.949590	0.250720	1.646894
C	4.764720	-0.188258	2.961380
C	5.674116	1.427018	1.436399
C	5.305958	0.518897	4.031909
H	4.172942	-1.081543	3.163491
C	6.208720	2.141868	2.503298
H	5.815293	1.783675	0.415031
C	6.030117	1.686265	3.807097
H	5.154719	0.156792	5.047650
H	6.774485	3.053220	2.314588
H	4.888434	-0.171342	-0.433033
N	4.386683	-1.891839	0.587969
H	4.284968	-2.297221	1.507616
C	3.984834	-2.745837	-0.401391
O	3.718158	-3.922908	-0.222866
O	3.964444	-2.094077	-1.590862
C	3.264042	-2.687940	-2.729201
C	1.848235	-3.076142	-2.330595
H	1.277606	-3.369163	-3.220879
H	1.848693	-3.908225	-1.621358
H	1.329968	-2.224783	-1.866469
C	3.235143	-1.542372	-3.728793
H	4.251200	-1.215626	-3.976934
H	2.736828	-1.855720	-4.653803
H	2.689266	-0.683636	-3.316610
C	4.055533	-3.871823	-3.260129
H	4.094139	-4.674369	-2.519530
H	3.589411	-4.256856	-4.175800
H	5.080457	-3.569014	-3.503371
H	6.453947	2.238140	4.644364

IM6''

SCF energy in MeCN: -2990.51086 a.u.

Free energy in MeCN: -2989.715103 a.u.

Pd	0.204780	-0.516425	0.281191
P	-0.035447	1.812443	-0.359261
P	-1.920897	-1.289858	-0.366692
C	-1.674734	2.455195	0.130911
C	-2.403672	3.414785	-0.576432
C	-2.173297	1.991277	1.356806
C	-3.592927	3.916601	-0.053549
H	-2.056578	3.763736	-1.547105
C	-3.357715	2.498620	1.881166
H	-1.626356	1.219456	1.901182
C	-4.067012	3.469658	1.177939
H	-4.155042	4.659323	-0.617030
H	-3.728715	2.123627	2.834591
H	-4.994861	3.869750	1.582347
C	0.207155	1.981971	-2.158412
C	0.139194	3.218718	-2.814442
C	0.556287	0.842900	-2.894175
C	0.349392	3.298355	-4.186777
H	-0.053457	4.127149	-2.244561
C	0.777883	0.925004	-4.266160
H	0.656898	-0.115735	-2.374933
C	0.660064	2.151151	-4.915719
H	0.285484	4.262252	-4.687600
H	1.050702	0.031829	-4.825935
H	0.831357	2.218774	-5.988209
C	1.093694	3.104248	0.287568
C	0.697326	4.033287	1.258402
C	2.422769	3.111851	-0.162637
C	1.613900	4.949992	1.767957
H	-0.333134	4.049768	1.612522
C	3.333841	4.027362	0.354225
H	2.745900	2.395454	-0.916275
C	2.932453	4.947083	1.321184
H	1.290923	5.673552	2.513950

H	4.361786	4.020106	-0.003478
H	3.645864	5.663511	1.722941
C	-3.037299	-0.181050	-1.313531
C	-2.698537	0.186737	-2.623213
C	-4.197851	0.365449	-0.748335
C	-3.499981	1.055640	-3.354261
H	-1.796771	-0.196904	-3.088125
C	-5.005205	1.224792	-1.487273
H	-4.471421	0.133251	0.277637
C	-4.663018	1.572663	-2.790945
H	-3.208261	1.324735	-4.368066
H	-5.904308	1.633999	-1.029536
H	-5.295987	2.249238	-3.361852
C	-2.863426	-1.724863	1.130470
C	-2.297174	-1.528044	2.395483
C	-4.165734	-2.243079	1.040143
C	-3.019855	-1.831524	3.546686
H	-1.280966	-1.131772	2.475342
C	-4.881830	-2.550490	2.191006
H	-4.618934	-2.399675	0.061069
C	-4.310304	-2.342523	3.445974
H	-2.565688	-1.672581	4.522855
H	-5.889515	-2.952388	2.108505
H	-4.873924	-2.582773	4.345234
C	-1.840668	-2.821964	-1.364858
C	-2.271891	-4.054676	-0.858999
C	-1.221211	-2.793836	-2.623767
C	-2.118003	-5.219456	-1.607138
H	-2.724894	-4.113574	0.128395
C	-1.084447	-3.954606	-3.374949
H	-0.798361	-1.867463	-3.009065
C	-1.534183	-5.172397	-2.869588
H	-2.461486	-6.167363	-1.198115
H	-0.607186	-3.909623	-4.352000
H	-1.420638	-6.082852	-3.454343
C	-0.182965	-0.228310	5.209112
C	-0.193190	0.913935	4.404175
C	0.606072	0.976716	3.275633
C	1.438428	-0.107330	2.907873
C	1.435435	-1.255264	3.735243
C	0.634192	-1.308827	4.865558
H	-0.818421	1.765817	4.667303
H	0.625961	1.879522	2.665328
H	2.053894	-2.118269	3.488438
H	0.649050	-2.199148	5.490690
C	2.242642	0.022613	1.725198
C	0.624373	-2.584080	0.639003
H	1.385428	-2.445143	1.411830
C	1.149731	-3.137091	-0.613374
H	0.667283	-4.041974	-0.993022
C	2.131511	-2.597998	-1.360652
H	2.624989	-1.664242	-1.089635
H	2.448919	-3.058530	-2.294443
H	-0.211760	-3.157187	1.055723
H	2.324215	0.988826	1.228587
H	-0.798962	-0.272960	6.104945
N	3.322657	-0.794580	1.494804
H	3.549643	-1.552381	2.127279
C	4.194208	-0.576408	0.429314
O	5.203727	-1.435668	0.524898
C	6.282336	-1.431179	-0.505971
C	6.966701	-0.076285	-0.513865
H	6.304404	0.709489	-0.884848
H	7.308845	0.190713	0.492372
H	7.847591	-0.120978	-1.163991
C	5.684933	-1.798619	-1.851811
H	5.160178	-2.758973	-1.791264
H	4.990369	-1.032937	-2.208092
H	6.489629	-1.901438	-2.588498
C	7.212503	-2.516996	-0.000280
H	8.060250	-2.626674	-0.684535
H	7.603994	-2.269469	0.992031
H	6.695885	-3.480730	0.061117
O	3.985961	0.273224	-0.416430

IM7''

SCF energy in MeCN: -2990.654747 a.u.

Free energy in MeCN: -2989.859736 a.u.

Pd	0.329182	-0.444689	0.322486
P	-0.093434	1.791360	-0.432207
P	-1.850280	-1.348795	-0.237128
C	-1.738334	2.392094	0.112288
C	-2.551055	3.245413	-0.639596
C	-2.172285	1.987441	1.382206
C	-3.765224	3.692640	-0.126149
H	-2.246160	3.546800	-1.641330
C	-3.383861	2.438660	1.897386

H	-1.554314	1.303614	1.965813	H	-4.626462	-2.166764	0.519167
C	-4.183008	3.295265	1.142534	C	-3.993031	-1.864257	3.845122
H	-4.394712	4.347575	-0.727008	H	-2.097590	-1.266069	4.694763
H	-3.706465	2.102845	2.882967	H	-5.737673	-2.428511	2.707815
H	-5.135072	3.646235	1.537933	H	-4.489195	-1.970985	4.808618
C	-0.081079	1.943784	-2.256135	C	-1.755649	-3.025164	-0.981178
C	-0.045899	3.185600	-2.905222	C	-2.433747	-4.142119	-0.481332
C	-0.066281	0.778853	-3.028909	C	-0.913805	-3.192891	-2.087900
C	-0.033416	3.254383	-4.294035	C	-2.291697	-5.385868	-1.091319
H	-0.010877	4.101015	-2.313595	H	-3.063850	-4.047603	0.401315
C	-0.052494	0.846171	-4.419064	C	-0.784924	-4.431150	-2.707496
H	-0.056858	-0.186491	-2.516978	H	-0.315904	-2.350359	-2.437495
C	-0.042288	2.084947	-5.053437	C	-1.475789	-5.532135	-2.210326
H	-0.006774	4.224818	-4.787158	H	-2.820329	-6.246539	-0.684433
H	-0.043760	-0.071910	-5.005821	H	-0.117565	-4.539334	-3.561021
H	-0.027142	2.142211	-6.140547	H	-1.365287	-6.506641	-2.682834
C	0.998875	3.187143	0.036188	C	0.387143	0.270571	5.362884
C	0.572215	4.291057	0.784000	C	0.176518	1.288424	4.429602
C	2.345061	3.100914	-0.345377	C	0.786358	1.231936	3.185249
C	1.475764	5.292262	1.133625	C	1.612653	0.153506	2.813388
H	-0.469213	4.373207	1.094246	C	1.846054	-0.838800	3.780323
C	3.243454	4.099520	0.011270	C	1.235003	-0.782886	5.031725
H	2.703347	2.232177	-0.896803	H	-0.458166	2.139285	4.678655
C	2.810791	5.199457	0.749462	H	0.634163	2.042107	2.469981
H	1.132121	6.148186	1.712520	H	2.528930	-1.658467	3.559906
H	4.288266	4.002358	-0.278664	H	1.433918	-1.569737	5.758553
H	3.515151	5.979929	1.032988	C	2.135757	0.101731	1.429359
C	-3.117082	-0.543291	-1.305461	C	0.793809	-2.454828	0.902126
C	-2.999239	-0.638614	-2.699683	H	1.286070	-2.414236	1.888384
C	-4.145579	0.251635	-0.782540	C	1.633740	-3.198427	-0.076205
C	-3.871870	0.040660	-3.541598	H	1.737275	-4.278804	0.099910
H	-2.218764	-1.259254	-3.137427	C	2.263110	-2.698949	-1.144568
C	-5.031196	0.914939	-1.626717	H	2.196482	-1.635513	-1.396156
H	-4.253578	0.365105	0.293974	H	2.864073	-3.327660	-1.801873
C	-4.896538	0.818320	-3.008112	H	-0.122601	-3.038898	1.095091
H	-3.750088	-0.044243	-4.620456	H	2.393657	1.097232	1.061283
H	-5.825331	1.521900	-1.193454	H	-0.085314	0.312517	6.343198
H	-5.584982	1.345729	-3.666326	N	3.295349	-0.721478	1.248449
C	-2.721266	-1.580944	1.358899	H	3.208798	-1.712347	1.438446
C	-2.026912	-1.335260	2.551698	C	4.219954	-0.427004	0.287992
C	-4.064938	-1.979404	1.434836	O	5.043018	-1.492328	0.127493
C	-2.658892	-1.472734	3.784869	C	6.124876	-1.427680	-0.854593
H	-0.981129	-1.019771	2.512688	C	7.119923	-0.344640	-0.464540
C	-4.694149	-2.120617	2.667685	H	6.668965	0.647667	-0.541450

H	7.466485	-0.495917	0.564575
H	7.994327	-0.387445	-1.125769
C	5.568991	-1.212920	-2.255121
H	4.820349	-1.977658	-2.492114
H	5.108021	-0.228153	-2.355184
H	6.380967	-1.296993	-2.988220
C	6.752163	-2.807454	-0.738411
H	7.588423	-2.905716	-1.440240
H	7.129555	-2.980513	0.275599
H	6.014434	-3.585760	-0.965703
O	4.301128	0.635778	-0.311490

TS2a''

SCF energy in MeCN: -2990.520653 a.u.

Free energy in MeCN: -2989.723391 a.u.

C	1.224906	-1.724826	1.451805
H	1.413315	-2.369891	0.589075
H	0.848614	-2.235538	2.336430
C	1.929819	-0.514087	1.579616
H	1.994662	-0.035681	2.559240
C	2.528554	0.149298	0.480335
H	2.397920	-0.248275	-0.526831
P	-2.144562	-1.142806	0.810223
C	-2.256970	-2.085800	2.369182
C	-1.571314	-1.619549	3.498632
C	-3.055795	-3.229222	2.477038
C	-1.690022	-2.280434	4.717523
H	-0.938947	-0.731731	3.414321
C	-3.162246	-3.895444	3.694431
H	-3.593979	-3.601099	1.605630
C	-2.483014	-3.422147	4.814350
H	-1.157070	-1.908997	5.590634
H	-3.780019	-4.788095	3.767114
H	-2.569295	-3.945108	5.764594
C	-2.507487	-2.362809	-0.495596
C	-1.442114	-3.143335	-0.963597
C	-3.788644	-2.578774	-1.017856
C	-1.649201	-4.118061	-1.933462
H	-0.443847	-2.984413	-0.553697
C	-3.991181	-3.547577	-1.997886
H	-4.631762	-1.992776	-0.655734
C	-2.925215	-4.316594	-2.458171
H	-0.813162	-4.724106	-2.278354
H	-4.990789	-3.705849	-2.397707
H	-3.089067	-5.075067	-3.220872
Pd	-0.019021	-0.124118	0.592577
C	-3.598065	-0.041708	0.872286
C	-4.083387	0.541715	-0.307906
C	-4.170547	0.329731	2.096626
C	-5.107476	1.481368	-0.260798
H	-3.674169	0.242349	-1.271493
C	-5.197465	1.268389	2.136866
H	-3.816013	-0.118585	3.024019
C	-5.663442	1.852037	0.961372
H	-5.473983	1.919174	-1.187796
H	-5.638366	1.540672	3.094204
H	-6.465009	2.587042	0.997175
P	-0.499503	1.858515	-0.628403
C	1.019007	2.634687	-1.289684
C	1.762154	3.515206	-0.489823
C	1.544904	2.228623	-2.520692
C	3.005940	3.971533	-0.915313
H	1.363071	3.845297	0.469916
C	2.794615	2.679823	-2.938656
H	0.969592	1.561981	-3.163519
C	3.530508	3.547352	-2.135928
H	3.568422	4.662377	-0.289346
H	3.187916	2.358776	-3.901857
H	4.503877	3.904731	-2.466257
C	-1.464720	1.431914	-2.120093
C	-2.381518	2.300912	-2.719592
C	-1.316690	0.136255	-2.635773
C	-3.142886	1.875123	-3.804626
H	-2.529081	3.301864	-2.316712
C	-2.075104	-0.287572	-3.722956
H	-0.620482	-0.556511	-2.155349
C	-2.995909	0.582051	-4.304272
H	-3.862386	2.555101	-4.256815
H	-1.959740	-1.303889	-4.097506
H	-3.602402	0.252148	-5.145285
C	-1.364284	3.220040	0.208375
C	-1.424120	4.509902	-0.341453
C	-1.975942	2.975472	1.442903
C	-2.108902	5.522208	0.321189
H	-0.919246	4.722907	-1.284354
C	-2.659563	3.991721	2.104405
H	-1.916188	1.979594	1.884302

C	-2.730930	5.262743	1.542099	C	-1.836680	1.974865	1.533147
H	-2.152503	6.519106	-0.112883	C	-2.822476	2.957932	1.671109
H	-3.135751	3.787521	3.061677	C	-1.872147	0.844717	2.361223
H	-3.263021	6.058345	2.059512	C	-3.829286	2.802157	2.621675
H	2.747605	1.212784	0.546325	H	-2.811563	3.835098	1.024359
C	4.603519	-0.465175	0.405114	C	-2.872740	0.695589	3.313554
C	5.191105	0.188080	1.553558	H	-1.121663	0.060815	2.236007
C	5.303357	-0.425705	2.814565	C	-3.858440	1.673776	3.440133
C	5.618240	1.523113	1.417784	H	-4.597632	3.566497	2.721871
C	5.846093	0.265721	3.889112	H	-2.894366	-0.197179	3.937380
H	4.958774	-1.448670	2.968863	H	-4.652138	1.555712	4.175094
C	6.158143	2.209453	2.494044	C	-0.947719	3.406407	-0.828964
H	5.529293	2.008513	0.445153	C	-0.551960	4.724582	-0.569634
C	6.278235	1.582578	3.735192	C	-1.731329	3.126813	-1.956567
H	5.934756	-0.226183	4.855441	C	-0.941469	5.749192	-1.427022
H	6.496756	3.235642	2.366450	H	0.059826	4.946389	0.304847
H	4.720562	0.015632	-0.564018	C	-2.124095	4.156515	-2.804864
N	4.543360	-1.843398	0.335590	H	-2.033133	2.097935	-2.165532
H	4.657459	-2.391272	1.179013	C	-1.727581	5.466556	-2.542575
C	3.967339	-2.571938	-0.699247	H	-0.630535	6.771745	-1.222920
O	3.695378	-3.749654	-0.584341	H	-2.735973	3.931335	-3.676521
O	3.780414	-1.782030	-1.764768	H	-2.028591	6.270388	-3.211540
C	3.001459	-2.293090	-2.917682	C	0.954399	2.587319	1.214472
C	1.611971	-2.673117	-2.432885	C	0.898356	2.940225	2.569893
H	0.951468	-2.853964	-3.290211	C	2.198766	2.583756	0.563944
H	1.634436	-3.573947	-1.811643	C	2.063292	3.277015	3.255041
H	1.173930	-1.849589	-1.846107	H	-0.057118	2.953415	3.092202
C	2.940572	-1.079568	-3.826065	C	3.358837	2.923015	1.251036
H	3.945462	-0.758611	-4.121596	H	2.258901	2.301562	-0.488686
H	2.374529	-1.316637	-4.733438	C	3.292499	3.266000	2.601114
H	2.446919	-0.242102	-3.318190	H	2.007102	3.552701	4.306250
C	3.736757	-3.446149	-3.574163	H	4.313801	2.903917	0.730000
H	3.788851	-4.316332	-2.916550	H	4.199530	3.525405	3.143293
H	3.213884	-3.733833	-4.493564	C	-3.313927	-0.301676	-1.347538
H	4.754581	-3.147919	-3.847985	C	-3.475974	-0.249644	-2.738432
H	6.707449	2.117958	4.579102	C	-4.016410	0.617916	-0.553162
				C	-4.318752	0.696131	-3.317787
TS2b''				H	-2.954900	-0.962138	-3.376848
SCF energy in MeCN: -2990.50878 a.u.				C	-4.856737	1.560865	-1.136503
Free energy in MeCN: -2989.710156 a.u.				H	-3.918350	0.586928	0.531129
				C	-5.008660	1.606222	-2.520382
Pd	-0.042333	-0.027220	-0.680213	H	-4.441890	0.713172	-4.399213
P	-0.516791	2.037897	0.283826	H	-5.394768	2.261982	-0.500145
P	-2.063960	-1.395310	-0.573347	H	-5.667231	2.343708	-2.975014

C	-2.859201	-2.035592	0.936742	H	4.393780	-2.308523	0.624151
C	-2.019258	-2.583509	1.912926	C	5.001217	-0.581412	-0.333380
C	-4.244975	-2.066672	1.133685	O	6.190622	-1.172638	-0.279104
C	-2.551468	-3.140537	3.070778	C	7.395933	-0.470194	-0.808251
H	-0.939001	-2.570972	1.759432	C	7.618869	0.807186	-0.019100
C	-4.774716	-2.613868	2.298966	H	6.834631	1.543410	-0.211121
H	-4.913442	-1.666803	0.372929	H	7.659265	0.597593	1.055734
C	-3.930821	-3.149987	3.269646	H	8.579671	1.246490	-0.309731
H	-1.885172	-3.565736	3.819871	C	7.220550	-0.220975	-2.294859
H	-5.853202	-2.630403	2.443889	H	6.987727	-1.154079	-2.820159
H	-4.348775	-3.579536	4.178111	H	6.430380	0.506791	-2.493632
C	-2.010094	-2.875280	-1.656216	H	8.157758	0.168582	-2.707712
C	-2.664058	-4.068946	-1.325869	C	8.495118	-1.480958	-0.542700
C	-1.278581	-2.820932	-2.852287	H	9.454468	-1.086050	-0.892614
C	-2.594852	-5.168967	-2.175570	H	8.583443	-1.695008	0.527675
H	-3.234636	-4.140499	-0.401805	H	8.300512	-2.421323	-1.069204
C	-1.218956	-3.917388	-3.705926	O	4.709954	0.510590	-0.785771
H	-0.756477	-1.901286	-3.121112				
C	-1.877366	-5.096946	-3.366710	**TS2c''**			
H	-3.112091	-6.087630	-1.905349	SCF energy in MeCN: -2990.610345 a.u.			
H	-0.653316	-3.851586	-4.633374	Free energy in MeCN: -2989.816774 a.u.			
H	-1.828685	-5.959178	-4.028288				
C	0.906240	-2.982584	3.727984	Pd	0.055649	-0.389059	-0.055221
C	0.813611	-1.600080	3.560459	P	-0.113258	1.958601	-0.018690
C	1.345932	-0.999032	2.426766	P	-2.076375	-1.334592	-0.453678
C	1.998873	-1.772252	1.450608	C	-1.633121	2.478587	0.868360
C	2.052120	-3.165282	1.609646	C	-2.413962	3.577839	0.496871
C	1.504343	-3.763513	2.739624	C	-2.037747	1.697831	1.959591
H	0.334275	-0.985208	4.321599	C	-3.581310	3.879234	1.195849
H	1.316092	0.086750	2.310872	H	-2.115642	4.189235	-0.355445
H	2.520663	-3.781115	0.840844	C	-3.198221	2.003240	2.662897
H	1.555869	-4.843950	2.855674	H	-1.447051	0.821503	2.234294
C	2.741558	-1.069880	0.410455	C	-3.977095	3.093521	2.276766
C	1.965207	-1.379286	-1.799575	H	-4.187938	4.731144	0.891025
H	2.944155	-1.849397	-1.802231	H	-3.502786	1.375054	3.499387
C	1.869183	-0.013857	-2.182484	H	-4.894428	3.328409	2.814573
H	2.739314	0.603526	-1.948288	C	-0.260002	2.795588	-1.641246
C	0.748912	0.633109	-2.691055	C	0.230977	4.085223	-1.881390
H	-0.054303	0.098386	-3.202580	C	-0.903501	2.113165	-2.682401
H	0.799835	1.699078	-2.907335	C	0.082030	4.675104	-3.133923
H	1.153029	-2.065897	-2.054002	H	0.736081	4.629152	-1.083777
H	2.584921	0.005739	0.318833	C	-1.063909	2.710037	-3.928954
H	0.507854	-3.451418	4.625758	H	-1.279751	1.104044	-2.507242
N	4.059654	-1.428869	0.247922	C	-0.567066	3.990917	-4.159068

H	0.474201	5.676115	-3.308054
H	-1.572576	2.166228	-4.723574
H	-0.682244	4.454779	-5.137480
C	1.183562	2.941649	0.822561
C	0.950633	3.764357	1.932894
C	2.504180	2.752954	0.386787
C	2.014322	4.386102	2.583298
H	-0.066196	3.922184	2.291769
C	3.562536	3.377774	1.036273
H	2.710213	2.093179	-0.457148
C	3.320338	4.196054	2.138414
H	1.818039	5.024651	3.443651
H	4.578243	3.202687	0.686186
H	4.148481	4.677737	2.655757
C	-3.240085	-0.401037	-1.523926
C	-3.385561	-0.691606	-2.887104
C	-3.884577	0.736376	-1.011801
C	-4.147687	0.130767	-3.712732
H	-2.903400	-1.572924	-3.308408
C	-4.651425	1.550869	-1.838312
H	-3.790369	0.983264	0.045754
C	-4.781898	1.256306	-3.193631
H	-4.249646	-0.116602	-4.768787
H	-5.145597	2.425286	-1.416466
H	-5.376758	1.898931	-3.840350
C	-3.035121	-1.598573	1.084195
C	-2.309898	-1.807109	2.264517
C	-4.434681	-1.618316	1.138004
C	-2.966973	-2.035893	3.469690
H	-1.217014	-1.771555	2.229902
C	-5.091189	-1.834374	2.346576
H	-5.011610	-1.454560	0.227791
C	-4.359325	-2.045904	3.513616
H	-2.384442	-2.195495	4.375837
H	-6.179804	-1.840850	2.376132
H	-4.875293	-2.214805	4.457820
C	-2.068058	-2.994441	-1.236538
C	-2.823113	-4.082660	-0.781329
C	-1.191856	-3.191383	-2.316482
C	-2.714949	-5.325341	-1.400083
H	-3.500268	-3.958511	0.063280
C	-1.094732	-4.430395	-2.941593
H	-0.570842	-2.360463	-2.663016
C	-1.855713	-5.502631	-2.482393
H	-3.310132	-6.161232	-1.034930
H	-0.408891	-4.559446	-3.777473
H	-1.771580	-6.477643	-2.959490
C	0.339979	-1.586991	4.757389
C	0.350783	-0.299374	4.219325
C	0.990036	-0.051421	3.011242
C	1.630865	-1.084108	2.304020
C	1.608766	-2.373883	2.857833
C	0.970530	-2.621442	4.069815
H	-0.135282	0.521004	4.746909
H	1.023892	0.961285	2.606614
H	2.095434	-3.198877	2.336145
H	0.969553	-3.629950	4.480766
C	2.314599	-0.778785	1.035406
C	1.552214	-2.186745	-0.502061
H	1.999681	-2.942248	0.147733
C	2.333834	-1.863335	-1.696200
H	3.330165	-2.310998	-1.775302
C	1.937668	-1.038983	-2.681195
H	0.977010	-0.517952	-2.628585
H	2.566682	-0.830734	-3.544287
H	0.541309	-2.535290	-0.737863
H	2.371254	0.284642	0.803135
H	-0.149884	-1.780073	5.710715
N	3.622719	-1.303172	0.901394
H	3.774191	-2.289654	1.072448
C	4.563348	-0.705491	0.098399
O	5.559307	-1.595109	-0.124020
C	6.707269	-1.193691	-0.950027
C	7.433513	-0.021719	-0.307635
H	6.824121	0.884454	-0.328517
H	7.686760	-0.252426	0.733658
H	8.369048	0.170946	-0.846807
C	6.240060	-0.880081	-2.363307
H	5.713671	-1.740124	-2.795189
H	5.572939	-0.014673	-2.379005
H	7.108250	-0.665529	-2.998190
C	7.576363	-2.439667	-0.932390
H	8.478877	-2.277599	-1.532340
H	7.881808	-2.688510	0.089919
H	7.036161	-3.297557	-1.348096
O	4.505095	0.437668	-0.315812

IM1’’’

SCF energy in MeCN: -3218.648089 a.u.

Free energy in MeCN: -3217.815837 a.u.

C	-1.347797	-0.297872	-0.491665
H	-1.152128	0.036522	0.535345
H	-1.318749	-1.393386	-0.494407
C	-0.423511	0.321854	-1.476978
H	-0.450375	-0.115300	-2.478608
C	0.005495	1.660813	-1.334475
H	-0.350300	2.263106	-0.494463
P	2.303756	-1.832604	-0.309245
C	2.628421	-2.780430	-1.843694
C	2.221937	-2.231361	-3.065183
C	3.258478	-4.032875	-1.840243
C	2.429853	-2.920917	-4.257732
H	1.743895	-1.249235	-3.065412
C	3.466496	-4.720653	-3.030885
H	3.590996	-4.464849	-0.896020
C	3.050981	-4.166404	-4.241158
H	2.108727	-2.481993	-5.200818
H	3.955183	-5.693669	-3.015720
H	3.217391	-4.705518	-5.172452
C	0.955686	-2.752311	0.522796
C	0.362289	-2.154051	1.645899
C	0.411461	-3.941152	0.027544
C	-0.742280	-2.732340	2.258920
H	0.757218	-1.202856	2.012660
C	-0.703733	-4.513264	0.636814
H	0.846801	-4.415287	-0.850727
C	-1.283455	-3.911501	1.749083
H	-1.210777	-2.239762	3.108624
H	-1.125693	-5.431427	0.230895
H	-2.168188	-4.347231	2.209474
Pd	1.597396	0.392212	-0.689108
O	-2.727666	0.094987	-0.818268
C	-3.642193	-0.242150	0.091127
O	-3.417178	-0.849661	1.121919
C	3.786769	-2.249711	0.694797
C	3.703510	-2.599375	2.046939
C	5.057594	-2.127756	0.112504
C	4.857346	-2.831609	2.790749
H	2.729813	-2.702377	2.523666
C	6.208508	-2.365884	0.855388
H	5.146211	-1.860715	-0.940442
C	6.111988	-2.720616	2.199480
H	4.770920	-3.102337	3.842308
H	7.183887	-2.272668	0.379703
H	7.011898	-2.907600	2.783519
P	3.337215	1.715240	0.136535
C	3.060606	3.518384	0.356543
C	2.491067	4.215423	-0.717879
C	3.391163	4.225116	1.518200
C	2.268490	5.585035	-0.638789
H	2.219174	3.667358	-1.621141
C	3.155900	5.596511	1.600648
H	3.836505	3.703551	2.365086
C	2.596949	6.279193	0.524608
H	1.826198	6.111206	-1.483212
H	3.415300	6.133365	2.512008
H	2.412901	7.350079	0.592576
C	3.848573	1.194039	1.815455
C	5.164977	0.911938	2.189794
C	2.827840	1.043674	2.767252
C	5.455277	0.504119	3.490274
H	5.969076	0.994924	1.459627
C	3.121267	0.650001	4.067646
H	1.794426	1.245965	2.476140
C	4.439532	0.380037	4.432689
H	6.484681	0.276093	3.763382
H	2.318937	0.545754	4.796604
H	4.671417	0.063535	5.448500
C	4.883077	1.713028	-0.848860
C	5.903274	2.652140	-0.649285
C	5.034220	0.754329	-1.856699
C	7.055373	2.618907	-1.428206
H	5.785515	3.418723	0.117748
C	6.188966	0.717845	-2.634413
H	4.224421	0.041227	-2.031436
C	7.200891	1.650022	-2.420159
H	7.840467	3.355613	-1.265676
H	6.292098	-0.033361	-3.416063
H	8.100455	1.629541	-3.033117
H	0.285344	2.238538	-2.215889
C	-5.010816	0.286406	-0.294638
H	-5.269008	-0.051607	-1.307736
N	-5.983290	-0.250195	0.621615
H	-5.631332	-0.617349	1.496755
C	-7.210894	-0.651670	0.178220

O	-7.610710	-0.503322	-0.963626
O	-7.891024	-1.209160	1.207692
C	-9.279798	-1.630939	0.995891
C	-10.132206	-0.434895	0.598925
H	-10.022742	0.371099	1.334603
H	-9.845679	-0.050153	-0.383109
H	-11.188888	-0.728096	0.571772
C	-9.339451	-2.748207	-0.034541
H	-9.049555	-2.388340	-1.024062
H	-8.673234	-3.570434	0.252788
H	-10.360544	-3.145605	-0.089074
C	-9.679560	-2.145210	2.368989
H	-10.717568	-2.496721	2.354056
H	-9.037872	-2.978998	2.675428
H	-9.594208	-1.353206	3.121238
C	-4.995896	1.835217	-0.289984
H	-4.689829	2.167447	0.712782
H	-4.221412	2.166985	-0.992920
C	-6.332369	2.413082	-0.648319
C	-6.666237	2.651566	-1.983880
C	-7.295257	2.657876	0.335007
C	-7.931598	3.109792	-2.331976
H	-5.923545	2.461282	-2.759834
C	-8.562887	3.117668	-0.008878
H	-7.047403	2.470467	1.380336
C	-8.886494	3.340928	-1.344405
H	-8.175176	3.286489	-3.378542
H	-9.302732	3.300018	0.769608
H	-9.878963	3.697812	-1.615351

1a'''

SCF energy in MeCN: -1017.597956 a.u.

Free energy in MeCN: -1017.270107 a.u.

C	5.226636	-0.628172	-0.793934
C	4.094477	-1.283592	-0.318586
C	3.081200	-0.582821	0.342459
C	3.228959	0.797544	0.511487
C	4.359241	1.457726	0.039044
C	5.362019	0.746481	-0.615924
H	6.008768	-1.192819	-1.299181
H	3.995362	-2.362236	-0.451766
H	2.445163	1.353044	1.028157
H	4.459875	2.532144	0.185574
H	6.248952	1.261263	-0.981796
C	1.847301	-1.286416	0.822126
H	2.067511	-2.318627	1.117105
H	1.425851	-0.790910	1.704765
C	0.748534	-1.337313	-0.247899
C	-0.436435	-2.157520	0.263664
O	-0.367101	-2.969877	1.157270
O	-1.553939	-1.894762	-0.442123
C	-2.747944	-2.504463	0.092525
H	-2.542530	-3.569485	0.266346
H	-2.959829	-2.044817	1.067295
C	-3.849592	-2.291927	-0.878910
H	-3.663498	-2.643062	-1.895711
C	-5.020910	-1.743792	-0.562182
H	-5.224585	-1.379915	0.444956
H	-5.823723	-1.641819	-1.288470
N	0.344626	-0.022157	-0.702472
H	1.143581	-1.857939	-1.132879
H	0.377739	0.196739	-1.686291
C	-0.515726	0.703392	0.071300
O	-0.801824	0.393577	1.218200
O	-0.955601	1.775915	-0.613045
C	-1.944670	2.665485	0.015196
C	-2.197631	3.694441	-1.073546
H	-2.928925	4.434123	-0.729211
H	-1.272835	4.220309	-1.335667
H	-2.589849	3.217684	-1.978678
C	-1.345100	3.319942	1.249459
H	-1.157291	2.585823	2.035990
H	-0.401488	3.818798	0.997798
H	-2.034784	4.080181	1.635623
C	-3.213633	1.885465	0.325946
H	-3.565308	1.355850	-0.567557
H	-3.050385	1.156353	1.123728
H	-4.002791	2.578818	0.641398

2a'''

SCF energy in MeCN: -828.979486 a.u.

Free energy in MeCN: -828.662012 a.u.

C	2.433805	3.198400	-0.232858
H	2.753837	3.392130	0.791804
H	3.218368	3.137858	-0.984140
C	1.146330	3.047063	-0.542089

H	0.867945	2.840986	-1.577075
C	0.039103	3.098705	0.457416
H	0.455281	3.375787	1.437144
H	-0.683376	3.886887	0.190974
C	-0.750820	1.783531	0.614883
H	-1.418110	1.911113	1.480497
C	-1.654522	1.476117	-0.588786
H	-2.276317	2.369032	-0.747926
H	-1.039187	1.339721	-1.483033
N	0.111432	0.666779	0.980135
C	-2.531503	0.275938	-0.364441
C	-2.133975	-0.995796	-0.788562
C	-3.746362	0.401158	0.316442
C	-2.928670	-2.109914	-0.535689
H	-1.189038	-1.100886	-1.320775
C	-4.544829	-0.710541	0.569572
H	-4.072075	1.389197	0.647741
C	-4.136364	-1.972295	0.144584
H	-2.602814	-3.092458	-0.875116
H	-5.491216	-0.590267	1.095198
H	-4.758827	-2.843945	0.340292
H	0.338070	0.558312	1.957934
C	0.952888	0.025623	0.117495
O	0.913002	0.099761	-1.101061
O	1.808792	-0.738861	0.837749
C	2.763702	-1.600655	0.131837
C	3.480373	-2.299735	1.275547
H	4.244915	-2.980234	0.883959
H	3.971119	-1.571448	1.930780
H	2.776184	-2.883640	1.878761
C	2.021698	-2.610875	-0.731489
H	1.256272	-3.128396	-0.140034
H	1.538384	-2.129942	-1.584779
H	2.725512	-3.364121	-1.106322
C	3.734377	-0.748909	-0.671393
H	3.226100	-0.229061	-1.486420
H	4.211712	-0.002813	-0.024726
H	4.521498	-1.385371	-1.093991

IM4'''

SCF energy in MeCN: -3029.87849 a.u.

Free energy in MeCN: -3029.047307 a.u.

C	1.212098	1.462700	-0.220251
H	1.149716	2.059719	0.692266
H	1.168926	2.020953	-1.154197
C	1.711145	0.181217	-0.185594
H	1.965495	-0.301499	-1.131956
C	2.124362	-0.522512	1.068044
H	1.809772	0.072375	1.937980
P	-2.135345	1.805115	0.151711
C	-1.572464	3.401818	-0.519552
C	-1.079773	3.443507	-1.832299
C	-1.602220	4.577579	0.238902
C	-0.647318	4.644608	-2.383005
H	-1.030670	2.523719	-2.419829
C	-1.156243	5.775576	-0.313174
H	-1.971536	4.559029	1.263049
C	-0.682429	5.812088	-1.621235
H	-0.272898	4.668277	-3.404310
H	-1.179947	6.684184	0.284748
H	-0.333051	6.749966	-2.047588
C	-2.287088	2.041473	1.949671
C	-1.209706	1.679487	2.769154
C	-3.428621	2.607651	2.532829
C	-1.269527	1.878250	4.144136
H	-0.326692	1.222745	2.316736
C	-3.488557	2.798717	3.910000
H	-4.272306	2.895816	1.906798
C	-2.411437	2.435928	4.716089
H	-0.426515	1.593665	4.770604
H	-4.379773	3.237287	4.354227
H	-2.462308	2.588441	5.792261
Pd	-0.607333	0.084131	-0.342401
C	-3.837322	1.599798	-0.457931
C	-4.721014	0.754041	0.231626
C	-4.246217	2.164985	-1.674719
C	-5.980675	0.479627	-0.289097
H	-4.426817	0.319988	1.186261
C	-5.508156	1.884473	-2.190075
H	-3.581062	2.834524	-2.217892
C	-6.375804	1.037993	-1.503162
H	-6.656937	-0.172102	0.261115
H	-5.816828	2.337986	-3.129977
H	-7.361715	0.821052	-1.909105
P	-1.901330	-1.861602	-0.379612
C	-0.642649	-3.161052	-0.140824
C	0.374590	-3.286531	-1.102709

C	-0.614582	-3.979730	0.993945	H	5.395019	-3.339219	2.107113
C	1.385529	-4.225071	-0.936886	C	8.349017	-2.603518	0.592073
H	0.363454	-2.648682	-1.988836	H	8.555933	-1.434513	-1.205840
C	0.407835	-4.910803	1.160519	H	7.826171	-3.737642	2.349490
H	-1.398003	-3.897017	1.745139	H	9.417403	-2.782474	0.696274
C	1.407040	-5.035995	0.199141	H	4.999753	0.685770	1.900101
H	2.164045	-4.320823	-1.691378	C	4.750133	1.068371	-0.065370
H	0.415779	-5.547782	2.042592	O	4.262411	0.784793	-1.152076
H	2.202775	-5.766476	0.330227	O	5.665368	2.020669	0.179126
C	-3.028719	-2.019062	1.036982	C	6.121304	2.899528	-0.915631
C	-4.290282	-2.615049	0.942398	C	7.101850	3.817209	-0.206904
C	-2.618173	-1.462572	2.256962	H	7.526326	4.535134	-0.916935
C	-5.128528	-2.646378	2.054473	H	6.605462	4.377330	0.592938
H	-4.624347	-3.038462	-0.004309	H	7.924014	3.243666	0.234136
C	-3.456325	-1.497442	3.365354	C	6.821905	2.077185	-1.984256
H	-1.637779	-0.984295	2.325510	H	7.620498	1.473077	-1.538408
C	-4.716791	-2.086199	3.261943	H	6.122391	1.416464	-2.502454
H	-6.110914	-3.108027	1.974891	H	7.279386	2.747864	-2.721043
H	-3.130364	-1.056220	4.305678	C	4.942929	3.686295	-1.466626
H	-5.378983	-2.107535	4.125008	H	4.239703	3.036995	-1.993349
C	-2.849668	-2.367841	-1.841965	H	4.413081	4.202973	-0.657337
C	-2.898396	-3.704735	-2.259486	H	5.305906	4.445948	-2.168816
C	-3.587843	-1.400315	-2.536265				
C	-3.678534	-4.063706	-3.354266	**IM5’’’**			
H	-2.326369	-4.463742	-1.726563	SCF energy in MeCN: -3030.032221 a.u.			
C	-4.373073	-1.767669	-3.623644	Free energy in MeCN: -3029.202198 a.u.			
H	-3.549108	-0.356867	-2.222580				
C	-4.417030	-3.097891	-4.035340	C	1.301965	1.382750	-0.249827
H	-3.710209	-5.102639	-3.675523	H	1.397251	1.952998	0.679629
H	-4.945161	-1.008109	-4.153563	H	1.365120	1.989812	-1.153643
H	-5.024557	-3.382960	-4.891753	C	1.658713	0.021277	-0.285059
H	1.630024	-1.504650	1.146287	H	1.981227	-0.391745	-1.244361
C	3.646970	-0.779761	1.172876	C	2.189556	-0.681745	0.935116
H	3.817513	-1.160079	2.189493	H	1.792861	-0.181210	1.833932
C	4.122195	-1.871251	0.197900	P	-2.293446	1.665223	0.118523
H	3.537160	-2.773944	0.427505	C	-2.082175	3.381056	-0.503141
H	3.877717	-1.577849	-0.829333	C	-1.277775	3.576234	-1.631567
N	4.412419	0.456362	1.111415	C	-2.703414	4.488253	0.085613
C	5.592851	-2.152902	0.318052	C	-1.105712	4.849534	-2.168599
C	6.497871	-1.623565	-0.606364	H	-0.780556	2.713776	-2.079455
C	6.090533	-2.911436	1.382358	C	-2.520436	5.762649	-0.442374
C	7.865444	-1.847266	-0.471965	H	-3.328853	4.351503	0.968149
H	6.116604	-1.035586	-1.441493	C	-1.723700	5.945097	-1.571277
C	7.456750	-3.137636	1.519604	H	-0.478862	4.986715	-3.048313

H	-3.002513	6.617631	0.029456	C	-4.187145	-2.414743	3.271973
H	-1.581770	6.943251	-1.982418	H	-5.398224	-3.710531	2.047935
C	-2.509658	1.909751	1.926807	H	-2.778092	-1.098054	4.247161
C	-1.363804	1.829985	2.731103	H	-4.861334	-2.461067	4.125638
C	-3.742153	2.162769	2.540562	C	-2.339259	-2.568614	-1.798312
C	-1.448003	1.994970	4.109988	C	-2.372682	-3.906112	-2.213759
H	-0.403018	1.619306	2.255516	C	-3.116325	-1.626100	-2.483761
C	-3.828220	2.317772	3.922047	C	-3.169608	-4.290504	-3.288531
H	-4.645534	2.228006	1.935358	H	-1.768756	-4.648633	-1.691649
C	-2.683223	2.233274	4.710018	C	-3.921623	-2.014756	-3.549767
H	-0.547851	1.929561	4.719311	H	-3.085073	-0.580288	-2.175260
H	-4.796345	2.505883	4.383870	C	-3.947486	-3.346803	-3.955991
H	-2.753084	2.352068	5.790106	H	-3.183795	-5.332330	-3.604938
Pd	-0.500766	0.193288	-0.299809	H	-4.522983	-1.269560	-4.068519
C	-3.989298	1.258298	-0.450493	H	-4.569023	-3.649242	-4.797401
C	-4.683488	0.211374	0.176232	H	1.842105	-1.726191	0.983351
C	-4.535100	1.822822	-1.610600	C	3.729151	-0.704364	1.037543
C	-5.887427	-0.253074	-0.339829	H	3.983424	-1.074195	2.043437
H	-4.274365	-0.244966	1.078080	C	4.377738	-1.678175	0.044587
C	-5.739086	1.350008	-2.129515	H	3.903982	-2.654812	0.222246
H	-4.013659	2.637247	-2.113535	H	4.133903	-1.379705	-0.979836
C	-6.418032	0.310781	-1.498797	N	4.314545	0.630084	0.986394
H	-6.409089	-1.065418	0.164447	C	5.866186	-1.789700	0.221838
H	-6.148975	1.801650	-3.032143	C	6.752762	-1.115121	-0.622889
H	-7.356811	-0.058576	-1.908111	C	6.395905	-2.553445	1.267061
P	-1.351760	-1.990687	-0.367031	C	8.128402	-1.202905	-0.426637
C	-0.119304	-3.336111	-0.174008	H	6.349172	-0.511809	-1.435255
C	0.923222	-3.420384	-1.109901	C	7.770059	-2.643199	1.466874
C	-0.126567	-4.226755	0.904315	H	5.715373	-3.092597	1.929374
C	1.916530	-4.384002	-0.979538	C	8.642893	-1.965801	0.618609
H	0.954184	-2.714013	-1.941679	H	8.803036	-0.670552	-1.096447
C	0.881250	-5.179092	1.044957	H	8.161164	-3.248718	2.283691
H	-0.925859	-4.177228	1.642271	H	9.719042	-2.035978	0.769806
C	1.902008	-5.263790	0.103779	H	4.311638	1.163770	1.843382
H	2.716695	-4.438035	-1.716531	C	4.475913	1.374295	-0.145024
H	0.862566	-5.861396	1.893636	O	4.412443	0.963814	-1.293059
H	2.688297	-6.008773	0.212601	O	4.765715	2.649461	0.225875
C	-2.475738	-2.268829	1.056316	C	5.126663	3.630726	-0.798242
C	-3.638243	-3.045379	1.003051	C	5.456163	4.861956	0.030949
C	-2.175662	-1.580914	2.240779	H	5.728191	5.698365	-0.622890
C	-4.489102	-3.113094	2.104874	H	4.594318	5.163883	0.636298
H	-3.891784	-3.580624	0.087501	H	6.296662	4.663760	0.705418
C	-3.020637	-1.653417	3.342281	C	6.352575	3.165869	-1.572320
H	-1.282599	-0.952441	2.274205	H	7.143563	2.851789	-0.880214

H	6.116015	2.329908	-2.233614
H	6.741545	3.993794	-2.178046
C	3.935796	3.897881	-1.706107
H	3.679902	3.011606	-2.291419
H	3.061564	4.192493	-1.112791
H	4.172062	4.719139	-2.394215

IM6'''

SCF energy in MeCN: -3029.82121 a.u.

Free energy in MeCN: -3028.998636 a.u.

Pd	-0.048040	-0.045523	-0.871638
P	0.857993	-1.976561	0.243357
P	1.833507	1.603676	-0.194206
C	0.943181	-1.687136	2.047896
C	1.716683	-2.454851	2.927977
C	0.216689	-0.604888	2.561416
C	1.773981	-2.131136	4.279858
H	2.290451	-3.302142	2.557779
C	0.272490	-0.279493	3.914102
H	-0.365852	0.017277	1.878123
C	1.057573	-1.041512	4.774741
H	2.384794	-2.731626	4.950981
H	-0.284566	0.578502	4.286679
H	1.113598	-0.788094	5.831329
C	2.543882	-2.337486	-0.382966
C	3.258624	-3.466933	0.044783
C	3.106269	-1.529259	-1.375822
C	4.524620	-3.735312	-0.462111
H	2.808948	-4.164214	0.750372
C	4.368640	-1.804100	-1.892966
H	2.539941	-0.674067	-1.747037
C	5.086975	-2.899191	-1.425498
H	5.068381	-4.612018	-0.116333
H	4.792541	-1.155517	-2.658245
H	6.076621	-3.114257	-1.823247
C	0.117403	-3.641123	0.089230
C	-0.536984	-4.288778	1.141220
C	0.163469	-4.256338	-1.170331
C	-1.137325	-5.529551	0.934838
H	-0.582341	-3.824904	2.126256
C	-0.434306	-5.494328	-1.371495
H	0.676309	-3.759673	-1.995590
C	-1.090260	-6.131923	-0.318581
H	-1.642416	-6.026456	1.760532
H	-0.387498	-5.964884	-2.351583
H	-1.560547	-7.100166	-0.475833
C	3.500235	1.135700	0.404930
C	4.682593	1.457650	-0.269989
C	3.579253	0.367002	1.575532
C	5.909909	0.998785	0.203857
H	4.657146	2.080427	-1.161201
C	4.804581	-0.089218	2.044618
H	2.674875	0.144288	2.138050
C	5.974965	0.216134	1.352469
H	6.820966	1.262697	-0.329941
H	4.840429	-0.684851	2.955357
H	6.935359	-0.144525	1.714923
C	1.144677	2.571997	1.193556
C	-0.243906	2.736273	1.272238
C	1.954471	3.161093	2.172029
C	-0.815674	3.453572	2.317724
H	-0.880299	2.290500	0.505075
C	1.380038	3.880461	3.217024
H	3.036501	3.052978	2.121094
C	-0.003310	4.022982	3.296244
H	-1.898822	3.552317	2.366165
H	2.019392	4.331598	3.973179
H	-0.448071	4.579180	4.119144
C	2.146732	2.832161	-1.507715
C	1.711955	4.158624	-1.407857
C	2.744636	2.405552	-2.704368
C	1.873576	5.034322	-2.479074
H	1.243000	4.510885	-0.490197
C	2.912443	3.284052	-3.768616
H	3.096101	1.375551	-2.797454
C	2.470203	4.601017	-3.659456
H	1.530910	6.062966	-2.387241
H	3.384234	2.938673	-4.686410
H	2.591765	5.287965	-4.494129
C	-2.155364	-0.611304	-0.780566
C	-0.641647	1.335320	-2.527287
H	-1.731117	1.350254	-2.542068
C	0.065284	0.325545	-3.234357
H	1.121742	0.514644	-3.443511
C	-0.437751	-0.894966	-3.638843
H	-1.491663	-1.147420	-3.528886
H	0.199471	-1.629854	-4.124984

H	-0.174234	2.314886	-2.434002
H	-2.536301	-0.328905	-1.764932
N	-2.555885	0.367777	0.146454
C	-2.561520	-2.014758	-0.389150
H	-2.076391	-2.736779	-1.056063
H	-2.213192	-2.242114	0.629514
C	-4.062884	-2.128505	-0.482330
C	-4.878062	-1.824598	0.612137
C	-4.667117	-2.457358	-1.699119
C	-6.264406	-1.860536	0.496812
H	-4.421573	-1.574964	1.572117
C	-6.052721	-2.494112	-1.818170
H	-4.040504	-2.694970	-2.560455
C	-6.854888	-2.192735	-0.720262
H	-6.885490	-1.632909	1.361240
H	-6.507718	-2.759695	-2.770427
H	-7.938591	-2.221064	-0.811455
H	-2.538545	0.137843	1.134233
C	-3.337859	1.466063	-0.209030
O	-3.600803	1.747718	-1.360676
O	-3.704304	2.109263	0.904838
C	-4.656814	3.253946	0.795455
C	-4.881492	3.633677	2.247133
H	-5.601469	4.456587	2.306747
H	-5.279809	2.788730	2.818660
H	-3.953265	3.967713	2.724997
C	-5.949151	2.775129	0.158088
H	-5.810476	2.499795	-0.889435
H	-6.352058	1.912991	0.702133
H	-6.693370	3.577907	0.207251
C	-3.997244	4.382535	0.023345
H	-3.032093	4.649204	0.471936
H	-3.840033	4.116803	-1.024591
H	-4.637844	5.270979	0.061235

IM7'''

SCF energy in MeCN: -3029.98155 a.u.

Free energy in MeCN: -3029.153157 a.u.

Pd	0.080091	0.690057	0.750403
P	-0.217878	0.187964	-1.590533
P	2.466805	0.098478	0.808974
C	0.368100	-1.531972	-1.870680
C	0.875031	-2.009870	-3.084544
C	0.316558	-2.399431	-0.771778
C	1.339580	-3.316797	-3.189404
H	0.945609	-1.349064	-3.946303
C	0.790872	-3.706155	-0.874811
H	-0.080908	-2.035874	0.179827
C	1.307866	-4.165424	-2.083104
H	1.742236	-3.671185	-4.137407
H	0.764654	-4.356256	-0.001096
H	1.688125	-5.182493	-2.164679
C	0.749564	1.271854	-2.708862
C	0.691275	1.194360	-4.108948
C	1.531972	2.275948	-2.128702
C	1.425020	2.072505	-4.898648
H	0.037695	0.463312	-4.584333
C	2.260205	3.161804	-2.918153
H	1.554837	2.356935	-1.039174
C	2.214760	3.055911	-4.304095
H	1.370790	1.997448	-5.983403
H	2.866978	3.932748	-2.444629
H	2.784055	3.745924	-4.924851
C	-1.846459	0.144029	-2.440578
C	-2.652068	-0.999831	-2.357096
C	-2.356630	1.276830	-3.089332
C	-3.931904	-1.008443	-2.902360
H	-2.280594	-1.888441	-1.845983
C	-3.628327	1.258729	-3.655726
H	-1.750734	2.180070	-3.157455
C	-4.422425	0.117863	-3.560169
H	-4.546277	-1.902975	-2.812819
H	-4.004042	2.146542	-4.162179
H	-5.421443	0.108028	-3.992769
C	3.591956	-0.072001	-0.633931
C	4.374514	1.010022	-1.060639
C	3.588505	-1.238091	-1.412638
C	5.118507	0.933958	-2.232771
H	4.399778	1.927302	-0.472946
C	4.336801	-1.312919	-2.583234
H	2.998323	-2.098997	-1.099825
C	5.101240	-0.226761	-3.001450
H	5.714872	1.789777	-2.546205
H	4.314499	-2.229998	-3.170912
H	5.682847	-0.285059	-3.919938
C	2.630434	-1.508977	1.671256
C	1.517051	-1.995477	2.371302

C	3.801398	-2.279855	1.639842	H	-7.774509	3.009741	1.454866
C	1.577256	-3.220790	3.028793	H	-3.524747	-0.020620	0.029157
H	0.585999	-1.426908	2.376829	C	-2.611145	-1.385104	1.216584
C	3.857722	-3.504338	2.298907	O	-1.776225	-1.688109	2.062649
H	4.667521	-1.926757	1.079380	O	-3.497778	-2.241154	0.633884
C	2.746585	-3.976795	2.995672	C	-3.561906	-3.632028	1.081410
H	0.697760	-3.581840	3.560611	C	-4.668003	-4.204947	0.209490
H	4.772684	-4.093791	2.265228	H	-4.836661	-5.260324	0.452724
H	2.793595	-4.937082	3.507350	H	-5.606388	-3.660412	0.362487
C	3.409734	1.299089	1.828045	H	-4.399987	-4.136526	-0.851655
C	4.482406	0.941932	2.649220	C	-3.948470	-3.695356	2.551354
C	3.046755	2.647815	1.734117	H	-3.155202	-3.295728	3.187205
C	5.177771	1.916075	3.360771	H	-4.865621	-3.122530	2.731315
H	4.769727	-0.104921	2.741813	H	-4.138398	-4.736570	2.839868
C	3.748319	3.622942	2.436456	C	-2.247096	-4.345151	0.803456
H	2.184201	2.921471	1.120910	H	-1.973781	-4.249261	-0.254712
C	4.815318	3.256604	3.253242	H	-1.436458	-3.934825	1.411905
H	6.007030	1.625466	4.003745	H	-2.351239	-5.414187	1.028702
H	3.449881	4.667254	2.359406				
H	5.359082	4.015496	3.813135	**TS2a'''**			
C	-1.996128	0.991076	1.134003	SCF energy in MeCN: -3029.836479 a.u.			
C	0.261197	1.118329	2.869322	Free energy in MeCN: -3029.013137 a.u.			
H	-0.417931	0.403647	3.353050				
C	-0.093271	2.508432	3.139982	C	0.030019	-2.248892	-1.790038
H	0.619377	3.263786	2.789203	H	0.036250	-3.073107	-1.072897
C	-1.209781	2.947336	3.751088	H	0.542296	-2.449231	-2.729098
H	-1.937023	2.249763	4.167642	C	-0.991579	-1.285250	-1.731346
H	-1.417829	4.007994	3.884354	H	-1.189195	-0.647148	-2.594037
H	1.294700	0.897995	3.164439	C	-1.671702	-0.980617	-0.531961
H	-2.082597	1.069272	2.225151	H	-1.534105	-1.593079	0.359804
N	-2.773825	-0.146159	0.697834	P	3.054251	-0.880069	-0.796166
C	-2.506463	2.272103	0.489983	C	3.455552	-1.342005	-2.516339
H	-1.905281	3.091876	0.906590	C	2.648341	-0.852062	-3.550891
H	-2.327520	2.252207	-0.595978	C	4.575271	-2.119123	-2.832331
C	-3.972709	2.520166	0.742964	C	2.957409	-1.129896	-4.879134
C	-4.928520	2.219921	-0.232364	H	1.768287	-0.252548	-3.304005
C	-4.413485	2.996504	1.981773	C	4.876033	-2.404794	-4.161036
C	-6.288424	2.391590	0.019630	H	5.210317	-2.508598	-2.036986
H	-4.594230	1.857539	-1.207253	C	4.070528	-1.910674	-5.184190
C	-5.768897	3.175669	2.235252	H	2.324615	-0.743298	-5.675631
H	-3.671277	3.225498	2.748379	H	5.744286	-3.016219	-4.397882
C	-6.712965	2.871182	1.255165	H	4.308299	-2.137247	-6.221349
H	-7.017183	2.153691	-0.754747	C	3.730551	-2.221235	0.237982
H	-6.093483	3.555388	3.203368	C	2.883174	-3.275450	0.604224

C	5.067852	-2.249221	0.654576	C	1.007164	2.816904	0.753486
C	3.359555	-4.335967	1.367222	C	0.633063	3.889956	1.577189
H	1.838302	-3.252389	0.289172	C	1.740115	3.072700	-0.410187
C	5.540757	-3.307440	1.425203	C	1.004307	5.188271	1.247021
H	5.739783	-1.436937	0.379950	H	0.039672	3.706082	2.473097
C	4.690050	-4.351263	1.781782	C	2.113659	4.373641	-0.735691
H	2.691980	-5.150439	1.642102	H	2.020822	2.243701	-1.061121
H	6.580822	-3.317686	1.744510	C	1.748233	5.430659	0.092838
H	5.063508	-5.177413	2.383549	H	0.710085	6.015001	1.890495
Pd	0.726926	-0.575089	-0.530182	H	2.688259	4.559369	-1.641193
C	4.142518	0.549289	-0.478369	H	2.035666	6.448365	-0.163440
C	4.438120	0.915838	0.842935	H	-2.115837	-0.001797	-0.396206
C	4.592620	1.362579	-1.526731	C	-3.874663	-1.583353	-0.690242
C	5.156126	2.077047	1.107286	H	-3.735016	-1.954102	-1.703443
H	4.121750	0.277877	1.667670	C	-4.047576	-2.525556	0.459480
C	5.313709	2.522019	-1.255690	H	-3.481471	-3.440572	0.244987
H	4.382882	1.087197	-2.559734	H	-3.597405	-2.075463	1.360186
C	5.590344	2.886578	0.059766	N	-4.560973	-0.394060	-0.618893
H	5.380457	2.344557	2.138538	C	-5.499211	-2.835508	0.744474
H	5.665301	3.140535	-2.079614	C	-6.166541	-2.175301	1.779581
H	6.152137	3.794794	0.268522	C	-6.212626	-3.733744	-0.054021
P	0.571542	1.100253	1.157714	C	-7.519321	-2.407948	2.016948
C	-1.128147	1.216758	1.829312	H	-5.608757	-1.490122	2.422610
C	-2.065679	2.059238	1.212940	C	-7.561715	-3.972207	0.184714
C	-1.561958	0.338957	2.829881	H	-5.703059	-4.253953	-0.865685
C	-3.401138	2.034890	1.603661	C	-8.219283	-3.307328	1.218513
H	-1.745129	2.740260	0.423319	H	-8.024030	-1.893313	2.832311
C	-2.900725	0.313128	3.215141	H	-8.103715	-4.681290	-0.438050
H	-0.846773	-0.322044	3.320040	H	-9.274591	-3.495744	1.404085
C	-3.823252	1.160979	2.605199	H	-5.082910	-0.163719	0.220196
H	-4.117920	2.697009	1.120371	C	-4.428729	0.586929	-1.589946
H	-3.220107	-0.363351	4.006795	O	-3.694695	0.456490	-2.552910
H	-4.866195	1.152733	2.918825	O	-5.206330	1.625439	-1.266341
C	1.597372	0.619874	2.589961	C	-5.257546	2.812817	-2.156161
C	2.235120	1.543429	3.425010	C	-6.259650	3.705231	-1.447305
C	1.809699	-0.749501	2.801223	H	-6.392322	4.636516	-2.008147
C	3.072968	1.101453	4.444980	H	-7.234436	3.213343	-1.364664
H	2.105250	2.611867	3.257480	H	-5.916658	3.962922	-0.438595
C	2.645851	-1.190339	3.822175	C	-5.763885	2.405356	-3.528051
H	1.338682	-1.474114	2.132013	H	-5.045179	1.773168	-4.053689
C	3.283029	-0.262166	4.643052	H	-6.715435	1.868735	-3.444534
H	3.572031	1.827782	5.083942	H	-5.939172	3.304028	-4.130276
H	2.812440	-2.256985	3.962430	C	-3.885840	3.463344	-2.208294
H	3.948217	-0.601003	5.434722	H	-3.942873	4.390177	-2.790464

H	-3.542772	3.726760	-1.200224
H	-3.147882	2.808293	-2.678162

TS2b'''

SCF energy in MeCN: -3029.822855 a.u.

Free energy in MeCN: -3028.997188 a.u.

Pd	-0.057801	0.495394	0.068417
P	-0.071516	-1.720742	-0.723688
P	2.230368	1.000571	0.147488
C	0.173805	-3.000183	0.546153
C	-0.140966	-4.347281	0.315082
C	0.674836	-2.621896	1.796581
C	0.071001	-5.296326	1.309340
H	-0.555099	-4.649825	-0.647087
C	0.889476	-3.573836	2.790647
H	0.885849	-1.566204	1.985376
C	0.592090	-4.912082	2.544870
H	-0.171697	-6.340004	1.120411
H	1.278523	-3.266865	3.760321
H	0.756034	-5.657769	3.320067
C	1.139036	-2.018190	-2.048401
C	1.911572	-3.180184	-2.126745
C	1.270469	-1.039130	-3.045746
C	2.784629	-3.368175	-3.194463
H	1.837485	-3.938738	-1.349023
C	2.131771	-1.238260	-4.119068
H	0.686191	-0.117328	-2.977184
C	2.888798	-2.406387	-4.195566
H	3.387292	-4.273291	-3.241841
H	2.219167	-0.476601	-4.891678
H	3.568365	-2.560740	-5.031584
C	-1.674820	-2.175529	-1.477544
C	-2.778052	-2.364192	-0.626111
C	-1.864035	-2.280484	-2.862086
C	-4.030934	-2.668809	-1.148187
H	-2.644802	-2.297056	0.453289
C	-3.121114	-2.588440	-3.377872
H	-1.024364	-2.145442	-3.541911
C	-4.205132	-2.787469	-2.526269
H	-4.871954	-2.821272	-0.473515
H	-3.248542	-2.684472	-4.454311
H	-5.182329	-3.038019	-2.934758
C	3.468181	-0.290012	-0.211035
C	4.187282	-0.323980	-1.411017
C	3.663655	-1.312837	0.727778
C	5.092124	-1.353264	-1.656672
H	4.048134	0.462049	-2.152179
C	4.560648	-2.344036	0.474946
H	3.131556	-1.285861	1.677873
C	5.281027	-2.363882	-0.717529
H	5.652742	-1.362254	-2.589787
H	4.705374	-3.126030	1.218300
H	5.992250	-3.164289	-0.912788
C	2.630893	1.451962	1.875894
C	1.580009	1.660602	2.778670
C	3.951002	1.560459	2.337263
C	1.837265	2.000827	4.103719
H	0.547436	1.548994	2.437309
C	4.206537	1.904688	3.659972
H	4.783217	1.346885	1.666891
C	3.151534	2.130575	4.543218
H	1.007705	2.163064	4.789680
H	5.234794	1.988386	4.006088
H	3.357476	2.397276	5.577793
C	2.719079	2.400138	-0.920920
C	3.978215	3.006776	-0.834880
C	1.796389	2.877885	-1.860339
C	4.302400	4.073080	-1.665982
H	4.710439	2.643186	-0.115441
C	2.123231	3.942889	-2.695602
H	0.806999	2.413987	-1.914439
C	3.376098	4.542304	-2.596466
H	5.281315	4.541235	-1.586812
H	1.396852	4.308825	-3.419102
H	3.631919	5.379561	-3.242504
C	-2.047006	2.078299	0.112017
C	-0.288754	3.674470	0.813832
C	-0.895503	4.759584	0.148303
H	-0.441206	5.094973	-0.787445
C	-2.047452	5.356376	0.567107
H	-2.518037	5.069513	1.508163
H	-2.509248	6.172441	0.017282
H	-0.592339	3.423685	1.828783
H	-2.460222	2.835563	0.775691
N	-2.245884	0.770832	0.589328
C	-2.292150	2.241298	-1.359542
H	-1.968010	3.247827	-1.650660

H	-1.682723	1.517434	-1.927456
C	-3.755934	2.031741	-1.667720
C	-4.209353	0.803963	-2.156341
C	-4.683944	3.038675	-1.387370
C	-5.569309	0.590464	-2.372101
H	-3.489228	0.016991	-2.395736
C	-6.040429	2.828196	-1.609650
H	-4.330320	3.993419	-0.993530
C	-6.486347	1.601338	-2.100106
H	-5.908767	-0.367176	-2.763858
H	-6.753889	3.623011	-1.401029
H	-7.547918	1.437243	-2.273571
H	0.704011	3.347049	0.517691
H	-2.746810	0.092530	0.004439
C	-2.340908	0.571452	1.995210
O	-2.668600	-0.691593	2.226194
C	-2.770613	-1.196872	3.632510
C	-1.474987	-0.927068	4.376666
H	-0.613229	-1.250399	3.780993
H	-1.357765	0.129019	4.627805
H	-1.473121	-1.507253	5.306549
C	-2.979256	-2.683456	3.413438
H	-3.113083	-3.184905	4.377694
H	-3.872839	-2.870928	2.806979
H	-2.112896	-3.132890	2.912373
C	-3.971469	-0.544932	4.289176
H	-3.832362	0.534068	4.398998
H	-4.883340	-0.730773	3.711286
H	-4.115269	-0.970866	5.288421
O	-2.103900	1.460665	2.783409

TS2c'''

SCF energy in MeCN: -3029.929077 a.u.

Free energy in MeCN: -3029.107717 a.u.

Pd	-0.176487	-0.362104	-0.864723
P	0.266495	1.807225	0.035134
P	-2.449085	-0.795128	-0.345747
C	-0.365468	1.716539	1.766933
C	-0.912424	2.804747	2.456393
C	-0.338437	0.467826	2.401972
C	-1.435288	2.642593	3.736979
H	-0.966781	3.780781	1.976218
C	-0.859423	0.303929	3.683255
H	0.070390	-0.391636	1.866312
C	-1.416533	1.391620	4.351423
H	-1.872059	3.496916	4.252859
H	-0.857796	-0.684329	4.144212
H	-1.841738	1.264314	5.345621
C	-0.679892	3.181112	-0.722638
C	-0.496120	4.530769	-0.385990
C	-1.639040	2.855817	-1.688505
C	-1.266490	5.521151	-0.986261
H	0.267600	4.807482	0.341076
C	-2.411102	3.846836	-2.288057
H	-1.766361	1.807143	-1.965965
C	-2.228779	5.180539	-1.935561
H	-1.111742	6.564533	-0.715135
H	-3.157214	3.572489	-3.032261
H	-2.828871	5.957932	-2.405958
C	1.910501	2.585331	0.319595
C	2.671139	2.260167	1.455051
C	2.505291	3.388401	-0.668963
C	3.966944	2.746640	1.609011
H	2.238880	1.628417	2.232516
C	3.791562	3.889896	-0.501863
H	1.942482	3.639088	-1.568771
C	4.528520	3.574425	0.639299
H	4.534715	2.485494	2.501050
H	4.225224	4.524380	-1.273401
H	5.537422	3.963292	0.765446
C	-3.669907	0.555901	-0.151591
C	-4.520015	0.928737	-1.201692
C	-3.646020	1.353160	1.003883
C	-5.316944	2.065039	-1.101685
H	-4.560684	0.324381	-2.107451
C	-4.439155	2.491664	1.097179
H	-3.005648	1.073288	1.840378
C	-5.275934	2.855383	0.044199
H	-5.973620	2.334601	-1.928156
H	-4.401055	3.095165	2.003552
H	-5.894244	3.748405	0.117431
C	-2.627286	-1.783341	1.188219
C	-1.587647	-2.676865	1.487176
C	-3.728091	-1.717533	2.051051
C	-1.659141	-3.499262	2.606794
H	-0.708236	-2.714140	0.836714
C	-3.785402	-2.523007	3.186250

H	-4.543534	-1.027695	1.834476	C	3.051547	-0.943373	4.509104
C	-2.755832	-3.419164	3.463362	H	3.229942	-1.383081	5.496888
H	-0.849923	-4.196839	2.815078	H	3.903300	-0.300948	4.257795
H	-4.644720	-2.455791	3.851996	H	2.152791	-0.317330	4.565994
H	-2.806195	-4.053368	4.346976	C	4.128224	-2.897697	3.359754
C	-3.265634	-1.854689	-1.603633	H	4.010079	-3.664975	2.590264
C	-4.241892	-2.809929	-1.300125	H	4.999757	-2.281178	3.111825
C	-2.886889	-1.677948	-2.941858	H	4.323658	-3.392576	4.318873
C	-4.832015	-3.560274	-2.312858	C	1.638187	-2.865461	3.761198
H	-4.541194	-2.966652	-0.263709	H	0.737494	-2.240886	3.706451
C	-3.483951	-2.421408	-3.955851	H	1.534057	-3.688271	3.050537
H	-2.106664	-0.947500	-3.175550	H	1.700885	-3.279799	4.775171
C	-4.458344	-3.365265	-3.641206	H	0.735874	-3.263692	-1.219145
H	-5.590190	-4.301337	-2.064128	H	2.553863	-2.252314	-1.497703
H	-3.178454	-2.271913	-4.990331				
H	-4.921335	-3.955501	-4.430196				
C	2.084829	-1.289513	-1.278794				
C	0.439217	-2.479383	-1.919013				
C	0.890272	-2.671507	-3.289374				
H	0.381176	-2.073569	-4.052592				
C	1.893482	-3.479454	-3.673021				
H	2.425457	-4.101837	-2.952370				
H	2.191037	-3.576385	-4.715209				
H	-0.646377	-2.347636	-1.888980				
N	2.403777	-0.978888	0.069589				
C	2.601146	-0.244707	-2.256829				
H	2.164604	-0.455477	-3.240556				
H	2.258525	0.756092	-1.959752				
C	4.106974	-0.270334	-2.328089				
C	4.857865	0.556869	-1.489348				
C	4.778528	-1.148289	-3.181850				
C	6.248464	0.522417	-1.512294				
H	4.340311	1.240184	-0.815220				
C	6.169644	-1.184114	-3.210312				
H	4.194288	-1.810414	-3.823904				
C	6.909338	-0.347479	-2.375979				
H	6.816340	1.179420	-0.853829				
H	6.679963	-1.868037	-3.887253				
H	7.997648	-0.376395	-2.398904				
H	2.424187	-0.004604	0.354977				
C	2.478685	-1.914445	1.061626				
O	2.350689	-3.116663	0.896965				
O	2.702944	-1.268781	2.233815				
C	2.879474	-2.037497	3.468343				