

SUPPORTING INFORMATION

A Computational mechanistic study on the Pd(II)-catalyzed γ -C(sp³)-H lactamization and Further Rational Design

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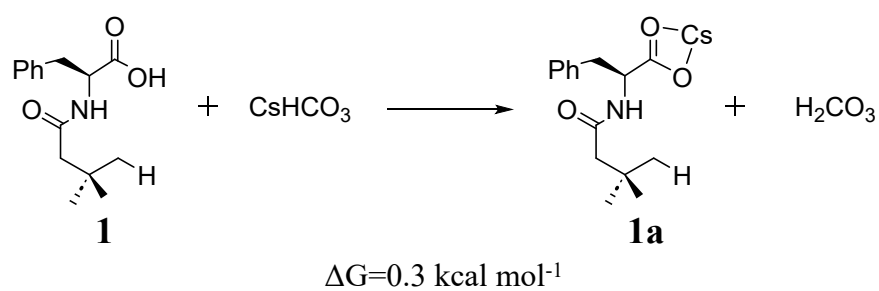
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Scheme S1. Reaction and reaction energies of the aliphatic amide with CsHCO_3 .

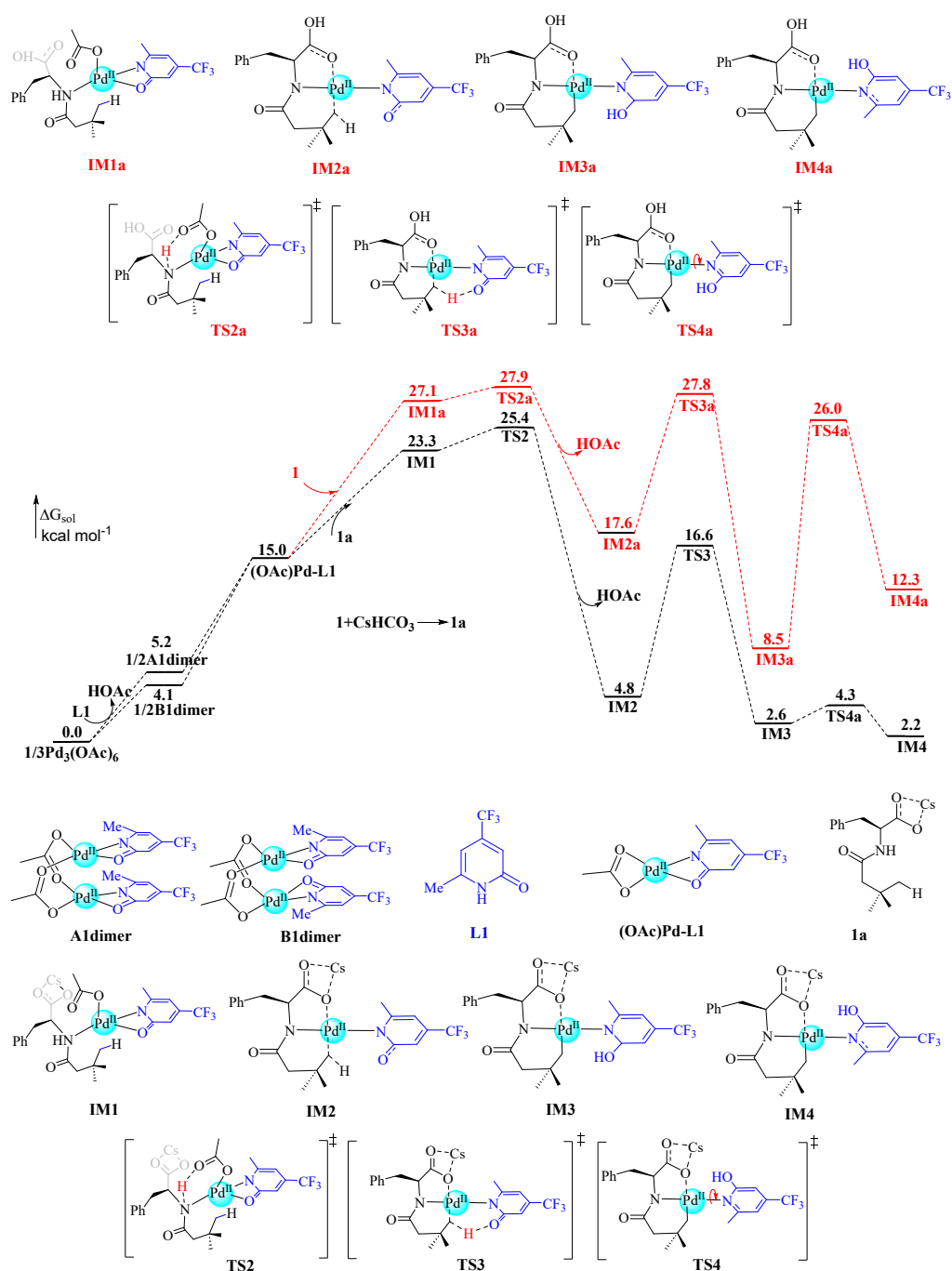


Fig.S1 Computed free energy profiles (in kcal mol⁻¹) for Stage I, together with the optimized key transitions states. (Red path: without Cs; Black path: with Cs).

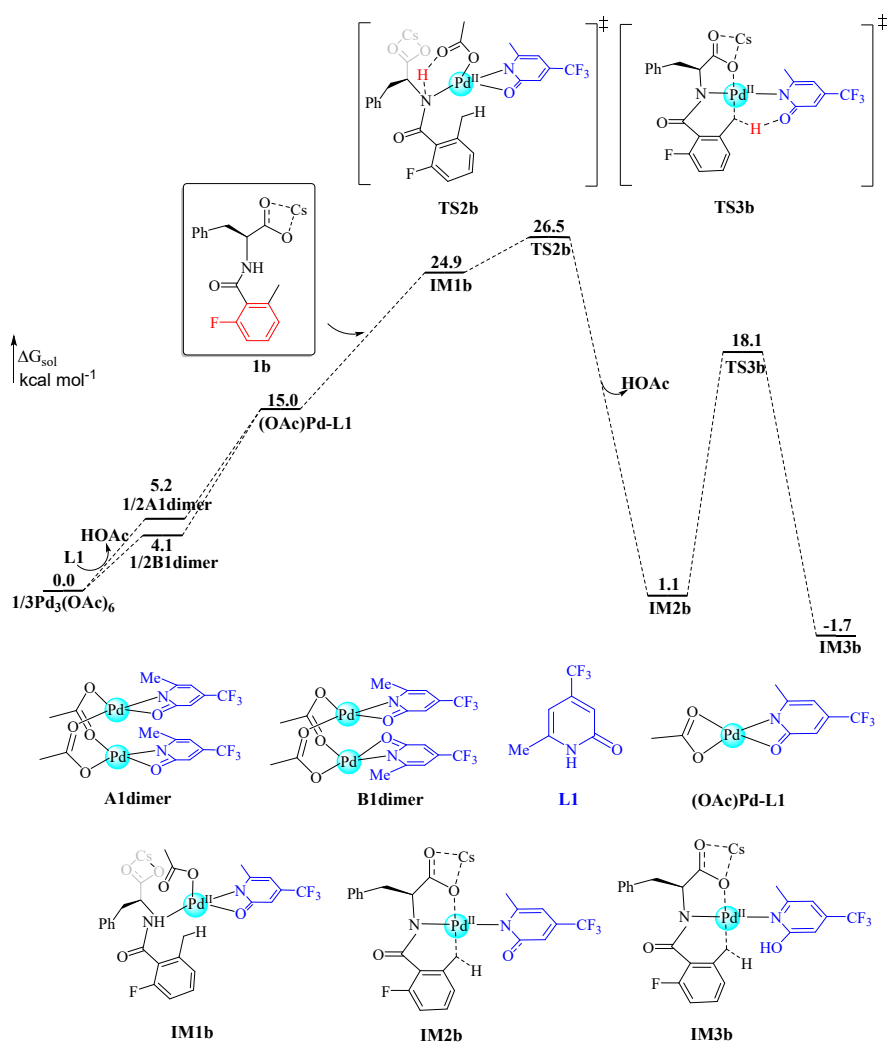


Fig.S2 Computed free energy profiles (in kcal mol⁻¹) for Stage I, together with the optimized key transitions states. Selection of more acidic benzyl substrates.

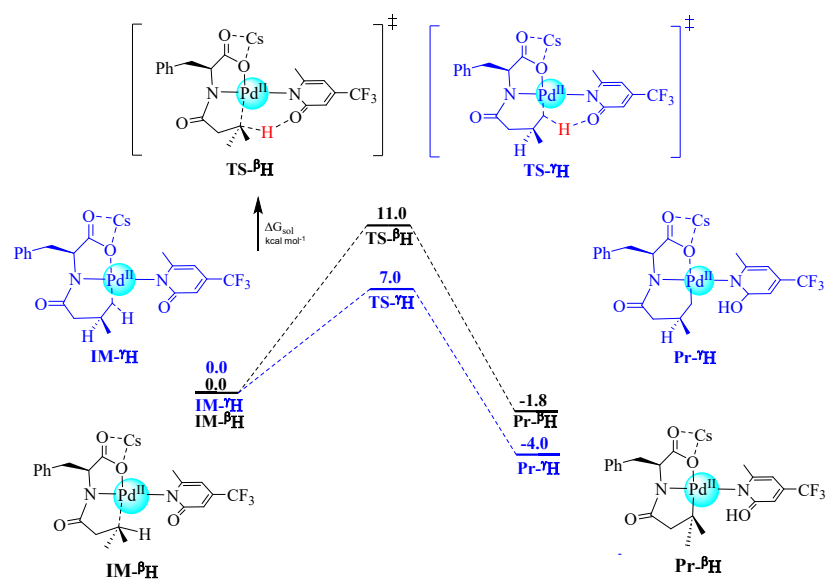


Fig.S3 Substrate **1b** reacts with Pd(II) via five-membered and six-membered chelation reactions between β -C(sp³)-H and γ -C(sp³)-H, respectively., together with the optimized key transitions states. Bond distances in Å.

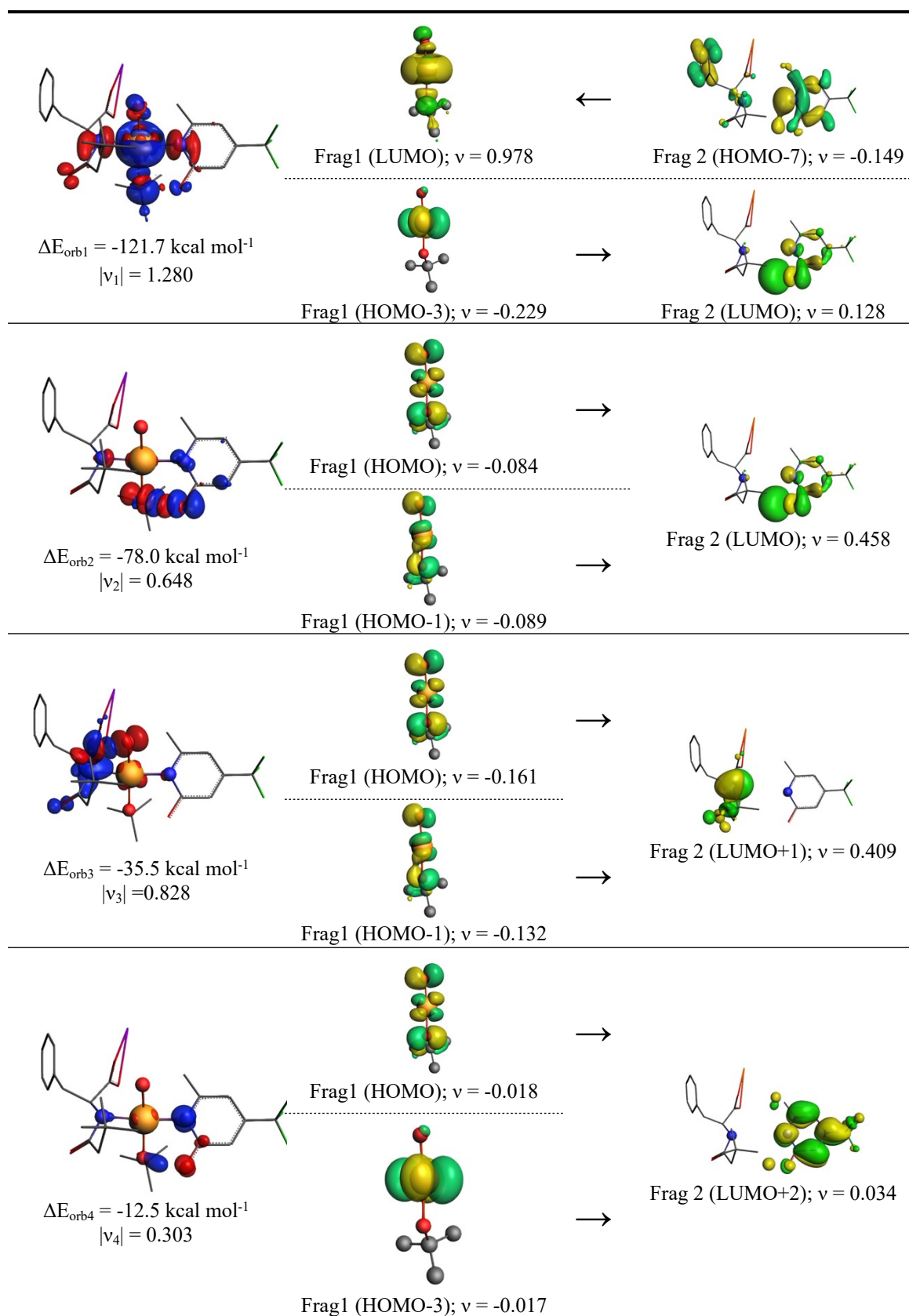


Fig. S4 Plot of deformation densities $\Delta\rho$ of the pairwise orbital interactions and the associated interaction energies (ΔE_{orb}) as well as the shape of the most important interacting MOs of the two fragments in **TS6**. The direction of the charge flow is red to blue.

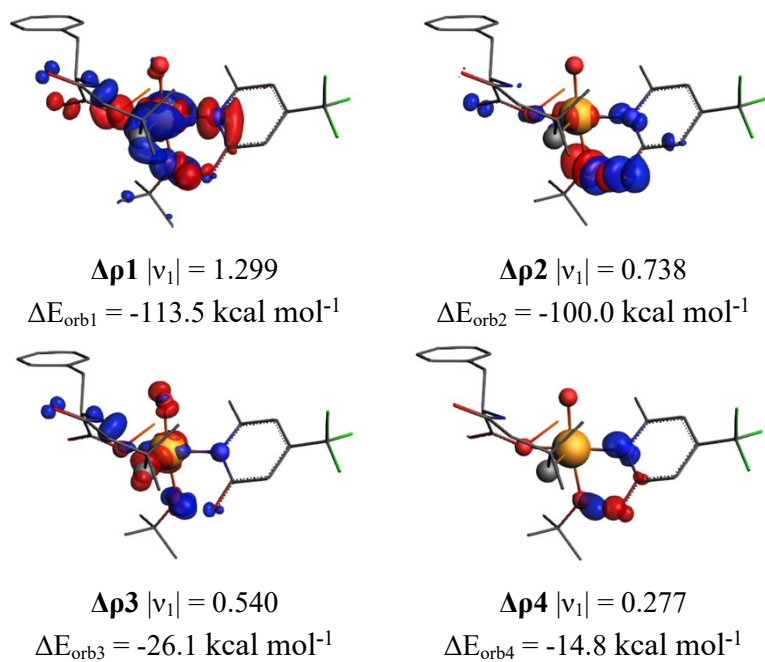


Fig. S5 Plot of deformation densities $\Delta\rho_{1-4}$ of the pairwise orbital interactions in **TS6a** together with the associated interaction energies ΔE_{orb} (in kcal mol^{-1}). The eigenvalues v are a measure for the relative amount of charge transfer. The direction of the charge flow is from red to blue.

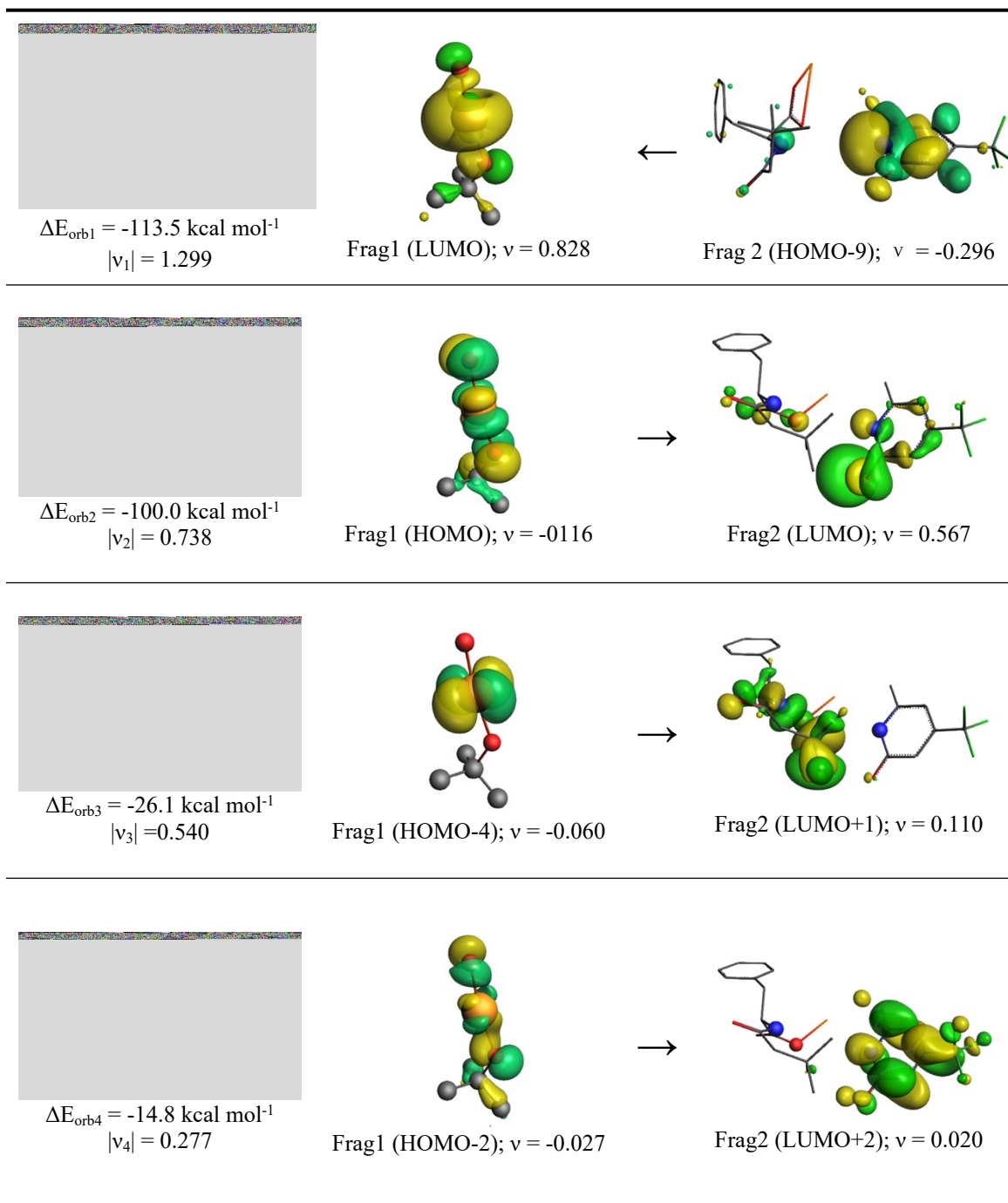


Fig. S6 Plot of deformation densities $\Delta\rho$ of the pairwise orbital interactions and the associated interaction energies (ΔE_{orb}) as well as the shape of the most important interacting MOs of the two fragments in **TS6a**. The direction of the charge flow is red to blue.

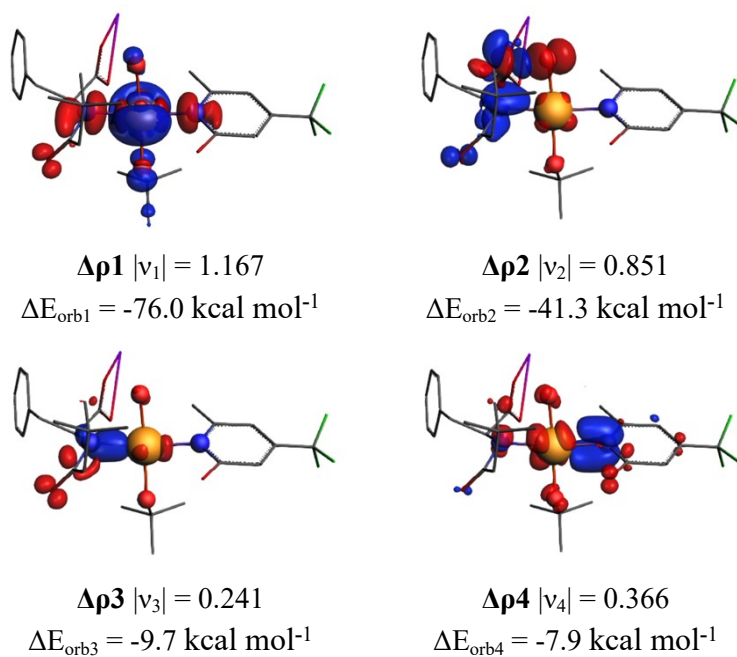


Fig. S7 Plot of deformation densities $\Delta\rho_{1-4}$ of the pairwise orbital interactions in **TS6b** together with the associated interaction energies ΔE_{orb} (in kcal mol⁻¹). The eigenvalues v are a measure for the relative amount of charge transfer. The direction of the charge flow is from red to blue.

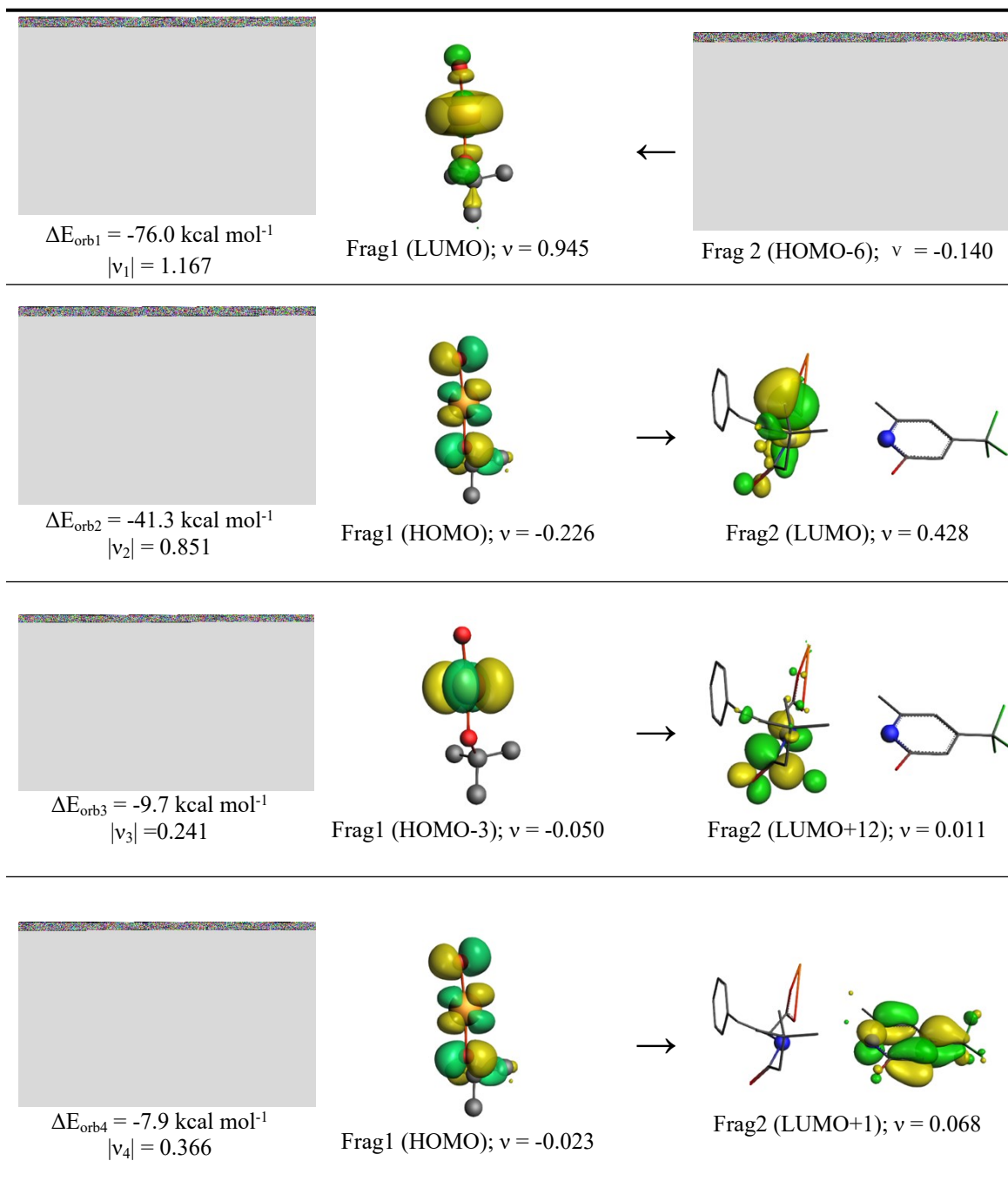


Fig. S8 Plot of deformation densities $\Delta\rho$ of the pairwise orbital interactions and the associated interaction energies (ΔE_{orb}) as well as the shape of the most important interacting MOs of the two fragments in **TS6b**. The direction of the charge flow is red to blue.

Table S1. Calculated Gibbs free energy barriers (in kcal mol⁻¹) on the Pd₃(OAc)₆ trimer dissociates into dimers and monomers step using different functionals.

Different computational levels	$\Delta G^\ddagger$ (1/2 B1 dimer)	$\Delta\Delta G^\ddagger$	$\Delta G^\ddagger$ ((OAc)Pd- L1)	$\Delta\Delta G^\ddagger$
BP86+D3(BJ)/def2-TZVPP(SMD, 2,2,2-TriFluoroEthanol) // BP86+D3(BJ)/def2-SVP((SMD, 2,2,2-TriFluoroEthanol)	4.1	0	15.0	0
PBE0+D3(BJ)/def2-TZVPP(SMD, 2,2,2-TriFluoroEthanol) // BP86+D3(BJ)/def2-SVP((SMD, 2,2,2-TriFluoroEthanol)	5.4	1.3	13.3	-1.7
WB97XD/def2-TZVPP(SMD, 2,2,2-TriFluoroEthanol) // BP86+D3(BJ)/def2-SVP((SMD, 2,2,2-TriFluoroEthanol)	5.3	1.2	13.8	-1.2
B3LYP+D3(BJ)/def2-TZVPP(SMD, 2,2,2-TriFluoroEthanol) // BP86+D3(BJ)/def2-SVP((SMD, 2,2,2-TriFluoroEthanol)	6.5	2.4	16.6	1.6
M06L+D3/def2-TZVPP(SMD, 2,2,2-TriFluoroEthanol) // BP86+D3(BJ)/def2-SVP((SMD, 2,2,2-TriFluoroEthanol)	7.1	3.0	15.0	0

Table S2. Cartesian coordinates of the optimized geometry at BP86+D3(BJ)/def2-SVP(SMD, solvent = 2, 2, 2-TriFluoroEthanol) (Hartree).

E = -1754.27605230 Hartree				H	2.812843	-2.845382	3.333846
Pd₃(OAC)₆				H	2.721054	-1.166282	3.982225
Pd	-1.543813	0.888012	-0.018282	H	2.801615	-2.682221	-3.394437
C	0.034860	2.561253	1.906537	H	3.341045	-0.976433	-3.733634
O	-1.034695	2.434692	1.222529	H	4.188624	-1.966362	-2.497929
O	1.132882	1.940026	1.702385	H	-2.726227	-1.161896	-3.980816
C	2.284281	-1.238661	-1.869834	H	-4.084060	-1.613896	-2.899234
O	1.605937	-2.103054	-1.223047	H	-2.813490	-2.842520	-3.335463
O	2.286110	0.022543	-1.660493	E = -2110.46215060 Hartree			
C	3.199011	-1.748717	-2.954065	A1dimer			
C	-0.012077	3.508710	3.077995	O	2.994407	-1.784450	0.414687
Pd	-0.000823	-1.768176	-0.000057	O	2.823430	-0.032163	1.875596
C	2.181238	-1.328449	1.924796	C	3.211219	-1.203419	1.535641
O	2.619672	-0.331500	1.260532	Pd	1.749341	-0.979531	-0.989932
O	1.093820	-1.960122	1.697794	C	3.960692	-1.998966	2.574199
C	-0.032733	2.560757	-1.907061	H	4.565976	-1.329704	3.214232
O	-1.131358	1.940675	-1.702658	H	3.217050	-2.515612	3.218122
O	1.036719	2.433415	-1.223036	H	4.597634	-2.764913	2.093896
C	0.015109	3.507664	-3.078922	O	3.776519	1.517685	-0.301562
C	3.006195	-1.781592	3.102067	O	3.407190	-0.118397	-1.848948
Pd	1.544608	0.886616	0.018230	C	4.081542	0.846028	-1.349422
C	-2.182735	-1.326915	-1.924511	Pd	1.947777	1.310344	0.591970
O	-2.620177	-0.329581	-1.260168	C	5.334823	1.262127	-2.077053
O	-1.095675	-1.959336	-1.697845	H	5.741324	0.423161	-2.671791
C	-3.008528	-1.779552	-3.101393	H	5.076457	2.094098	-2.766723
C	-2.284870	-1.236378	1.870222	H	6.089880	1.635827	-1.359248
O	-2.285646	0.024793	1.660725	C	-0.946057	0.748303	1.804522
O	-1.607884	-2.101503	1.222957	C	-2.296620	1.017840	1.516422
C	-3.199335	-1.745723	2.955014	C	-2.617028	1.915754	0.477923
H	-1.001921	3.826434	-3.372809	C	-1.623170	2.539268	-0.290840
H	0.489292	2.979379	-3.933505	C	-0.290683	2.232312	0.040028
H	0.643440	4.385293	-2.832381	H	-3.082613	0.530636	2.106677
H	-0.640603	4.386234	2.831605	H	-1.849062	3.221999	-1.121391
H	-0.485541	2.980768	3.933192	C	-4.065195	2.193483	0.133997
H	1.005195	3.827567	3.370953	F	-4.918433	1.782439	1.099836
H	-3.346602	-0.970790	3.730907	F	-4.285276	3.519755	-0.060768
H	-2.798335	-2.675456	3.400166	F	-4.429171	1.566617	-1.019088
H	-4.186847	-1.970573	2.497801	C	-0.503106	-0.149091	2.916804
H	4.081709	-1.613399	2.902016				

H	-0.340170	0.450441	3.839393	C	-4.234078	-1.234304	-0.524240
H	-1.265957	-0.918045	3.141181	O	-5.343999	-0.625811	-0.553949
H	0.460182	-0.632773	2.669302	C	-4.196175	-2.752232	-0.352401
O	0.819731	2.641219	-0.543255	H	-3.859515	-3.229544	-1.302130
N	-0.002569	1.373168	1.068018	C	-3.282368	-3.221922	0.798808
C	-0.657765	-2.496993	0.410248	C	-3.633375	-4.663341	1.213763
C	-2.060468	-2.543902	0.387745	H	-3.499164	-5.364695	0.360734
C	-2.769379	-1.768490	-0.558600	H	-2.980346	-5.014614	2.041287
C	-2.111111	-0.950296	-1.483133	H	-4.687851	-4.747101	1.555719
C	-0.701158	-0.950265	-1.426877	C	-1.797176	-3.111583	0.435864
H	-2.589199	-3.195256	1.096915	H	-1.558577	-3.844995	-0.373827
H	-2.641083	-0.336107	-2.221922	H	0.830770	-0.826763	3.079420
C	-4.281742	-1.820116	-0.533459	H	-1.163097	-3.373207	1.313843
F	-4.781308	-1.143621	0.538435	O	-0.668688	0.614130	-1.126270
F	-4.841655	-1.285727	-1.641679	H	-5.243467	-3.074859	-0.179501
F	-4.733380	-3.097507	-0.428415	C	-3.093807	1.350710	0.877353
C	0.185388	-3.307136	1.344769	H	-4.167678	1.422659	1.145042
H	0.822674	-2.651781	1.971321	H	-2.643216	0.545602	1.493792
H	-0.444341	-3.928881	2.007543	C	-2.365836	2.639496	1.160970
H	0.867636	-3.967899	0.769864	C	-1.061600	2.597244	1.705510
O	0.155124	-0.292386	-2.180785	C	-2.916599	3.897351	0.830230
N	-0.040727	-1.696151	-0.487921	C	-0.327525	3.778659	1.915910
E = -2110.46505366 Hartree				H	-0.621597	1.619054	1.963494
B1dimer				C	-2.184714	5.079326	1.035014
Pd	-1.185010	-1.314856	-0.275721	H	-3.930816	3.946363	0.400829
C	1.672361	-2.017806	-0.934757	C	-0.885900	5.025051	1.576500
C	3.063202	-1.948632	-0.756782	H	0.685213	3.726360	2.349197
C	3.575752	-1.533025	0.485311	H	-2.630519	6.052194	0.771082
C	2.704074	-1.232506	1.536752	H	-0.313916	5.952736	1.739674
C	1.319852	-1.332500	1.291055	Cs	1.999053	2.130436	-0.996102
H	3.730899	-2.197693	-1.592540	H	-3.483432	-2.560307	1.674524
H	3.065473	-0.912795	2.524756	C	1.064408	-2.406702	-2.248723
C	5.061142	-1.301449	0.648792	H	0.350819	-3.245864	-2.115517
F	5.391406	-0.037629	0.245968	H	0.483910	-1.556794	-2.666639
F	5.465038	-1.421455	1.934484	H	1.844733	-2.702982	-2.975477
F	5.798475	-2.156971	-0.096879	E = -584.703488746 Hartree			
O	0.394917	-1.047412	2.227116	Pd(OAC)₂			
N	0.820452	-1.693543	0.084576	Pd	-0.000003	0.000179	-0.017775
C	-1.722420	1.360785	-1.271555	C	-3.943192	-0.000046	0.058319
O	-1.706235	2.471783	-1.847082	H	-4.347234	-0.886111	-0.468507
C	-3.013215	0.842516	-0.614645	H	-4.255496	-0.057685	1.123484
H	-3.879494	1.250370	-1.175651	H	-4.346783	0.934608	-0.375735
N	-3.041139	-0.620966	-0.622633	C	-2.457180	0.000703	-0.001226

O	-1.764774	-1.088414	-0.013686	H	-4.486537	-3.214643	-0.953414
O	-1.764533	1.089480	-0.012939	C	-3.121497	-1.837148	-0.049903
C	3.943204	-0.000700	0.058330	O	-2.091736	-2.585396	0.079106
H	4.347557	0.886380	-0.466525	O	-3.081072	-0.558957	-0.128032
H	4.255498	0.054361	1.123634	C	0.637522	-0.992492	1.237063
H	4.346505	-0.934542	-0.377761	C	1.994328	-0.760385	1.199685
C	2.457180	-0.000892	-0.001234	C	2.648082	-0.620201	-0.068977
O	1.765136	1.088448	-0.013506	C	1.971713	-0.785286	-1.254935
O	1.764176	-1.089469	-0.013126	C	0.554326	-1.098860	-1.246036

E = -699.415838087 Hartree

L1

C	1.668436	-1.061350	-0.000080
C	0.285213	-1.151695	-0.000117
C	-0.477765	0.053043	-0.000111
C	0.123758	1.297069	-0.000021
C	1.568470	1.418803	-0.000014
H	-0.197575	-2.137648	-0.000155
H	-0.458412	2.228314	0.000028
C	-1.987442	-0.068033	0.000022
F	-2.424611	-0.750795	1.091838
F	-2.613199	1.131304	-0.000873
F	-2.424624	-0.752422	-1.090837
C	2.589289	-2.241474	0.000076
H	2.014959	-3.186005	-0.000070
H	3.248903	-2.223765	-0.893792
H	3.248232	-2.223906	0.894482
O	2.214308	2.484577	0.000043
N	2.243044	0.183335	-0.000074
H	3.270285	0.252080	-0.000008

E = -1284.13384544 Hartree

TS1

Pd	-1.399037	0.574234	-0.031378
C	-0.755506	4.469136	0.033970
H	-0.676020	4.776592	1.099111
H	0.204176	4.706038	-0.465366
H	-1.590040	5.025931	-0.433055
C	-1.014549	3.005147	-0.019577
O	-2.204321	2.516217	-0.104395
O	-0.054805	2.140596	0.047276
C	-4.474933	-2.491507	-0.112193
H	-4.637911	-3.067405	0.822216
H	-5.277958	-1.744147	-0.240972

H	2.562363	-0.687190	2.137082
H	2.464213	-0.698174	-2.232747
C	4.123595	-0.279295	-0.063544
F	4.839922	-1.214455	0.613904
F	4.648738	-0.188564	-1.305434
F	4.340450	0.910506	0.557548
C	-0.146540	-1.153594	2.505904
H	-0.791422	-2.055708	2.453497
H	0.530112	-1.237232	3.376701
H	-0.818146	-0.281785	2.662986
O	-0.119494	-1.356886	-2.256720
N	-0.087277	-1.085253	0.040830
H	-1.065999	-1.885364	0.070749

E = -228.929225440 Hartree

HOAc

C	1.377164	-0.015093	0.000139
H	1.705947	-0.582870	-0.895881
H	1.849364	0.983879	0.001647
H	1.706551	-0.586720	0.893351
C	-0.124953	0.127604	0.000114
O	-0.727441	1.191986	-0.000080
O	-0.839469	-1.027464	0.000167
H	-0.239849	-1.805529	-0.001332

E = -1055.19258737 Hartree

(OAc)Pd-L1

Pd	-1.759377	0.394536	0.006563
C	-5.597551	-0.541478	-0.041833
H	-5.904081	-0.630453	-1.106552
H	-5.762211	-1.519590	0.449679
H	-6.212543	0.246869	0.433008
C	-4.156429	-0.171666	0.007252
O	-3.754444	1.051295	0.012371
O	-3.223514	-1.066943	0.015632

C	0.847456	-1.406876	0.006404	H	-1.707442	-1.092890	-1.551627
C	2.246782	-1.287993	0.009557	C	2.098322	1.374080	-0.500869
C	2.834713	-0.000790	0.008872	H	2.032601	1.656272	-1.572180
C	2.062171	1.166231	0.005492	H	2.833449	2.050295	-0.018078
C	0.662353	0.986795	0.001896	C	2.522699	-0.067618	-0.353612
H	2.866935	-2.195109	0.013817	C	2.216290	-1.010599	-1.357591
H	2.500226	2.172922	0.006405	C	3.123700	-0.520321	0.840693
C	4.346450	0.092494	-0.005525	C	2.493799	-2.375952	-1.169264
F	4.858256	-0.411706	-1.159985	H	1.745431	-0.669423	-2.293668
F	4.792066	1.365219	0.108312	C	3.406280	-1.882686	1.030196
F	4.896480	-0.621210	1.011430	H	3.360109	0.205466	1.636519
C	0.109367	-2.709189	0.008053	C	3.086269	-2.816432	0.027250
H	-0.545683	-2.780825	-0.885924	H	2.244259	-3.099908	-1.961676
H	0.807844	-3.566300	0.011799	H	3.874225	-2.220053	1.969120
H	-0.549965	-2.776343	0.899224	H	3.301202	-3.886526	0.178113
O	-0.294247	1.891730	-0.000357	H	1.664205	3.604742	1.127155
N	0.122197	-0.266340	0.002381				

E = -883.886715654 Hartree

E = -284.533754823 Hartree

1

C	0.216751	3.034549	-0.028797
O	0.946271	3.991074	0.577563
C	0.694517	1.593876	0.150764
H	0.777212	1.380987	1.238919
N	-0.298303	0.694127	-0.388087
H	-0.750565	0.963576	-1.266998
C	-0.679448	-0.452783	0.244078
O	-0.190794	-0.800785	1.336243
C	-1.764778	-1.251540	-0.453980
H	-1.553318	-2.321657	-0.251950
C	-3.212282	-0.917347	0.029828
C	-3.569572	0.542967	-0.311940
H	-3.495923	0.730950	-1.404742
H	-4.611461	0.770869	-0.001728
H	-2.901357	1.267276	0.198244
C	-4.174089	-1.865270	-0.713286
H	-3.948880	-2.928358	-0.482909
H	-5.227123	-1.669323	-0.418604
H	-4.099978	-1.733375	-1.813894
C	-3.343658	-1.142597	1.548772
H	-4.391721	-0.972032	1.875008
H	-3.064488	-2.180421	1.829221
H	-2.693499	-0.453071	2.125414
O	-0.753931	3.345180	-0.703369

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C	-0.713530	-1.664869	0.703783
O	-1.174639	-2.687376	0.116581
C	0.683742	-1.168352	0.238881
H	0.676208	-1.102339	-0.870088
N	0.909201	0.165023	0.765604
H	0.333623	0.373317	1.592667
C	1.390478	1.195592	0.020637
O	1.910132	1.028257	-1.103332
C	1.196594	2.572819	0.631568
H	2.113321	3.167814	0.437926
C	-0.039864	3.330488	0.047166
C	-1.305131	2.453197	0.151653
H	-1.481840	2.110783	1.193407
H	-2.200840	3.022898	-0.175829
H	-1.227318	1.551469	-0.491515
C	-0.235366	4.615230	0.875102
H	0.675221	5.251191	0.851276
H	-1.079786	5.217735	0.477028
H	-0.457100	4.380041	1.938038
C	0.206571	3.702876	-1.427720
H	-0.672036	4.238198	-1.847248
H	1.090175	4.368413	-1.530440
H	0.391779	2.802196	-2.047263
O	-1.294078	-0.997385	1.618602
H	1.075249	2.480339	1.731280

C	1.788324	-2.179298	0.653403	O	1.292830	-0.863058	-1.585012
H	1.741512	-2.320907	1.754059	C	2.829252	0.225464	-0.097433
H	1.542143	-3.148846	0.174065	H	3.307952	0.626386	-1.012155
C	3.159100	-1.700135	0.243226	N	1.933012	1.318375	0.383214
C	3.953009	-0.945036	1.133303	H	1.722367	1.197684	1.429225
C	3.628062	-1.898425	-1.074199	C	2.397293	2.642761	0.078218
C	5.179001	-0.396227	0.717515	O	3.372987	2.818402	-0.643318
H	3.598694	-0.779857	2.163805	C	1.582237	3.780268	0.641263
C	4.854476	-1.356858	-1.491912	H	2.299275	4.576095	0.926696
H	3.015192	-2.480030	-1.783049	C	0.568430	4.370314	-0.394170
C	5.633176	-0.598544	-0.597742	C	-0.563030	3.354832	-0.633873
H	5.783489	0.193673	1.425661	H	-0.137058	2.425851	-1.202281
H	5.204335	-1.522957	-2.523816	H	-1.132589	3.177405	0.302852
H	6.593172	-0.168385	-0.925797	H	-1.299681	3.684150	-1.395721
Cs	-3.725141	-0.787502	-0.307385	C	-0.055051	5.633164	0.231319
E = -1939.10798471 Hartree				H	0.717450	6.414866	0.386010
IM1				H	-0.838689	6.053067	-0.433492
Pd	-0.186293	1.130033	0.058038	H	-0.520996	5.407497	1.213208
C	0.279952	-1.805629	3.182801	C	1.247635	4.724389	-1.728262
H	0.540809	-1.617717	4.240947	H	0.524243	5.239583	-2.394240
H	-0.743389	-2.220686	3.102957	H	2.113541	5.400378	-1.572859
H	0.991080	-2.551521	2.767453	H	1.610210	3.821102	-2.260396
C	0.423048	-0.534092	2.374052	O	2.191331	-2.114595	0.069138
O	-0.190184	-0.564161	1.224031	H	1.027850	3.452799	1.545557
O	1.120396	0.423210	2.787920	C	3.918862	-0.059857	0.954623
C	-2.720282	0.326090	-1.274786	H	4.276739	0.915662	1.348419
C	-4.042930	-0.124755	-1.289549	H	3.474309	-0.619684	1.800839
C	-4.783457	-0.090985	-0.080382	C	5.094796	-0.812226	0.370656
C	-4.229407	0.421556	1.081296	C	5.368453	-2.149691	0.726250
C	-2.872882	0.922997	1.089776	C	5.938497	-0.177892	-0.569560
H	-4.479702	-0.500714	-2.224586	C	6.457366	-2.836506	0.160400
H	-4.789171	0.464471	2.025953	H	4.714962	-2.656669	1.453965
C	-6.175630	-0.678412	-0.071637	C	7.024713	-0.862256	-1.139902
F	-6.131063	-2.039034	-0.175929	H	5.736717	0.869075	-0.852525
F	-6.864300	-0.392407	1.058290	C	7.287889	-2.196351	-0.776816
F	-6.918851	-0.235182	-1.119879	H	6.656789	-3.880428	0.452421
C	-1.868930	0.317602	-2.513363	H	7.672264	-0.350516	-1.870356
H	-0.876340	-0.137609	-2.315170	H	8.139716	-2.734654	-1.222736
H	-2.370858	-0.233928	-3.330769	Cs	-0.759651	-3.083091	-0.556346
H	-1.680336	1.356842	-2.858867	E = -1939.09749366 Hartree			
O	-2.320567	1.436909	2.098388	TS2			
N	-2.169637	0.791100	-0.116906	Pd	0.926553	-0.945416	0.129954
C	2.033643	-1.032562	-0.563712	C	0.318275	-0.372947	4.389551

H	0.362817	-1.205942	5.116780	H	0.557093	-5.446002	-2.781317
H	1.178913	0.309299	4.513772	H	-0.647541	-4.119256	-2.893333
H	-0.617812	0.196554	4.576428	O	-1.731609	0.940339	0.695947
C	0.256523	-0.912746	2.990884	H	1.329435	-3.520781	0.364851
O	0.785337	-0.221959	2.058612	C	-3.099245	-1.526469	1.238864
O	-0.355642	-2.027640	2.795259	H	-3.335509	-2.607179	1.346825
C	2.597634	1.473909	-0.383690	H	-2.637615	-1.188390	2.186389
C	3.776033	2.224378	-0.389082	C	-4.358520	-0.728202	0.974546
C	4.976176	1.600839	0.037840	C	-4.742676	0.321814	1.837870
C	4.985996	0.278624	0.453425	C	-5.141300	-0.967286	-0.178323
C	3.764360	-0.492733	0.461683	C	-5.873055	1.111464	1.561064
H	3.755335	3.272202	-0.718088	H	-4.136538	0.526456	2.735481
H	5.904109	-0.220902	0.792510	C	-6.268824	-0.176266	-0.462746
C	6.248989	2.415616	0.028035	H	-4.864693	-1.785635	-0.863283
F	6.137446	3.521301	0.814768	C	-6.638149	0.869101	0.404616
F	7.326183	1.721972	0.467219	H	-6.154667	1.924749	2.249782
F	6.544134	2.860633	-1.224708	H	-6.865053	-0.379636	-1.367165
C	1.275893	2.055280	-0.797319	H	-7.521654	1.489112	0.182401
H	0.575338	2.083285	0.064224	Cs	-3.236076	3.015632	-1.029474
H	1.400465	3.082935	-1.188543	E = -1710.17146132 Hartree			
H	0.788258	1.428423	-1.572513	IM2			
O	3.691668	-1.697115	0.838609	Pd	0.604125	0.632343	-0.096399
N	2.618534	0.172209	0.017137	C	2.461221	-1.982897	0.339730
C	-1.786831	0.109155	-0.261374	C	3.778752	-2.426605	0.144225
O	-1.644756	0.383479	-1.496160	C	4.716410	-1.557221	-0.461041
C	-2.092134	-1.381542	0.079205	C	4.360281	-0.268359	-0.870518
H	-2.538122	-1.828683	-0.830959	C	3.018812	0.122241	-0.648834
N	-0.813123	-2.098765	0.320579	H	4.065381	-3.439348	0.460211
H	-0.550609	-2.162762	1.638620	H	5.071206	0.423552	-1.341219
C	-0.747481	-3.394145	-0.217867	C	6.135343	-2.049213	-0.643492
O	-1.761878	-4.007113	-0.575834	F	6.171015	-3.224020	-1.327844
C	0.646390	-3.945145	-0.403348	F	6.912623	-1.168991	-1.317473
H	0.618701	-5.047581	-0.292741	F	6.736645	-2.279347	0.555460
C	1.203255	-3.581736	-1.822161	C	1.385271	-2.830974	0.948141
C	1.044838	-2.074111	-2.094717	H	0.614192	-3.062616	0.182331
H	1.733023	-1.471485	-1.389727	H	1.792469	-3.783840	1.334907
H	1.524670	-1.765316	-3.048551	H	0.879231	-2.288082	1.772795
H	-0.001952	-1.716991	-2.138417	O	2.455668	1.269205	-0.945008
C	2.696366	-3.954418	-1.854306	N	2.128490	-0.733234	-0.057810
H	2.839179	-5.033310	-1.636397	C	-2.092379	0.357356	0.744690
H	3.131615	-3.746426	-2.854609	O	-3.107464	-0.083501	1.312769
H	3.264280	-3.371216	-1.099276	C	-2.104990	1.631246	-0.088828
C	0.436729	-4.350704	-2.915748	H	-2.727421	2.388011	0.432799
H	0.823161	-4.085700	-3.922333				

N	-0.736127	2.122352	-0.238386	H	-4.516986	0.082047	-1.750420
C	-0.564221	3.462087	-0.344014	H	-3.482679	0.711941	2.449389
O	-1.542813	4.262236	-0.355154	C	-5.471252	-0.277245	0.796478
C	0.856911	3.986882	-0.429078	F	-5.473937	-1.629479	0.604110
H	0.845875	4.842069	-1.138209	F	-5.779347	-0.063929	2.096919
C	1.453975	4.479960	0.927418	F	-6.489651	0.222343	0.050946
C	1.369597	3.374618	1.998054	C	-2.083957	0.930673	-2.761594
H	1.850364	2.436104	1.645680	H	-1.250599	0.224177	-2.956378
H	1.881139	3.694847	2.931058	H	-2.917930	0.702598	-3.451722
H	0.317603	3.132742	2.256621	H	-1.699988	1.949073	-2.980994
C	2.935419	4.823963	0.675274	O	-1.058177	1.630702	1.807848
H	3.040848	5.599598	-0.113442	N	-1.635881	1.202642	-0.369802
H	3.419816	5.210271	1.597870	C	1.867172	-0.826216	-1.440658
H	3.497548	3.924806	0.343477	O	2.174425	-1.962408	-1.847676
C	0.705947	5.732729	1.422556	C	2.857127	0.051311	-0.668506
H	1.131889	6.092676	2.383954	H	3.858006	-0.033337	-1.141913
H	0.780908	6.562235	0.686897	N	2.400327	1.441089	-0.688449
H	-0.371716	5.522769	1.581036	C	3.292801	2.408509	-0.400070
O	-0.950976	-0.296101	0.788109	O	4.522827	2.180132	-0.228850
H	1.524940	3.208985	-0.841641	C	2.758266	3.833081	-0.301456
C	-2.739215	1.359458	-1.491360	H	2.414650	4.165245	-1.306542
H	-2.823432	2.352111	-1.981644	C	1.607906	4.052882	0.715170
H	-2.014186	0.754707	-2.074925	C	1.966561	3.434350	2.080300
C	-4.077735	0.664005	-1.453147	H	2.905238	3.870428	2.482635
C	-4.207417	-0.668160	-1.902616	H	1.159538	3.616628	2.820770
C	-5.216435	1.306415	-0.916093	H	2.106756	2.336693	1.999682
C	-5.437455	-1.345863	-1.813826	C	1.406955	5.575860	0.881972
H	-3.326393	-1.180462	-2.325070	H	1.159779	6.057333	-0.088101
C	-6.445294	0.632880	-0.823282	H	0.578754	5.791832	1.590021
H	-5.134185	2.347632	-0.562973	H	2.327259	6.056971	1.276179
C	-6.560387	-0.698385	-1.268147	C	0.289143	3.467072	0.179276
H	-5.517909	-2.385195	-2.172487	H	0.080102	3.824415	-0.854266
H	-7.322157	1.149541	-0.400358	H	-0.124431	2.266212	0.881787
H	-7.524865	-1.226149	-1.195044	H	-0.570283	3.843091	0.779858
Cs	-2.674541	-3.107073	0.930422	O	0.657130	-0.341328	-1.582433
E = -1710.15305306 Hartree				H	3.624370	4.467154	-0.023823
TS3				C	2.962825	-0.443387	0.810250
Pd	0.393555	1.478949	-0.617617	H	3.725667	0.207224	1.288056
C	-2.529113	0.838220	-1.331044	H	1.988630	-0.231832	1.300108
C	-3.804028	0.383249	-0.970824	C	3.323554	-1.897037	0.989586
C	-4.137950	0.316348	0.401931	C	2.440671	-2.779830	1.649042
C	-3.240663	0.739321	1.378575	C	4.537302	-2.416624	0.483684
C	-1.953502	1.211112	0.977175	C	2.750907	-4.144899	1.792221
				H	1.492826	-2.385864	2.054569

C	4.850727	-3.778222	0.623836	H	0.094579	5.720320	1.512530
H	5.243294	-1.742942	-0.029084	H	1.824685	6.156192	1.308164
C	3.956863	-4.650233	1.275288	C	0.103397	3.393115	0.067798
H	2.045910	-4.815563	2.310286	H	-0.197213	3.895453	-0.883037
H	5.801041	-4.164838	0.221134	H	-0.244630	1.185375	1.515006
H	4.203207	-5.718782	1.382848	H	-0.760892	3.465317	0.766936
Cs	-0.912362	-2.774630	-0.461066	O	0.748806	-0.531210	-1.246079
E = -1710.17948201 Hartree				H	3.337884	4.698156	0.014910
IM3				C	3.235163	-0.244598	0.785647
Pd	0.360396	1.457767	-0.486748	H	4.006289	0.437032	1.200756
C	-2.541441	0.935419	-1.258992	H	2.298110	-0.093128	1.361952
C	-3.850723	0.499657	-1.008665	C	3.672305	-1.682903	0.888873
C	-4.236087	0.210397	0.315126	C	2.775179	-2.672105	1.348276
C	-3.331256	0.369237	1.368020	C	4.958331	-2.088318	0.466120
C	-2.028205	0.798076	1.046586	C	3.146199	-4.028098	1.384715
H	-4.554076	0.384193	-1.844440	H	1.769283	-2.366672	1.683052
H	-3.590965	0.152815	2.412829	C	5.333604	-3.441526	0.500216
C	-5.610355	-0.362509	0.585086	H	5.671946	-1.329774	0.103953
F	-5.611887	-1.713967	0.395111	C	4.427705	-4.418391	0.956308
F	-6.021313	-0.142148	1.855441	H	2.430595	-4.783114	1.749781
F	-6.548905	0.151864	-0.244635	H	6.341404	-3.738666	0.167182
C	-2.043934	1.241535	-2.638712	H	4.722760	-5.479687	0.981880
H	-1.203477	0.564104	-2.900318	Cs	-0.953235	-2.897985	-0.335393
H	-2.849610	1.125235	-3.387761	E = -1710.13700073 Hartree			
H	-1.648069	2.277600	-2.687505	TS4			
O	-1.100140	0.914337	2.003538	Pd	-1.185010	-1.314856	-0.275721
N	-1.654127	1.070448	-0.230293	C	1.672361	-2.017806	-0.934757
C	2.025235	-0.760226	-1.366331	C	3.063202	-1.948632	-0.756782
O	2.492568	-1.772464	-1.929629	C	3.575752	-1.533025	0.485311
C	2.958516	0.247318	-0.675524	C	2.704074	-1.232506	1.536752
H	3.924725	0.270729	-1.222040	C	1.319852	-1.332500	1.291055
N	2.359118	1.582469	-0.642650	H	3.730899	-2.197693	-1.592540
C	3.180251	2.629656	-0.432542	H	3.065473	-0.912795	2.524756
O	4.438330	2.521642	-0.354731	C	5.061142	-1.301449	0.648792
C	2.531452	4.006272	-0.304731	F	5.391406	-0.037629	0.245968
H	2.201238	4.340659	-1.314789	F	5.465038	-1.421455	1.934484
C	1.327988	4.102406	0.666329	F	5.798475	-2.156971	-0.096879
C	1.694783	3.505579	2.039376	O	0.394917	-1.047412	2.227116
H	2.565743	4.029189	2.489246	N	0.820452	-1.693543	0.084576
H	0.842935	3.593895	2.747094	C	-1.722420	1.360785	-1.271555
H	1.949031	2.429177	1.953093	O	-1.706235	2.471783	-1.847082
C	0.978902	5.597990	0.850935	C	-3.013215	0.842516	-0.614645
H	0.742848	6.079010	-0.122395	H	-3.879494	1.250370	-1.175651

N	-3.041139	-0.620966	-0.622633	C	-2.243343	1.404521	-0.994120
C	-4.234078	-1.234304	-0.524240	H	-3.616979	0.174576	2.397111
O	-5.343999	-0.625811	-0.553949	H	-4.273618	1.325718	-1.768152
C	-4.196175	-2.752232	-0.352401	C	-5.578725	0.352689	0.483212
H	-3.859515	-3.229544	-1.302130	F	-6.068848	0.711189	1.694674
C	-3.282368	-3.221922	0.798808	F	-6.356303	0.931139	-0.460297
C	-3.633375	-4.663341	1.213763	F	-5.750874	-0.996329	0.371482
H	-3.499164	-5.364695	0.360734	C	-0.877930	0.545730	2.350145
H	-2.980346	-5.014614	2.041287	H	-0.261588	1.451404	2.524519
H	-4.687851	-4.747101	1.555719	H	-1.380074	0.256974	3.292698
C	-1.797176	-3.111583	0.435864	H	-0.175676	-0.263822	2.055367
H	-1.558577	-3.844995	-0.373827	O	-1.712597	1.807739	-2.154310
H	0.830770	-0.826763	3.079420	N	-1.402133	1.213551	0.052003
H	-1.163097	-3.373207	1.313843	C	1.937561	-1.014921	-1.320190
O	-0.668688	0.614130	-1.126270	O	2.243514	-2.066869	-1.920623
H	-5.243467	-3.074859	-0.179501	C	3.024403	-0.096358	-0.737297
C	-3.093807	1.350710	0.877353	H	3.954854	-0.218439	-1.329924
H	-4.167678	1.422659	1.145042	N	2.580869	1.299084	-0.758857
H	-2.643216	0.545602	1.493792	C	3.517810	2.262651	-0.678399
C	-2.365836	2.639496	1.160970	O	4.761022	2.031141	-0.692815
C	-1.061600	2.597244	1.705510	C	3.010319	3.699480	-0.572010
C	-2.916599	3.897351	0.830230	H	2.562804	4.000720	-1.546355
C	-0.327525	3.778659	1.915910	C	1.971090	3.951950	0.551132
H	-0.621597	1.619054	1.963494	C	2.473486	3.370601	1.887426
C	-2.184714	5.079326	1.035014	H	3.468196	3.783716	2.161234
H	-3.930816	3.946363	0.400829	H	1.768609	3.612798	2.711394
C	-0.885900	5.025051	1.576500	H	2.563482	2.266140	1.835788
H	0.685213	3.726360	2.349197	C	1.794413	5.480314	0.707553
H	-2.630519	6.052194	0.771082	H	1.483403	5.948955	-0.250682
H	-0.313916	5.952736	1.739674	H	1.017604	5.714866	1.466812
Cs	1.999053	2.130436	-0.996102	H	2.741445	5.965294	1.030295
H	-3.483432	-2.560307	1.674524	C	0.610661	3.345337	0.166315
C	1.064408	-2.406702	-2.248723	H	0.200503	3.881740	-0.722412
H	0.350819	-3.245864	-2.115517	H	-0.710339	1.855855	-1.997796
H	0.483910	-1.556794	-2.666639	H	-0.120376	3.478455	0.996622
H	1.844733	-2.702982	-2.975477	O	0.709558	-0.660975	-1.071096
				H	3.906025	4.335329	-0.414929
E = -1710.17812468 Hartree				C	3.311956	-0.533557	0.743465
IM4				H	4.273714	-0.064313	1.036173
Pd	0.612776	1.384419	-0.358885	H	2.510818	-0.082109	1.365565
C	-1.876784	0.780353	1.257458	C	3.331309	-2.024045	0.962006
C	-3.245494	0.527476	1.425403	C	2.202489	-2.668607	1.515950
C	-4.117862	0.717605	0.334881	C	4.421635	-2.819152	0.544113
C	-3.628865	1.167463	-0.893559	C	2.160660	-4.067794	1.650677

H	1.346650	-2.055313	1.845242	H	0.526101	5.975438	-0.440529
C	4.383887	-4.217326	0.676500	H	1.213371	5.638302	-2.065981
H	5.308784	-2.332792	0.105945	H	-0.452293	6.293772	-1.914416
C	3.251935	-4.848152	1.227358	C	0.825517	3.269031	-0.843800
H	1.272342	-4.550833	2.090109	H	1.281434	3.710621	0.062458
H	5.244251	-4.821956	0.346339	H	3.947558	2.241366	1.567526
H	3.223609	-5.944813	1.330693	H	1.617836	3.077061	-1.598674
Cs	-1.385140	-2.828903	-0.628637	O	-1.572354	0.138998	-2.613647
E = -2018.77998100 Hartree				H	-2.189439	4.991606	-0.702660
TS5				C	-3.639675	0.328583	0.513034
Pd	0.290283	1.387563	-0.274134	H	-3.569606	1.094155	1.313099
C	2.432911	-0.475534	-1.340475	H	-4.539972	0.578257	-0.085793
C	3.435505	-1.425573	-1.100206	C	-3.804173	-1.038088	1.151176
C	4.358565	-1.196708	-0.063646	C	-4.846962	-1.909488	0.766885
C	4.318105	-0.001883	0.653837	C	-2.895247	-1.483661	2.139071
C	3.295845	0.921229	0.340303	C	-4.968256	-3.191178	1.332544
H	3.488354	-2.328858	-1.723435	H	-5.564397	-1.578239	-0.001146
H	5.054872	0.239619	1.432869	C	-3.010846	-2.764339	2.708296
C	5.378661	-2.262627	0.272561	H	-2.074843	-0.820686	2.455475
F	6.374023	-1.798649	1.063295	C	-4.046301	-3.627603	2.302743
F	4.792563	-3.300033	0.930856	H	-5.788596	-3.854418	1.012793
F	5.951407	-2.778276	-0.843638	H	-2.288087	-3.089350	3.474635
C	1.492601	-0.617307	-2.496775	H	-4.138657	-4.632456	2.745649
H	1.705103	0.184536	-3.237428	Cs	-1.045055	-3.364814	-0.988944
H	1.623444	-1.594896	-2.998053	O	-0.201896	-0.737874	0.380403
H	0.427544	-0.491297	-2.208421	O	0.692604	1.303071	1.787598
O	3.238991	2.138123	0.896820	H	-0.044033	-0.404646	1.300539
N	2.329300	0.645390	-0.563061	C	0.229786	2.119727	2.846033
C	-2.418660	-0.240321	-1.748241	C	0.802581	1.410027	4.103541
O	-3.249971	-1.189840	-1.878246	H	0.510478	1.959199	5.023020
C	-2.379415	0.453909	-0.358083	H	0.415927	0.372458	4.172990
H	-1.450022	-0.300360	0.104312	H	1.909798	1.370917	4.048606
N	-1.703682	1.688053	-0.365583	C	0.794157	3.551607	2.775976
C	-2.339020	2.888867	-0.532926	H	0.386777	4.091057	1.898552
O	-3.555414	2.943968	-0.821180	H	0.519825	4.130299	3.682459
C	-1.505898	4.154987	-0.455902	H	1.898915	3.536006	2.691585
H	-1.160478	4.305748	0.589568	C	-1.304807	2.150875	2.932695
C	-0.282513	4.160432	-1.404728	H	-1.729905	2.588252	2.008501
C	-0.694088	3.726612	-2.825008	H	-1.711780	1.125742	3.043697
H	-1.514528	4.365505	-3.214833	H	-1.650859	2.754928	3.796976
H	0.165948	3.814062	-3.522153	E = -2018.78456878 Hartree			
H	-1.039879	2.673063	-2.847902	IM5			
C	0.285318	5.599597	-1.457222	Pd	-0.42376	1.20461	0.09070

C	-2.56059	-0.65500	1.07200	C	4.22306	-0.57144	-0.92803
C	-3.61165	-1.57076	0.94218	C	5.46004	-1.15028	-0.56998
C	-4.55367	-1.38801	-0.08712	C	3.44376	-1.22208	-1.91364
C	-4.47704	-0.26676	-0.90957	C	5.90412	-2.34290	-1.16823
C	-3.40587	0.63358	-0.70576	H	6.07644	-0.66047	0.20160
H	-3.68711	-2.41109	1.64613	C	3.88178	-2.41601	-2.51322
H	-5.22220	-0.05914	-1.69042	H	2.46717	-0.79759	-2.19712
C	-5.64863	-2.41641	-0.27444	C	5.11525	-2.98392	-2.14147
F	-6.33982	-2.61666	0.87616	H	6.87217	-2.77700	-0.86914
F	-6.54033	-2.06069	-1.22756	H	3.25501	-2.90587	-3.27653
F	-5.12618	-3.61786	-0.63650	H	5.46067	-3.91958	-2.60998
C	-1.60077	-0.73600	2.21854	Cs	1.31352	-3.24985	0.85345
H	-1.82672	0.08050	2.93884	O	0.09777	-0.84439	-0.56966
H	-1.70020	-1.70017	2.75201	O	-0.64734	1.36547	-1.92105
H	-0.54229	-0.60031	1.91476	H	0.00746	-0.62303	-1.52196
O	-3.31634	1.79001	-1.37136	C	-0.03059	2.27722	-2.80975
N	-2.42916	0.38759	0.19575	C	-0.51536	1.72060	-4.18184
C	2.42963	-0.17018	1.82138	H	-0.11602	2.35522	-4.99980
O	3.38684	-0.98324	1.98792	H	-0.15733	0.68167	-4.32848
C	2.36196	0.53230	0.41963	H	-1.62288	1.72743	-4.22926
H	1.75097	-0.22669	-0.15102	C	-0.53914	3.71716	-2.63707
N	1.50225	1.69052	0.44390	H	-0.18008	4.14014	-1.67940
C	1.96205	2.84711	1.00104	H	-0.16486	4.37028	-3.45219
O	3.08643	2.88535	1.55615	H	-1.64739	3.74802	-2.64364
C	1.07530	4.07465	0.99443	C	1.50071	2.22583	-2.75048
H	0.92700	4.41846	-0.05197	H	1.84668	2.57257	-1.75632
C	-0.30020	3.84790	1.66317	H	1.86428	1.18940	-2.89989
C	-0.12706	3.19139	3.04760	H	1.95521	2.87185	-3.52931
H	0.52688	3.80645	3.70160	Pd	0.777679	-1.460436	-0.603650
H	-1.10988	3.08750	3.55447	C	2.677802	-0.147825	1.321525
H	0.32364	2.18030	2.97190	E = -2018.82276072 Hartree			
C	-0.99634	5.21919	1.83327	IM6			
H	-1.08364	5.75165	0.86283	Pd	0.777072	-1.232362	-0.435295
H	-2.01915	5.09801	2.24889	C	-1.852259	-0.207760	-1.849859
H	-0.42051	5.86724	2.52878	C	-3.212150	0.074762	-1.645960
C	-1.18736	3.00248	0.75243	C	-4.009269	-0.843734	-0.939417
H	-1.46591	3.55192	-0.16613	C	-3.476165	-2.075172	-0.570253
H	-4.04421	1.86348	-2.02524	C	-2.113518	-2.315948	-0.859558
H	-2.11348	2.68704	1.27761	H	-3.630328	1.017906	-2.024107
O	1.47133	0.04098	2.62184	H	-4.075463	-2.852416	-0.075341
H	1.63851	4.86718	1.52632	C	-5.423196	-0.462110	-0.562635
C	3.73201	0.70174	-0.27108	F	-6.103265	0.060679	-1.612394
H	3.62011	1.48595	-1.04962	F	-6.139161	-1.506224	-0.089512
H	4.48449	1.07702	0.44859				

F	-5.410780	0.492648	0.413224	H	2.617525	6.616502	-1.140293
C	-1.011453	0.770929	-2.617215	Cs	-1.889891	2.897643	0.924921
H	-0.482547	0.265891	-3.448614	C	-0.164260	-1.733077	2.602193
H	-1.649112	1.574048	-3.032017	C	-1.541735	-2.212973	3.123568
H	-0.254775	1.232529	-1.951444	H	-1.751261	-3.239803	2.757531
O	-1.559775	-3.516284	-0.662134	H	-1.576184	-2.220086	4.233641
N	-1.294401	-1.363878	-1.369674	H	-2.345487	-1.543637	2.750566
C	1.275198	1.405786	0.746536	C	0.090977	-0.301317	3.109325
O	1.184182	2.488343	1.371712	H	0.056305	-0.264053	4.218840
C	2.632723	0.690744	0.665181	H	1.090454	0.058228	2.799616
H	3.170740	0.890206	1.614821	H	-0.674006	0.397258	2.716465
N	2.470455	-0.760042	0.519230	C	0.937680	-2.661522	3.149073
C	3.511047	-1.556764	0.848840	H	0.827587	-3.685729	2.735485
O	4.558294	-1.078924	1.364358	H	1.940747	-2.275230	2.884793
C	3.397857	-3.058368	0.629554	H	0.890848	-2.730741	4.256596
H	2.761360	-3.484371	1.432709	O	-0.311645	-1.822386	1.195266
C	2.841468	-3.504723	-0.736401	O	1.608946	-0.750025	-2.225842
C	3.710512	-2.938586	-1.872616	H	1.373710	0.197107	-2.291554
H	4.750070	-3.320714	-1.786915				
H	3.315835	-3.242856	-2.864874	E = -2018.81094844 Hartree			
H	3.740335	-1.833519	-1.850931	TS6			
C	2.900520	-5.053966	-0.795202	Pd	0.771367	0.959641	-0.103977
H	2.330449	-5.513374	0.039448	C	2.539152	-1.483445	-0.370501
H	2.477876	-5.432696	-1.749722	C	3.748584	-2.183943	-0.438186
H	3.953006	-5.403439	-0.725769	C	4.951797	-1.492709	-0.170483
C	1.358963	-3.154602	-0.848569	C	4.925704	-0.154767	0.198983
H	0.766844	-3.714736	-0.102410	C	3.669735	0.527293	0.305816
H	-2.195972	-4.122000	-0.225244	H	3.746128	-3.252361	-0.693259
H	0.959053	-3.329150	-1.867232	H	5.838071	0.403326	0.449528
O	0.290713	0.865215	0.108126	C	6.260771	-2.236822	-0.296162
H	4.418886	-3.464554	0.777927	F	6.516696	-2.570424	-1.591585
C	3.479470	1.277462	-0.519687	F	7.320753	-1.518106	0.145210
H	4.539016	1.022936	-0.317048	F	6.244060	-3.401430	0.407300
H	3.158556	0.727892	-1.425271	C	1.229087	-2.176376	-0.613278
C	3.300708	2.758876	-0.729544	H	0.710817	-1.733742	-1.487305
C	2.332011	3.229472	-1.644714	H	1.381254	-3.258887	-0.785973
C	4.021296	3.704899	0.030964	H	0.553272	-2.037903	0.256858
C	2.085614	4.604904	-1.793567	O	3.588367	1.734305	0.746058
H	1.761839	2.501383	-2.245668	N	2.518019	-0.153809	-0.059404
C	3.779724	5.081508	-0.115318	C	-1.942328	-0.289901	-0.009617
H	4.778480	3.353080	0.751251	O	-1.902507	-1.036304	1.012182
C	2.807368	5.537117	-1.025486	C	-2.142932	1.231530	0.211390
H	1.327199	4.951687	-2.514468	H	-2.251960	1.406225	1.302041
H	4.353105	5.805669	0.486093	N	-0.966006	1.978041	-0.256981

C	-0.878816	3.309176	0.114477	H	3.059759	1.946813	3.710341
O	-1.626331	3.841159	0.951332	H	1.674592	3.051858	4.033259
C	0.178121	4.084885	-0.654065	H	1.922370	1.591608	5.055961
H	1.149128	3.938452	-0.133935	O	1.288360	1.795531	1.748902
C	0.289751	3.620276	-2.141688	O	0.372699	0.529747	-2.000279
C	-0.186679	4.763852	-3.089220	H	-0.511008	0.058540	-1.908996
H	0.497499	5.631891	-2.981495				
H	-0.167285	4.445019	-4.152159	E = -1710.11478962 Hartree			
H	-1.214595	5.097319	-2.839709	TS6a			
C	1.743274	3.253236	-2.485857	Pd	-0.048337	0.638758	-0.196187
H	2.120552	2.466341	-1.799959	C	-2.483412	-0.071301	1.499284
H	1.833155	2.885591	-3.529178	C	-3.788395	-0.544433	1.694913
H	2.395404	4.144391	-2.375766	C	-4.480087	-1.130996	0.618881
C	-0.678636	2.504976	-2.448600	C	-3.858755	-1.271026	-0.625114
H	-0.483907	1.946975	-3.374564	C	-2.550319	-0.774520	-0.758105
H	2.301404	1.856937	1.473755	H	-4.249057	-0.458287	2.688680
H	-1.745277	2.729810	-2.306464	H	-4.347974	-1.751293	-1.482419
O	-1.894052	-0.700466	-1.221694	C	-5.908959	-1.587579	0.815371
H	-0.068606	5.161165	-0.568133	F	-6.762063	-0.528781	0.847027
C	-3.460735	1.672496	-0.478532	F	-6.329236	-2.409635	-0.175340
H	-3.636786	2.743624	-0.249495	F	-6.064183	-2.252786	1.988353
H	-3.346159	1.561474	-1.574746	C	-1.666623	0.468961	2.632662
C	-4.614196	0.819147	-0.001158	H	-0.889410	1.167351	2.264825
C	-5.207121	-0.137007	-0.854552	H	-2.305001	0.969948	3.385459
C	-5.061078	0.895980	1.337579	H	-1.141143	-0.369670	3.140565
C	-6.219263	-0.994670	-0.385783	O	-1.885345	-0.911071	-1.910525
H	-4.861408	-0.212436	-1.898594	N	-1.898081	-0.153415	0.264967
C	-6.069845	0.039676	1.810037	C	2.902705	1.000930	-0.241657
H	-4.609096	1.637354	2.017136	O	4.114513	0.789518	-0.463669
C	-6.650681	-0.912398	0.950701	C	2.441827	1.694775	1.064985
H	-6.671710	-1.732392	-1.068675	H	3.307141	2.323674	1.377910
H	-6.406182	0.115210	2.856835	N	1.225676	2.473247	0.859868
H	-7.441386	-1.584490	1.321281	C	1.377323	3.438585	-0.063084
Cs	-2.884072	-3.538193	-0.472878	O	2.476482	3.746448	-0.627459
C	1.120902	1.170958	3.065550	C	0.125759	4.214078	-0.492769
C	1.556676	-0.297922	3.026916	H	0.429582	4.771625	-1.402598
H	2.633862	-0.398181	2.783679	C	-1.160862	3.394737	-0.797496
H	1.383054	-0.772398	4.014655	C	-2.045251	3.252464	0.454650
H	0.967266	-0.851431	2.267626	H	-2.428613	4.246772	0.768200
C	-0.363388	1.287086	3.414752	H	-2.919179	2.595497	0.259154
H	-0.538808	0.961615	4.460241	H	-1.470522	2.828005	1.297035
H	-0.710276	2.335221	3.309027	C	-1.975862	4.163510	-1.873043
H	-0.971106	0.640698	2.750198	H	-1.426700	4.220844	-2.836741
C	1.995321	1.989743	4.023412	H	-2.955388	3.674711	-2.060699

H	-2.172423	5.202911	-1.532297	O	-1.935682	-1.169013	0.921166
C	-0.835135	2.036220	-1.431379	C	-2.103800	1.171002	0.354957
H	-0.047348	2.115374	-2.212754	H	-2.123120	1.238693	1.461872
H	-0.963442	-0.497506	-1.706498	N	-0.969100	1.964549	-0.139186
H	-1.750167	1.587260	-1.869286	C	-0.883846	3.276276	0.294619
O	1.956288	0.591376	-1.040153	O	-1.561119	3.745553	1.224506
H	-0.111309	4.983385	0.276221	C	0.080612	4.115700	-0.527912
C	2.168646	0.616393	2.153152	H	1.102284	3.946508	-0.125775
H	2.038606	1.139726	3.124819	C	0.033600	3.746074	-2.045299
H	1.188785	0.140329	1.919136	C	-0.648623	4.896693	-2.843058
C	3.218248	-0.462696	2.249816	H	-0.021246	5.811124	-2.781508
C	2.952799	-1.758094	1.754915	H	-0.762753	4.634698	-3.915958
C	4.504764	-0.191967	2.766909	H	-1.651185	5.134774	-2.432251
C	3.940797	-2.759302	1.774703	C	1.455423	3.527106	-2.588261
H	1.951254	-1.979456	1.346765	H	1.972377	2.723924	-2.026462
C	5.494601	-1.188430	2.789629	H	1.439042	3.253857	-3.664260
H	4.731159	0.815112	3.154140	H	2.052206	4.456877	-2.479466
C	5.217916	-2.475809	2.290795	C	-0.867440	2.558428	-2.304160
H	3.711599	-3.764895	1.385337	H	-0.709016	2.055440	-3.268247
H	6.492323	-0.959428	3.198151	H	4.577334	2.295744	-0.242465
H	5.995536	-3.256263	2.308665	H	-1.934394	2.710217	-2.088831
Cs	1.887554	-2.232069	-2.125727	O	-1.923963	-0.616826	-1.267422
E = -2018.78253149 Hartree				H	-0.159801	5.182156	-0.349351
TS6b				C	-3.476695	1.669699	-0.176599
Pd	0.823536	1.020966	-0.106699	H	-3.625545	2.714476	0.164719
C	2.529848	-1.450671	-0.279518	H	-3.460183	1.661023	-1.284206
C	3.716114	-2.196733	-0.260073	C	-4.593428	0.776521	0.313138
C	4.950209	-1.524083	-0.202176	C	-5.254815	-0.102677	-0.572092
C	4.985729	-0.129466	-0.191541	C	-4.938734	0.738444	1.683121
C	3.756310	0.560681	-0.224724	C	-6.235287	-0.996920	-0.104225
H	3.664890	-3.293784	-0.286882	H	-4.988702	-0.087616	-1.641907
H	5.928937	0.433672	-0.165489	C	-5.915759	-0.154300	2.154473
C	6.230969	-2.326561	-0.125379	H	-4.431403	1.418023	2.387724
F	6.249543	-3.323244	-1.046585	C	-6.565794	-1.028889	1.262759
F	7.331893	-1.565688	-0.329211	H	-6.742713	-1.672821	-0.812048
F	6.367401	-2.913489	1.093475	H	-6.172621	-0.168815	3.226127
C	1.188008	-2.113035	-0.354403	H	-7.331844	-1.729325	1.632618
H	0.649834	-1.776284	-1.264177	Cs	-2.935037	-3.519266	-0.745097
H	1.290770	-3.214459	-0.372492	C	1.275971	1.077820	2.944220
H	0.550760	-1.819926	0.505987	C	2.032340	-0.268388	2.944168
O	3.679231	1.900195	-0.255317	H	3.088712	-0.128455	2.631500
N	2.568728	-0.085235	-0.238843	H	2.029549	-0.736271	3.951922
C	-1.948371	-0.323293	-0.021432	H	1.554517	-0.981509	2.243525
				C	-0.198669	0.833748	3.324498

H	-0.296606	0.393156	4.340227	H	1.356019	2.569026	-1.593834
H	-0.761157	1.791189	3.306466	C	2.547428	3.775946	1.459501
H	-0.675186	0.137148	2.604915	H	2.148103	3.992325	2.472233
C	1.923321	2.025869	3.978445	H	3.361935	3.029261	1.552920
H	2.989063	2.206460	3.722184	H	2.975731	4.716448	1.052128
H	1.399083	3.004944	3.978383	C	0.861023	2.097161	1.238416
H	1.878583	1.606568	5.005954	H	0.072295	2.318623	1.970575
O	1.386370	1.753342	1.702823	H	1.774660	-0.673804	2.267248
O	0.336556	0.655316	-2.022262	H	1.633856	1.398173	1.607842
H	-0.527312	0.157566	-1.915984	O	-1.640437	-0.060141	0.889655
E = -2018.79143858 Hartree				H	0.705389	5.120056	-0.463204
TS6c				C	-3.053877	1.849478	-1.537922
Pd	0.331124	-0.108089	0.372738	H	-3.117442	2.871530	-1.966697
C	2.539403	-1.161442	-1.390824	H	-2.277796	1.288930	-2.097144
C	3.837738	-1.163270	-1.907035	C	-4.378661	1.140224	-1.658470
C	4.882489	-0.592780	-1.142838	C	-4.437100	-0.187719	-2.134745
C	4.636807	-0.133787	0.141930	C	-5.582785	1.763429	-1.259635
C	3.310199	-0.212415	0.679287	C	-5.658896	-0.881990	-2.201215
H	4.030010	-1.622049	-2.886512	H	-3.504966	-0.680571	-2.459917
H	5.429403	0.264301	0.789730	C	-6.805089	1.075080	-1.325086
C	6.264455	-0.500444	-1.748044	H	-5.556728	2.801444	-0.888797
F	6.288621	0.392164	-2.775302	C	-6.848189	-0.253220	-1.791532
F	7.203565	-0.106576	-0.855577	H	-5.681373	-1.918235	-2.576888
F	6.669097	-1.693789	-2.258921	H	-7.733873	1.577434	-1.009081
C	1.423400	-1.860715	-2.113399	H	-7.807501	-0.793034	-1.840959
H	0.592839	-1.162914	-2.333905	Cs	-2.146928	-2.947203	-0.294487
H	1.791041	-2.311264	-3.054506	C	0.193706	-1.157986	3.505886
H	1.023038	-2.671666	-1.467143	C	1.233666	-1.775074	4.451332
O	3.061558	0.065335	1.908846	H	2.148544	-1.147346	4.494697
N	2.278893	-0.594340	-0.170344	H	0.822727	-1.855050	5.478365
C	-2.651195	0.747897	0.726582	H	1.520910	-2.790843	4.109444
O	-3.768914	0.437381	1.187533	C	-1.040239	-2.054032	3.383601
C	-2.522089	2.052566	-0.073679	H	-1.495378	-2.211253	4.382457
H	-3.210682	2.771831	0.426847	H	-1.798638	-1.585072	2.727525
N	-1.180832	2.584121	-0.099032	H	-0.760789	-3.046558	2.972683
C	-1.036351	3.911240	-0.020811	C	-0.184004	0.258127	3.948717
O	-1.963569	4.767328	-0.128073	H	0.710653	0.911403	3.999273
C	0.378400	4.386202	0.304449	H	-0.916527	0.704317	3.248139
H	0.273541	4.966755	1.248403	H	-0.644703	0.230455	4.957451
C	1.427576	3.272250	0.487537	O	0.841644	-1.126279	2.185564
C	2.101493	2.905468	-0.849688	O	-0.015000	0.612237	-1.433196
H	2.633645	3.792731	-1.250696	H	-0.387066	1.498876	-1.119788
H	2.842415	2.091325	-0.720730	E = -2018.88720001 Hartree			

IM7				H	-3.043674	2.410460	-2.325136
Pd	0.321887	-0.234784	0.254311	H	-2.016108	0.985240	-2.005520
C	2.624179	-1.375618	-1.263202	C	-4.099334	0.665309	-1.605066
C	3.960383	-1.421676	-1.672639	C	-4.063398	-0.568739	-2.293630
C	4.932418	-0.730212	-0.913161	C	-5.293120	1.020433	-0.935847
C	4.575323	-0.078468	0.258841	C	-5.177986	-1.426991	-2.311347
C	3.210046	-0.096448	0.693454	H	-3.140150	-0.856719	-2.824551
H	4.234067	-1.993592	-2.569711	C	-6.406431	0.162339	-0.944908
H	5.309329	0.434510	0.894783	H	-5.356375	1.978829	-0.397232
C	6.363157	-0.721669	-1.398789	C	-6.354231	-1.065970	-1.629620
F	6.478938	-0.055677	-2.580562	H	-5.124394	-2.383131	-2.857455
F	7.212782	-0.131495	-0.524547	H	-7.325463	0.457461	-0.412967
F	6.824526	-1.983031	-1.617831	H	-7.228822	-1.736145	-1.635612
C	1.562571	-2.149618	-1.992469	Cs	-2.056973	-2.933612	-0.098416
H	0.744473	-1.483579	-2.329079	C	0.091034	-0.846840	3.485290
H	1.993354	-2.675816	-2.865406	C	1.089248	-1.386622	4.520438
H	1.120068	-2.905759	-1.308839	H	2.032189	-0.800698	4.497634
O	2.842281	0.387915	1.824237	H	0.666548	-1.319882	5.543769
N	2.264406	-0.665611	-0.150818	H	1.332772	-2.448690	4.310389
C	-2.491349	1.044876	0.807418	C	-1.184138	-1.690215	3.457609
O	-3.385266	1.060604	1.676964	H	-1.651053	-1.705086	4.463395
C	-2.487669	2.171145	-0.254458	H	-1.916820	-1.264442	2.745191
H	-3.269712	2.890430	0.072543	H	-0.952390	-2.737622	3.171801
N	-1.206345	2.902661	-0.314698	C	-0.218718	0.632359	3.743775
C	-1.049310	4.001958	-1.141545	H	0.698496	1.249919	3.654713
O	-1.779496	4.295882	-2.096853	H	-0.975720	1.012068	3.032570
C	0.122360	4.825903	-0.631713	H	-0.621411	0.763252	4.769285
H	-0.314828	5.757497	-0.207151	O	0.764242	-1.009938	2.189343
C	0.802197	3.964267	0.456519	O	0.156077	0.500528	-1.586824
C	1.961077	3.149850	-0.148330	H	-0.196006	1.399336	-1.390193
H	2.753968	3.827945	-0.528022				
H	2.407915	2.486432	0.618892	E = -2020.06137662 Hartree			
H	1.622159	2.512781	-0.990767	IM9a			
C	1.307580	4.785061	1.649709	Pd	0.928792	0.660215	-0.523441
H	0.496195	5.399362	2.093701	O	1.075580	0.819604	-2.553920
H	1.706231	4.118565	2.444323	C	2.452059	-1.868892	-0.846808
H	2.126775	5.468573	1.341593	C	3.579615	-2.701748	-0.825667
C	-0.358085	3.025179	0.885084	C	4.827508	-2.163105	-0.467301
H	-0.951008	3.462800	1.720775	C	4.941557	-0.806346	-0.159964
H	1.636062	-0.433313	2.207165	C	3.773684	-0.021595	-0.202157
H	0.016934	2.030153	1.203275	H	3.471231	-3.762227	-1.092586
O	-1.665491	0.048772	0.698757	H	5.901733	-0.345002	0.108897
H	0.788551	5.127557	-1.465258	C	6.037541	-3.070971	-0.415606
C	-2.882283	1.564144	-1.627791	F	6.215958	-3.723725	-1.592737

F	7.180516	-2.396985	-0.149072	H	-5.083007	-3.154558	-2.784290
F	5.894638	-4.021452	0.544669	H	-7.089034	0.493363	-1.532401
C	1.114282	-2.380680	-1.289325	H	-7.186897	-1.953867	-2.103752
H	1.025154	-2.269926	-2.392214	H	1.978939	1.169013	-2.703370
H	1.002978	-3.455801	-1.048372	Cs	-4.304284	-2.004156	1.542260
H	0.286353	-1.797439	-0.839304	C	0.851096	-0.048111	2.515177
O	3.772621	1.298022	0.042834	C	-0.133332	0.338310	3.644488
N	2.563574	-0.550733	-0.498925	H	-1.177037	0.192513	3.296008
C	-2.306829	0.345314	0.241208	H	0.030159	-0.269540	4.559782
O	-2.960743	0.737073	1.253588	H	-0.010750	1.409180	3.911559
C	-2.116577	1.372752	-0.920091	C	2.301036	0.183507	2.995410
H	-2.811998	2.212643	-0.720131	H	2.531511	-0.410430	3.906211
N	-0.748034	1.949920	-0.979623	H	3.028646	-0.111130	2.213856
H	-0.338604	1.954793	-1.945283	H	2.465106	1.255823	3.232136
C	-0.498792	3.149670	-0.258594	C	0.649689	-1.538168	2.171210
O	-1.206337	3.451546	0.699331	H	-0.350588	-1.689367	1.718243
C	0.646790	3.978766	-0.805530	H	1.415066	-1.888542	1.451940
H	0.188714	4.655279	-1.565413	H	0.734460	-2.173312	3.078699
C	1.458961	4.825576	0.210682	O	0.520586	0.817014	1.442015
C	1.892064	3.967956	1.416288	H	4.676520	1.602250	0.278977
H	2.449654	3.068645	1.087797				
H	2.553223	4.557081	2.087278	E = -2020.07076663 Hartree			
H	1.021690	3.628645	2.011031	IM9b			
C	2.717130	5.323398	-0.529620	Pd	-0.843735	0.720847	-0.133128
H	2.450989	5.906795	-1.437205	O	-0.480075	0.376417	-2.091343
H	3.329054	5.977924	0.126948	C	-2.109195	-1.956306	0.094779
H	3.353075	4.469546	-0.848524	C	-3.115725	-2.920975	-0.047918
C	0.634418	6.036616	0.691318	C	-4.358752	-2.544183	-0.587045
H	1.224401	6.654426	1.401800	C	-4.576533	-1.225886	-0.988567
H	0.344464	6.686836	-0.162208	C	-3.521936	-0.305168	-0.825929
H	-0.292910	5.712167	1.203783	H	-2.919410	-3.955228	0.265481
O	-1.866019	-0.829038	0.048871	H	-5.529410	-0.893779	-1.423693
H	1.326387	3.305187	-1.367794	C	-5.438548	-3.588460	-0.770676
C	-2.429314	0.710372	-2.273471	F	-5.566292	-4.370536	0.330728
H	-2.417646	1.496797	-3.060794	F	-6.650091	-3.038612	-1.021368
H	-1.620075	-0.010287	-2.506981	F	-5.148624	-4.414292	-1.810700
C	-3.759604	-0.013562	-2.266032	C	-0.757619	-2.295953	0.636513
C	-3.829098	-1.388002	-2.583365	H	-0.484296	-1.606235	1.459795
C	-4.949337	0.649641	-1.888648	H	-0.724722	-3.341394	0.997189
C	-5.051345	-2.082090	-2.531724	H	0.012410	-2.153861	-0.152624
H	-2.905659	-1.920179	-2.864732	O	-3.610636	0.981155	-1.195542
C	-6.172641	-0.041917	-1.829868	N	-2.340185	-0.659521	-0.273104
H	-4.919345	1.721770	-1.634799	C	2.035763	-0.248515	-0.069043
C	-6.228733	-1.411525	-2.150088	O	1.901660	-1.073193	-1.032744

C	2.109866	1.254595	-0.444964	C	-2.562362	-0.177433	3.061440
H	2.096457	1.343056	-1.545598	H	-3.345804	-0.131229	3.847728
N	0.892278	1.949376	0.035811	H	-3.010668	-0.666182	2.174660
H	0.830608	2.027429	1.070438	H	-1.738224	-0.820621	3.435220
C	0.539585	3.168027	-0.633973	C	-3.167028	2.070110	2.097690
O	0.905145	3.359711	-1.790357	H	-2.819349	3.102812	1.888880
C	-0.244794	4.135426	0.221622	H	-3.509642	1.626795	1.142100
H	0.521116	4.783771	0.709578	H	-4.040903	2.135374	2.780711
C	-1.295309	5.019271	-0.499583	O	-0.899060	1.167021	1.854383
C	-2.303640	4.119305	-1.240126	H	-4.499473	1.176634	-1.564758
H	-2.824427	3.445420	-0.531733				
H	-3.072245	4.732839	-1.756648	E = -2020.05491008 Hartree			
H	-1.806030	3.484997	-2.002809	TS9a			
C	-2.031775	5.827533	0.588027	Pd	0.941829	0.596276	-0.463546
H	-1.329686	6.478836	1.151348	O	0.853364	0.850293	-2.558697
H	-2.810007	6.478295	0.135730	C	2.626092	-1.816572	-0.910291
H	-2.531752	5.157847	1.319407	C	3.807297	-2.571896	-0.919708
C	-0.627982	6.002186	-1.482707	C	5.007091	-1.978573	-0.490727
H	-1.389998	6.674703	-1.931680	C	5.020813	-0.645446	-0.074703
H	0.119592	6.639691	-0.962958	C	3.802139	0.058356	-0.081248
H	-0.109051	5.468654	-2.302085	H	3.777594	-3.613554	-1.267650
O	2.156627	-0.546100	1.156202	H	5.940877	-0.142186	0.253222
H	-0.723561	3.553891	1.036318	C	6.274690	-2.804956	-0.455490
C	3.378797	1.915672	0.129253	F	6.435559	-3.519042	-1.597725
H	3.450058	2.948294	-0.276638	F	7.382419	-2.044016	-0.292464
H	3.275584	1.990013	1.231249	F	6.245905	-3.698414	0.568773
C	4.615300	1.112758	-0.214487	C	1.334166	-2.376220	-1.426661
C	5.409675	0.540676	0.802952	H	1.246350	-2.159041	-2.513796
C	4.955740	0.852370	-1.561526	H	1.299404	-3.475229	-1.297763
C	6.519531	-0.264400	0.486537	H	0.461556	-1.904247	-0.931510
H	5.147760	0.725560	1.857678	O	3.696367	1.345314	0.281978
C	6.059631	0.043564	-1.881466	N	2.640616	-0.523708	-0.466159
H	4.345661	1.287475	-2.369913	C	-2.272391	0.237815	0.229344
C	6.845627	-0.519866	-0.858254	O	-2.786200	0.702670	1.293094
H	7.129201	-0.698676	1.295714	C	-2.093447	1.222093	-0.964047
H	6.308950	-0.148082	-2.937721	H	-2.816480	2.045520	-0.796248
H	7.711566	-1.153517	-1.109110	N	-0.746351	1.833564	-0.993082
H	0.328290	-0.187162	-2.015065	H	-0.036401	1.535661	-2.042574
Cs	3.649624	-3.174983	0.379100	C	-0.625555	3.121443	-0.463462
C	-2.030937	1.230148	2.711488	O	-1.535933	3.661073	0.183465
C	-1.524138	1.914485	4.000502	C	0.665648	3.846889	-0.823422
H	-1.134710	2.928853	3.771155	H	0.423617	4.455658	-1.726059
H	-2.331267	2.014682	4.756865	C	1.297005	4.772135	0.252448
H	-0.698488	1.323159	4.450227	C	1.450942	4.018509	1.587660

H	2.061587	3.102407	1.459767				
H	1.950087	4.662650	2.342874	E = -2020.06091926 Hartree			
H	0.467545	3.712931	1.999387	TS9b			
C	2.695475	5.171145	-0.262516	Pd	-0.843607	0.628866	-0.191996
H	2.634182	5.684902	-1.246085	O	-0.667876	0.433795	-2.179701
H	3.198110	5.861016	0.448706	C	-2.300125	-1.963807	-0.043442
H	3.343564	4.276944	-0.386202	C	-3.416849	-2.810713	-0.049797
C	0.450422	6.044768	0.455484	C	-4.694898	-2.261179	-0.255001
H	0.925358	6.716055	1.203082	C	-4.843869	-0.888206	-0.458467
H	0.352185	6.613366	-0.494704	C	-3.682416	-0.091858	-0.445865
H	-0.569358	5.795067	0.807994	H	-3.278305	-3.888502	0.110770
O	-1.927340	-0.972615	0.044908	H	-5.825656	-0.423455	-0.625156
H	1.420331	3.100884	-1.144483	C	-5.901278	-3.174350	-0.297354
C	-2.387853	0.524615	-2.306290	F	-5.860594	-4.099723	0.693900
H	-2.341854	1.290789	-3.111819	F	-7.065420	-2.494573	-0.171374
H	-1.596444	-0.223029	-2.512849	F	-5.958370	-3.855642	-1.472191
C	-3.738900	-0.160590	-2.309714	C	-0.912358	-2.476544	0.180150
C	-3.846579	-1.543452	-2.577393	H	-0.479130	-2.021981	1.094872
C	-4.917787	0.552006	-1.991144	H	-0.907954	-3.578006	0.283785
C	-5.090747	-2.197562	-2.529812	H	-0.246425	-2.177689	-0.656348
H	-2.934573	-2.114953	-2.815810	O	-3.704614	1.237577	-0.633698
C	-6.163887	-0.098388	-1.937604	N	-2.456093	-0.618996	-0.229035
H	-4.860584	1.632072	-1.778252	C	1.967151	-0.319800	-0.193827
C	-6.255770	-1.477424	-2.204520	O	1.790788	-0.854872	-1.342313
H	-5.149859	-3.277582	-2.742412	C	2.130811	1.225621	-0.167050
H	-7.070010	0.476573	-1.685935	H	2.445220	1.537258	-1.182336
H	-7.231389	-1.988043	-2.161725	N	0.831044	1.880482	0.107267
H	1.587527	1.463905	-2.777001	H	0.296579	1.659273	1.265362
Cs	-4.443949	-1.882742	1.600768	C	0.666039	3.147801	-0.480659
C	0.922804	-0.228219	2.520444	O	1.508723	3.623089	-1.253988
C	-0.023777	0.184086	3.672709	C	-0.577567	3.897771	-0.042904
H	-1.075386	0.142604	3.321255	H	-0.252536	4.576744	0.779535
H	0.091005	-0.482630	4.553476	C	-1.333487	4.722841	-1.118794
H	0.191198	1.225507	3.992406	C	-1.637712	3.841726	-2.346132
C	2.387493	-0.156986	3.006382	H	-2.222232	2.944937	-2.054147
H	2.536958	-0.768040	3.922379	H	-2.230890	4.407876	-3.095731
H	3.084877	-0.545999	2.238159	H	-0.707485	3.496960	-2.842657
H	2.671257	0.890051	3.241020	C	-2.664408	5.173130	-0.481585
C	0.590620	-1.667864	2.087401	H	-2.490613	5.773851	0.436982
H	-0.426619	-1.710977	1.649510	H	-3.251086	5.797669	-1.188821
H	1.311693	-2.028641	1.328144	H	-3.288729	4.298116	-0.200769
H	0.644039	-2.363917	2.951493	C	-0.525758	5.965994	-1.540331
O	0.661242	0.733439	1.504901	H	-1.089012	6.564090	-2.288698
H	4.558272	1.680180	0.612424	H	-0.321915	6.622747	-0.666991

H	0.448156	5.679548	-1.982895	C	0.007116	0.000002	0.012759
O	2.063837	-0.953072	0.899248	C	-0.679180	-1.265142	-0.527489
H	-1.278807	3.170859	0.406298	H	-1.756179	-1.273316	-0.252977
C	3.195528	1.677405	0.853850	H	-0.611829	-1.324949	-1.634073
H	3.316727	2.778086	0.753879	H	-0.207166	-2.174022	-0.099179
H	2.823680	1.470864	1.877712	C	1.502357	-0.001493	-0.323609
C	4.519817	0.977947	0.633737	H	1.663496	-0.001436	-1.420570
C	5.086645	0.161833	1.637734	H	1.996480	0.896569	0.102864
C	5.187014	1.070721	-0.609533	H	1.994553	-0.900773	0.102523
C	6.283176	-0.541864	1.410057	C	-0.676505	1.266846	-0.526923
H	4.572969	0.071151	2.608776	H	-1.753498	1.277166	-0.252496
C	6.380361	0.364662	-0.843624	H	-0.202590	2.174530	-0.098175
H	4.765162	1.705445	-1.406087	H	-0.608890	1.326996	-1.633474
C	6.932662	-0.447620	0.164837	O	-0.054295	-0.000276	1.459411
H	6.707929	-1.171958	2.208630				
H	6.884004	0.451046	-1.820224	E = -882.681342638 Hartree			
H	7.867856	-1.001185	-0.017907	2a			
H	0.226286	0.005750	-2.180724	C	0.136309	-0.666578	0.393255
Cs	3.708177	-3.153623	-0.552541	O	-0.412443	-1.121530	1.443971
C	-1.402740	1.171765	2.934593	C	1.115917	0.532857	0.570316
C	-0.527030	1.626698	4.113485	H	1.040042	0.884993	1.617457
H	0.035395	2.544839	3.842270	N	2.498221	0.098441	0.411649
H	-1.143479	1.850101	5.009101	C	3.453898	0.313142	1.367773
H	0.205555	0.837065	4.381426	O	3.272928	0.904195	2.445707
C	-2.134489	-0.137852	3.267910	C	4.746421	-0.325516	0.876379
H	-2.785580	-0.016484	4.158502	H	4.853774	-1.308776	1.387739
H	-2.773076	-0.455563	2.418603	C	4.537397	-0.498176	-0.648785
H	-1.405383	-0.947790	3.477076	C	4.954482	0.792254	-1.378952
C	-2.418992	2.262487	2.567022	H	6.040096	0.985995	-1.249618
H	-1.921301	3.237960	2.400226	H	4.745814	0.716737	-2.466948
H	-2.971833	1.986128	1.646203	H	4.404523	1.674571	-0.987733
H	-3.156420	2.396428	3.385903	C	5.274753	-1.708595	-1.230401
O	-0.491425	0.883913	1.853272	H	4.993998	-2.644734	-0.703335
H	-4.623499	1.547193	-0.792144	H	5.037075	-1.838975	-2.308011
				H	6.374615	-1.583044	-1.141359
E = -76.3691573034 Hartree				C	2.994438	-0.667453	-0.733494
H2O				H	2.695374	-1.736687	-0.645760
O	0.000000	0.000000	0.123345	H	2.574300	-0.282445	-1.684833
H	0.000000	0.758766	-0.493381	O	-0.058013	-1.083750	-0.791092
H	0.000000	-0.758766	-0.493381	H	5.624999	0.291891	1.151731
				C	0.770819	1.693183	-0.393172
E = -233.517446198 Hartree				H	1.391394	2.569935	-0.105043
^tBuOH				H	1.054921	1.412344	-1.427280
H	-1.002750	0.000162	1.701836	C	-0.700440	2.048148	-0.358142

C	-1.487061	1.985331	-1.529741	C	-2.602514	2.238847	1.159828
C	-1.335143	2.393380	0.857602	H	-3.501885	2.342156	0.517466
C	-2.864517	2.270834	-1.494810	H	-2.640336	1.241740	1.645578
H	-1.008643	1.704774	-2.482661	H	-2.653882	3.010929	1.956775
C	-2.712610	2.672961	0.898568	O	-1.290610	1.461323	-0.767690
H	-0.742151	2.445340	1.785247	H	1.368833	0.375951	-3.158563
C	-3.483822	2.613259	-0.278147	C	-5.634034	-0.571376	0.156519
H	-3.457784	2.220942	-2.422518	H	-5.908428	0.452751	0.490182
H	-3.187820	2.941391	1.856164	H	-5.924369	-0.671475	-0.907258
H	-4.563006	2.834144	-0.246569	H	-6.194983	-1.294541	0.779929
Cs	-3.094253	-1.495691	0.016247	C	-4.137795	-0.754318	0.356855

E = -1365.12054348 Hartree

TS7

Pd	-1.370991	-0.503847	-0.452087
O	-1.465001	-2.667548	-0.333982
C	1.257972	-0.882696	0.922610
C	2.641128	-0.737540	1.091003
C	3.419680	-0.268631	0.018412
C	2.819633	0.019089	-1.207275
C	1.426111	-0.157500	-1.318304
H	3.095169	-0.984064	2.060550
H	3.396821	0.373237	-2.072807
C	4.903686	-0.046821	0.220037
F	5.487653	-1.112515	0.823422
F	5.557394	0.169461	-0.945045
F	5.129477	1.031393	1.015812
C	0.393684	-1.407861	2.030507
H	0.224509	-2.497376	1.890604
H	0.880839	-1.258383	3.012567
H	-0.605235	-0.925457	2.025856
O	0.756190	0.055538	-2.460613
N	0.669425	-0.567415	-0.271304
H	-2.415682	-2.913234	-0.356050
H	-1.112776	-3.009438	-1.184385
C	-1.319603	2.384127	0.317076
C	-1.300329	3.766800	-0.371647
H	-2.177388	3.875062	-1.043451
H	-1.328210	4.586820	0.376044
H	-0.379934	3.880186	-0.982115
C	-0.079822	2.243764	1.223792
H	-0.026698	3.069065	1.965047
H	-0.113901	1.291573	1.788901
H	0.850632	2.259304	0.618488

E = -1288.72659658 Hartree

IM8

Pd	-1.199574	-0.695891	0.076174
C	1.516945	-1.285487	0.486686
C	2.906745	-1.226574	0.473978
C	3.517487	-0.081099	-0.094635
C	2.749170	0.944847	-0.627778
C	1.320295	0.849499	-0.606794
H	3.496344	-2.053365	0.893104
H	3.196216	1.843619	-1.073581
C	5.028244	-0.005013	-0.117192
F	5.560134	-1.016568	-0.854396
F	5.488139	1.156015	-0.637802
F	5.546173	-0.119693	1.134842
C	0.717851	-2.420995	1.064473
H	-0.050011	-2.793994	0.337041
H	1.354978	-3.296933	1.295680
H	0.207513	-2.112699	2.003044
O	0.564288	1.769538	-1.101094
N	0.764035	-0.273864	-0.037239
H	-0.695766	1.520941	-0.836510
C	-2.234340	2.138832	0.495302
C	-2.204422	3.504578	-0.213306
H	-2.835827	3.485993	-1.124691
H	-2.594616	4.287392	0.468498
H	-1.169170	3.778329	-0.502199
C	-1.318528	2.131664	1.723773
H	-1.689347	2.845365	2.487359
H	-1.296503	1.115954	2.175482
H	-0.283124	2.418821	1.450163

C	-3.663953	1.732740	0.851016	H	-3.874508	3.202050	-1.114372
H	-4.289713	1.675943	-0.062879	H	-2.174565	2.964148	-1.634934
H	-3.680210	0.744050	1.349256	C	-2.180847	4.014918	0.944087
H	-4.111605	2.480211	1.536869	H	-3.073076	4.673603	0.895940
O	-1.734577	1.194398	-0.516392	H	-1.805429	4.012246	1.988460
C	-5.302235	-1.836273	-0.304335	H	-1.395208	4.453303	0.293056
H	-5.840726	-2.163670	-1.214177	C	-3.570066	1.950234	1.411174
H	-5.269545	-2.654728	0.441496	H	-3.791661	0.912357	1.088468
H	-5.860423	-0.989397	0.149963	H	-3.202018	1.921515	2.458092
C	-3.910061	-1.356014	-0.666056	H	-4.513866	2.532005	1.392289
O	-3.616355	-0.957976	-1.804828	O	-1.320538	1.777464	0.643180
O	-3.069043	-1.371686	0.348335				

E = -1943.60105252 Hartree

E = -1288.72023894 Hartree

TS8

Pd	-1.228984	-0.588121	-0.306613
C	-4.406906	-2.972755	-0.236605
H	-4.402740	-3.580523	-1.167131
H	-4.360100	-3.664295	0.626930
H	-5.337820	-2.374542	-0.211745
C	-3.219224	-2.075732	-0.247521
O	-3.265278	-0.874748	-0.713785
O	-2.068097	-2.463719	0.186243
C	1.537068	-1.335596	0.797803
C	2.912929	-1.070182	0.769439
C	3.401134	-0.032654	-0.060415
C	2.542634	0.735085	-0.847622
C	1.153822	0.440181	-0.793606
H	3.591341	-1.669648	1.392207
H	2.898137	1.546783	-1.496551
C	4.888525	0.248194	-0.056675
F	5.608420	-0.880887	-0.290478
F	5.252070	1.157322	-0.991546
F	5.295992	0.728239	1.149491
C	0.918941	-2.408775	1.640966
H	0.460816	-3.192217	1.001164
H	1.676073	-2.882228	2.293234
H	0.107860	-1.988692	2.271554
O	0.195162	1.039817	-1.431425
N	0.721994	-0.580672	0.019200
H	-0.723921	1.957510	-0.128595
C	-2.522681	2.586124	0.492837
C	-2.974600	2.568267	-0.973786
H	-3.222719	1.538469	-1.299616

TS10a

Pd	0.773674	1.168330	-1.033922
C	2.339591	-1.269591	-1.617143
C	3.362046	-2.212079	-1.448046
C	4.546020	-1.825810	-0.793710
C	4.701623	-0.510391	-0.349245
C	3.637272	0.386613	-0.563751
H	3.221765	-3.237494	-1.816422
H	5.615085	-0.169158	0.157483
C	5.612887	-2.857367	-0.509227
F	5.812056	-3.683764	-1.566698
F	6.806966	-2.296129	-0.201882
F	5.258796	-3.644072	0.544465
C	1.041298	-1.606972	-2.285149
H	0.868916	-0.930473	-3.150390
H	1.035876	-2.654029	-2.644320
H	0.189979	-1.456246	-1.583588
O	3.679186	1.675770	-0.181573
N	2.482468	0.010971	-1.156625
C	-2.020436	0.299414	0.232858
O	-2.453545	0.588926	1.391405
C	-2.199465	1.374515	-0.877810
H	-3.003258	2.064058	-0.547348
N	-0.964875	2.149604	-0.993610
C	-1.026456	3.499588	-0.898566
O	-2.098561	4.162207	-0.871828
C	0.325653	4.183562	-0.753362
H	0.333519	5.131487	-1.331698
C	0.666562	4.448591	0.744066
C	0.255112	3.294041	1.620686
H	0.874496	1.686852	1.541968

H	0.724197	3.273166	2.624277	E = -1786.45203413 Hartree			
H	-0.816133	3.024723	1.635438	TS10b			
C	2.176674	4.722366	0.870972	Pd	1.103822	0.750758	-0.766002
H	2.489265	5.555654	0.206599	C	2.852974	-1.636954	-0.341571
H	2.443414	4.999284	1.913449	C	4.017488	-2.344191	-0.014889
H	2.758074	3.819983	0.594228	C	5.214281	-1.635325	0.198419
C	-0.122303	5.709786	1.222897	C	5.233675	-0.243974	0.073505
H	0.040330	5.892639	2.305432	C	4.027278	0.401403	-0.257502
H	0.217765	6.610279	0.665801	H	3.981856	-3.439324	0.067284
H	-1.207873	5.578616	1.044736	H	6.149314	0.344759	0.224807
O	-1.465599	-0.801351	-0.087331	C	6.463851	-2.388004	0.595969
H	1.116548	3.504460	-1.162093	F	6.650544	-3.487887	-0.177772
C	-2.600810	0.735860	-2.227847	F	7.579997	-1.627655	0.495149
H	-2.850000	1.562837	-2.928845	F	6.388536	-2.821085	1.883079
H	-1.724041	0.200099	-2.645981	C	1.553031	-2.332672	-0.618977
C	-3.768314	-0.216667	-2.089719	H	1.291482	-2.228510	-1.694600
C	-3.639187	-1.580128	-2.436969	H	1.617299	-3.410689	-0.377616
C	-4.995066	0.217942	-1.536201	H	0.725313	-1.870626	-0.042810
C	-4.700080	-2.482862	-2.242297	O	3.930307	1.734407	-0.415700
H	-2.685283	-1.937630	-2.858247	N	2.869975	-0.272495	-0.448595
C	-6.057009	-0.681834	-1.334140	C	-2.351943	0.615899	0.118107
H	-5.119543	1.277041	-1.256905	O	-3.285718	1.322419	0.591598
C	-5.913774	-2.037691	-1.684864	C	-1.842836	0.948743	-1.312666
H	-4.576434	-3.541874	-2.522501	H	-2.607485	1.609024	-1.768608
H	-7.004195	-0.321102	-0.900866	N	-0.591751	1.706612	-1.224829
H	-6.745307	-2.743519	-1.527313	C	-0.660896	3.064954	-1.205279
Cs	-3.403142	-2.364219	1.709583	O	-1.708529	3.725489	-1.428265
C	1.410493	-0.100430	2.531636	C	0.639390	3.763790	-0.832815
C	0.293948	0.007105	3.583201	H	0.779755	4.659062	-1.475129
H	-0.678610	-0.283401	3.137464	C	0.650722	4.155824	0.678592
H	0.499707	-0.644436	4.458745	C	-0.036052	3.109147	1.521605
H	0.200312	1.051140	3.949581	H	0.472120	1.373221	1.501760
C	2.748286	0.412115	3.088300	H	0.213583	3.120669	2.600497
H	3.072419	-0.180582	3.969888	H	-1.111267	2.940545	1.323365
H	3.541891	0.347369	2.316475	C	2.110251	4.349880	1.130714
H	2.659531	1.473052	3.403526	H	2.632108	5.095168	0.493228
C	1.542676	-1.542319	2.022383	H	2.155366	4.709530	2.181123
H	0.599928	-1.859042	1.531212	H	2.669075	3.393275	1.067897
H	2.366351	-1.627456	1.284753	C	-0.120655	5.502313	0.851622
H	1.759017	-2.236136	2.860651	H	-0.198642	5.779609	1.923674
O	1.038634	0.682799	1.376286	H	0.406289	6.324971	0.319426
H	4.538205	1.879411	0.247447	H	-1.143994	5.417664	0.434399
				O	-1.795950	-0.363289	0.736552
				H	1.491027	3.061603	-1.007907

C	-1.652891	-0.325387	-2.159749	C	-0.621464	3.125417	-1.031320
H	-1.473693	-0.013405	-3.212601	O	-1.628099	3.808170	-1.361651
H	-0.733229	-0.842830	-1.812298	C	0.754246	3.767956	-0.920421
C	-2.831965	-1.269685	-2.073878	H	0.990592	4.241342	-1.899013
C	-2.661622	-2.598152	-1.625178	C	0.888505	4.832603	0.209247
C	-4.140167	-0.826938	-2.377250	C	0.303089	4.282249	1.524218
C	-3.761657	-3.464552	-1.490628	H	0.773235	3.315047	1.797277
H	-1.648912	-2.951961	-1.370769	H	0.466392	4.998317	2.357930
C	-5.243766	-1.688057	-2.239542	H	-0.791002	4.110472	1.439941
H	-4.296442	0.207874	-2.723410	C	2.391579	5.117197	0.401231
C	-5.059214	-3.011256	-1.795101	H	2.861080	5.463056	-0.544963
H	-3.605422	-4.498237	-1.141054	H	2.553432	5.906295	1.166926
H	-6.255482	-1.323536	-2.481597	H	2.929637	4.203676	0.732837
H	-5.923343	-3.686697	-1.687780	C	0.165741	6.136345	-0.183155
Cs	-4.522436	-1.203873	1.918938	H	0.250619	6.893808	0.625923
O	0.607567	0.359134	1.546051	H	0.604897	6.574772	-1.105415
H	4.796654	2.162203	-0.241445	H	-0.909381	5.950881	-0.378173
H	-0.321486	0.029497	1.321565	O	-1.808140	-1.092966	0.074321
E = -1943.65554309 Hartree				H	1.509088	2.964802	-0.751920
IM10a				C	-2.281772	0.541749	-2.216683
Pd	0.955224	0.686633	-0.454786	H	-2.257183	1.375705	-2.952144
C	2.652174	-1.714014	-0.950306	H	-1.455978	-0.154551	-2.470172
C	3.827238	-2.474460	-1.003282	C	-3.608576	-0.181203	-2.284542
C	5.044561	-1.884310	-0.617816	C	-3.673332	-1.559552	-2.588739
C	5.077434	-0.550636	-0.206016	C	-4.814201	0.492469	-1.978670
C	3.861204	0.157828	-0.168410	C	-4.900691	-2.246517	-2.588059
H	3.782274	-3.514946	-1.353236	H	-2.741545	-2.101651	-2.819327
H	6.011060	-0.050064	0.085800	C	-6.043364	-0.191331	-1.970994
C	6.309855	-2.714235	-0.632375	H	-4.789524	1.569045	-1.742489
F	6.431770	-3.414942	-1.788074	C	-6.092041	-1.565417	-2.273631
F	7.424687	-1.958769	-0.495672	H	-4.926473	-3.321839	-2.829445
F	6.310766	-3.620702	0.380874	H	-6.970517	0.353538	-1.728913
C	1.339422	-2.254228	-1.434517	H	-7.054476	-2.102196	-2.268006
H	1.164216	-1.912798	-2.479137	Cs	-4.368085	-2.042134	1.544288
H	1.340004	-3.361132	-1.435581	C	1.106340	-0.038877	2.534285
H	0.490618	-1.877225	-0.826842	C	0.205963	0.398992	3.718371
O	3.778273	1.446674	0.195011	H	-0.859070	0.339702	3.415862
N	2.682267	-0.419555	-0.505392	H	0.370821	-0.255161	4.600361
C	-2.152460	0.108246	0.315760	H	0.430216	1.444989	4.013558
O	-2.644152	0.521710	1.412206	C	2.589055	0.042037	2.949585
C	-2.008056	1.156701	-0.822846	H	2.770836	-0.524825	3.887337
H	-2.763606	1.945936	-0.630081	H	3.249463	-0.393849	2.174234
N	-0.689429	1.788582	-0.780689	H	2.889853	1.096691	3.118065
				C	0.746698	-1.481123	2.140930

H	-0.286984	-1.536033	1.744901	C	-0.486475	5.393746	0.309818
H	1.437590	-1.860446	1.362826	H	-0.373599	5.975813	1.249919
H	0.835300	-2.155787	3.018405	H	-0.419412	6.106402	-0.540171
O	0.786675	0.924408	1.531041	H	-1.501191	4.949639	0.296746
H	4.664667	1.785904	0.446912	O	-2.101612	0.680530	0.959716
E = -1786.51546541 Hartree				H	1.419709	2.881085	-1.218638
IM10b				C	-1.584588	-0.893284	-1.749713
Pd	1.146265	0.526318	-0.839022	H	-1.045355	-0.956133	-2.721283
C	3.192796	-1.680445	-0.579393	H	-0.903914	-1.281199	-0.966833
C	4.412335	-2.263270	-0.209580	C	-2.838069	-1.738962	-1.783480
C	5.409745	-1.459665	0.372624	C	-3.002586	-2.799305	-0.865934
C	5.184527	-0.096832	0.568092	C	-3.881598	-1.476490	-2.700072
C	3.938315	0.426658	0.169392	C	-4.178889	-3.573243	-0.854781
H	4.571063	-3.337575	-0.377555	H	-2.195186	-3.014443	-0.145791
H	5.938725	0.564892	1.016340	C	-5.057201	-2.244849	-2.692085
C	6.718457	-2.093232	0.793795	H	-3.771714	-0.653728	-3.425336
F	7.285878	-2.780043	-0.230848	C	-5.212955	-3.294891	-1.766155
F	7.622566	-1.180462	1.219422	H	-4.286687	-4.396359	-0.129372
F	6.530505	-2.979073	1.806605	H	-5.860872	-2.023492	-3.413126
C	2.085510	-2.491933	-1.181561	H	-6.136058	-3.896628	-1.760063
H	1.665363	-1.983019	-2.073588	Cs	-4.545929	-0.786836	2.220821
H	2.444324	-3.499569	-1.464087	O	0.410724	-0.288247	0.803167
H	1.255612	-2.602677	-0.452231	H	4.344009	2.219792	0.734086
O	3.614371	1.722735	0.304397	H	-0.519981	0.102326	0.855683
N	2.974873	-0.343707	-0.387375	E = -1670.87158849 Hartree			
C	-2.711158	0.738345	-0.167711	IM-PH			
O	-3.964181	0.834024	-0.300789	Pd	0.057204	1.448536	0.342003
C	-1.850366	0.599688	-1.452538	C	2.921583	0.934353	1.131195
H	-2.457668	1.033630	-2.274440	C	4.182201	0.334301	1.048635
N	-0.596312	1.355601	-1.360396	C	4.431082	-0.563600	-0.017659
C	-0.740245	2.710338	-1.323351	C	3.451192	-0.832245	-0.963166
O	-1.858182	3.271174	-1.464741	C	2.154474	-0.208978	-0.858933
C	0.522225	3.539194	-1.134470	H	4.949440	0.561677	1.800834
H	0.573049	4.269947	-1.971694	H	3.624061	-1.526188	-1.797944
C	0.605261	4.309253	0.218251	C	5.763059	-1.275172	-0.074154
C	0.457962	3.325012	1.395280	F	5.828751	-2.268236	0.859051
H	1.255292	2.553456	1.371931	F	6.002222	-1.851208	-1.277513
H	0.528694	3.862443	2.365345	F	6.799756	-0.434457	0.182133
H	-0.518771	2.797851	1.368854	C	2.576489	1.901607	2.228814
C	1.989929	4.984551	0.282043	H	1.667302	1.568620	2.773242
H	2.126844	5.702350	-0.555148	H	3.410201	2.001815	2.950018
H	2.114071	5.546262	1.232737	H	2.351651	2.905485	1.808684
H	2.804524	4.233177	0.220558	O	1.201783	-0.439928	-1.670007

N	1.955701	0.663242	0.209845	C	-3.614471	0.077480	1.167147
C	-2.024778	-0.145030	1.431339	C	-2.360104	0.728926	0.950935
O	-2.621573	-1.067662	2.001342	H	-4.341947	-0.685768	-2.108486
C	-2.758643	1.013735	0.746928	H	-3.998502	-0.001417	2.193149
H	-3.574029	1.363738	1.416471	C	-5.575752	-1.229314	0.282729
N	-1.805757	2.083225	0.482242	F	-5.342406	-2.571234	0.182153
C	-2.211809	3.299545	0.056461	F	-6.131001	-1.017328	1.499335
O	-3.419119	3.641963	-0.001775	F	-6.515358	-0.928197	-0.649584
C	-1.080716	4.265435	-0.305747	C	-1.941768	0.520554	-2.771349
H	-0.762278	4.781806	0.626670	H	-0.981213	-0.029007	-2.851055
C	0.148401	3.651723	-0.999117	H	-2.625100	0.172299	-3.568637
H	0.729538	2.926126	-0.272656	H	-1.710363	1.594161	-2.937511
O	-0.704673	-0.162375	1.314726	O	-1.657024	1.249543	1.894381
H	-1.506341	5.046073	-0.969710	N	-1.858111	0.788751	-0.337880
C	-3.389909	0.503661	-0.589334	C	2.241048	-0.179421	-1.397168
H	-3.886642	1.387658	-1.040637	O	2.887667	-1.093996	-1.932645
H	-2.558856	0.204395	-1.261606	C	2.943040	0.936807	-0.595359
C	-4.372937	-0.629943	-0.435715	H	3.817750	1.294645	-1.181716
C	-4.104150	-1.900769	-0.988112	N	1.990653	2.006952	-0.387594
C	-5.573478	-0.453186	0.289414	C	2.289550	3.307441	-0.213293
C	-5.004022	-2.968825	-0.820862	O	3.446841	3.791388	-0.205963
H	-3.176304	-2.050507	-1.565262	C	1.004519	4.128923	-0.089809
C	-6.473479	-1.517435	0.461010	H	0.646404	4.343164	-1.120761
H	-5.803657	0.533810	0.723613	C	-0.116970	3.421576	0.726793
C	-6.191003	-2.781754	-0.090769	H	-0.601441	2.015978	1.066493
H	-4.775277	-3.951993	-1.263668	O	0.925560	-0.139332	-1.432629
H	-7.404525	-1.360163	1.029453	H	1.234076	5.109578	0.383340
H	-6.897478	-3.616372	0.044585	C	3.444409	0.395244	0.782358
Cs	-0.155347	-2.847930	-0.210694	H	4.017083	1.226422	1.245951
C	-0.179995	2.995408	-2.343090	H	2.546350	0.219318	1.411335
H	0.690999	2.442088	-2.747045	C	4.278849	-0.859501	0.717742
H	-1.033134	2.292325	-2.269129	C	3.779160	-2.078401	1.225150
H	-0.451042	3.789844	-3.072219	C	5.554975	-0.857213	0.110638
C	1.280196	4.682525	-1.137424	C	4.527159	-3.265513	1.127125
H	2.181849	4.228361	-1.596048	H	2.788394	-2.090787	1.710258
H	0.936650	5.510020	-1.795411	C	6.304953	-2.040115	0.009684
H	1.560485	5.116579	-0.156436	H	5.962839	0.085664	-0.289636
E = -1670.85400596 Hartree TS-PH				C	5.792458	-3.250975	0.513988
				H	4.118726	-4.205885	1.532009
				H	7.298230	-2.019254	-0.467471
				H	6.381196	-4.178803	0.433143
Pd	0.100976	1.460571	-0.351392	Cs	-0.165561	-2.623559	0.091352
C	-2.553859	0.325610	-1.414497	C	0.284394	3.499432	2.215271
C	-3.790395	-0.307672	-1.237101	H	-0.476214	3.055205	2.885477
C	-4.299928	-0.446331	0.075003				

H	1.252524	2.988887	2.398289	H	-4.280539	0.870804	1.241306
H	0.406784	4.569639	2.494751	H	-2.612807	0.287977	1.535756
C	-1.470670	4.082562	0.465427	C	-2.730086	2.394429	1.167753
H	-2.274923	3.623362	1.074742	C	-1.419074	2.603697	1.653412
H	-1.418409	5.161645	0.737402	C	-3.517408	3.522379	0.846162
H	-1.758128	4.019916	-0.603838	C	-0.907664	3.904068	1.815427
E = -1670.87762501 Hartree				H	-0.795731	1.728885	1.905298
Pr-^βH				C	-3.008883	4.822679	1.003952
Pd	-0.990029	-1.401561	-0.311568	H	-4.540758	3.375053	0.463359
C	1.954696	-1.779103	-1.001185	C	-1.700657	5.019139	1.486652
C	3.327674	-1.615628	-0.768318	H	0.114332	4.047577	2.203601
C	3.762037	-1.183264	0.500002	H	-3.637538	5.691371	0.748984
C	2.839164	-0.935005	1.519986	H	-1.303532	6.039294	1.612459
C	1.473688	-1.107822	1.217563	Cs	1.711944	2.348543	-0.968014
H	4.043158	-1.816636	-1.576972	H	-2.977664	-2.990930	1.718167
H	3.136395	-0.593582	2.520645	C	1.407402	-2.203332	-2.329733
C	5.228463	-0.888527	0.727805	H	0.793069	-3.121576	-2.222305
F	5.520567	0.393100	0.357837	H	0.737489	-1.414912	-2.734617
F	5.584927	-1.014561	2.026823	H	2.221256	-2.394505	-3.054207
F	6.032344	-1.699837	0.001051	E = -1670.87338820 Hartree			
O	0.539975	-0.837620	2.140097	IM-^γH			
N	1.054489	-1.517116	-0.009979	Pd	-1.344145	-1.170669	-0.169997
C	-1.925382	1.179352	-1.255168	C	1.343072	-2.392352	-0.704931
O	-2.078894	2.294985	-1.832171	C	2.733502	-2.454242	-0.559574
C	-3.111818	0.486527	-0.557709	C	3.314568	-1.866432	0.592130
H	-4.043605	0.762596	-1.093057	C	2.522835	-1.290845	1.576511
N	-2.934337	-0.968038	-0.561062	C	1.086613	-1.239972	1.418983
C	-4.026342	-1.746798	-0.429596	H	3.348389	-2.930657	-1.334882
O	-5.209959	-1.298383	-0.426013	H	2.956844	-0.823836	2.472198
C	-3.773301	-3.245707	-0.272550	C	4.818909	-1.763085	0.677172
H	-3.436009	-3.669268	-1.247262	F	5.270347	-0.711338	-0.077054
C	-2.739274	-3.601649	0.815509	F	5.265558	-1.554944	1.938558
C	-2.861412	-5.085759	1.210076	F	5.442591	-2.871181	0.203720
H	-2.677189	-5.744834	0.333176	O	0.311365	-0.693079	2.257153
H	-2.121785	-5.356325	1.993683	N	0.568505	-1.797340	0.244162
H	-3.873837	-5.322875	1.602705	C	-1.366175	1.425926	-1.245833
C	-1.307554	-3.282992	0.375340	O	-1.017475	2.485286	-1.788103
H	-1.026185	-3.936607	-0.486987	C	-2.728727	1.235502	-0.570282
H	-0.355897	-0.989335	1.670636	H	-3.487300	1.809481	-1.141619
H	-0.587894	-3.495404	1.198474	N	-3.042446	-0.193590	-0.582083
O	-0.771863	0.573056	-1.147738	C	-4.323439	-0.604390	-0.482459
H	-4.756462	-3.705422	-0.043837	O	-5.294194	0.198827	-0.449876
C	-3.222525	0.990327	0.930687	C	-4.565532	-2.113988	-0.468973

H	-4.137935	-2.559133	-1.395902	F	5.313266	-2.143478	-0.422193
C	-4.021694	-2.894763	0.748833	F	5.930696	-0.593779	-1.832546
C	-4.618420	-4.310860	0.775457	F	6.494650	-0.443634	0.273001
H	-4.328589	-4.879766	-0.134711	O	1.336586	1.461945	-1.893509
H	-4.263008	-4.881220	1.659108	N	1.759326	1.081371	0.328321
H	-5.726985	-4.275822	0.814989	C	-2.010750	-0.481961	1.387150
C	-2.489218	-2.989639	0.753851	O	-2.465493	-1.536440	1.866461
H	-2.094907	-3.324863	-0.233199	C	-2.891088	0.478299	0.582279
H	-2.038462	-2.024259	1.224784	H	-3.865917	0.586549	1.103814
H	-2.091950	-3.709149	1.500489	N	-2.238958	1.781760	0.464803
O	-0.543662	0.396273	-1.173929	C	-3.012352	2.847441	0.177034
H	-5.665149	-2.243005	-0.516429	O	-4.269552	2.773602	0.081936
C	-2.689423	1.767321	0.908338	C	-2.311885	4.187780	-0.015508
H	-3.740396	1.955178	1.208198	H	-1.960184	4.559704	0.974624
H	-2.301754	0.932591	1.527946	C	-1.125021	4.189952	-0.998336
C	-1.823612	2.982741	1.123614	C	-0.770879	5.634142	-1.395852
C	-0.520698	2.827812	1.649124	H	-0.462715	6.225337	-0.505901
C	-2.251120	4.274042	0.743169	H	0.067837	5.657016	-2.123299
C	0.333800	3.936253	1.792383	H	-1.638733	6.148688	-1.859867
H	-0.176697	1.820603	1.941425	C	0.111977	3.497518	-0.416824
C	-1.397716	5.381830	0.880800	H	0.349324	3.884265	0.601012
H	-3.264576	4.408777	0.330404	H	0.423351	2.230109	-1.044373
C	-0.100779	5.217048	1.403938	H	1.014714	3.746201	-1.019575
H	1.344692	3.798774	2.210658	O	-0.741184	-0.163171	1.483978
H	-1.746474	6.382930	0.579250	H	-3.094293	4.891145	-0.364420
H	0.566781	6.086811	1.514334	C	-3.161991	-0.108126	-0.840310
Cs	2.256152	1.781397	-1.108470	H	-3.833956	0.622207	-1.338762
H	-4.340958	-2.362857	1.673171	H	-2.198949	-0.108960	-1.393451
C	0.647728	-2.952091	-1.914964	C	-3.778093	-1.484723	-0.863243
H	-0.087655	-3.729832	-1.618585	C	-3.082345	-2.579353	-1.420396
H	0.081210	-2.155536	-2.443306	C	-5.054544	-1.717181	-0.301485
H	1.373208	-3.400968	-2.619866	C	-3.638193	-3.871902	-1.413941
				H	-2.088697	-2.411817	-1.870053
E = -1670.86060578 Hartree				C	-5.612615	-3.005580	-0.291650
TS-7H				H	-5.615799	-0.873807	0.133491
Pd	-0.242045	1.572899	0.461759	C	-4.905101	-4.090475	-0.844864
C	2.566391	0.684890	1.351612	H	-3.077696	-4.711496	-1.856736
C	3.812364	0.104429	1.080647	H	-6.608935	-3.166777	0.151229
C	4.208496	-0.054499	-0.267366	H	-5.343351	-5.101358	-0.835854
C	3.405876	0.404305	-1.308750	Cs	0.631587	-2.674834	0.194942
C	2.146605	1.003540	-0.998984	H	-1.439368	3.648963	-1.920427
H	4.454845	-0.223596	1.909108	C	2.060465	0.881242	2.751020
H	3.699803	0.307458	-2.362594	H	1.776628	1.942378	2.913402
C	5.490858	-0.796544	-0.568553	H	1.147732	0.274054	2.923108

H	2.829133	0.595708	3.493564	C	-0.327525	3.778659	1.915910
E = -1670.87857830 Hartree				H	-0.621597	1.619054	1.963494
Pr-^γH				C	-2.184714	5.079326	1.035014
Pd	-1.185010	-1.314856	-0.275721	H	-3.930816	3.946363	0.400829
C	1.672361	-2.017806	-0.934757	C	-0.885900	5.025051	1.576500
C	3.063202	-1.948632	-0.756782	H	0.685213	3.726360	2.349197
C	3.575752	-1.533025	0.485311	H	-2.630519	6.052194	0.771082
C	2.704074	-1.232506	1.536752	H	-0.313916	5.952736	1.739674
C	1.319852	-1.332500	1.291055	Cs	1.999053	2.130436	-0.996102
H	3.730899	-2.197693	-1.592540	H	-3.483432	-2.560307	1.674524
H	3.065473	-0.912795	2.524756	C	1.064408	-2.406702	-2.248723
C	5.061142	-1.301449	0.648792	H	0.350819	-3.245864	-2.115517
F	5.391406	-0.037629	0.245968	H	0.483910	-1.556794	-2.666639
F	5.465038	-1.421455	1.934484	H	1.844733	-2.702982	-2.975477
F	5.798475	-2.156971	-0.096879	E = -2112.020258 Hartree			
O	0.394917	-1.047412	2.227116	IM1b			
N	0.820452	-1.693543	0.084576	Pd	-0.240726	0.755657	-0.410201
C	-1.722420	1.360785	-1.271555	C	0.190781	-0.991031	3.509119
O	-1.706235	2.471783	-1.847082	H	0.455704	-0.456820	4.440829
C	-3.013215	0.842516	-0.614645	H	-0.847473	-1.370629	3.559217
H	-3.879494	1.250370	-1.175651	H	0.877243	-1.857265	3.393698
N	-3.041139	-0.620966	-0.622633	C	0.391991	-0.083117	2.316877
C	-4.234078	-1.234304	-0.524240	O	-0.293832	-0.424946	1.262014
O	-5.343999	-0.625811	-0.553949	O	1.197152	0.878959	2.366918
C	-4.196175	-2.752232	-0.352401	C	-2.805009	-0.339581	-1.450206
H	-3.859515	-3.229544	-1.302130	C	-4.158784	-0.671791	-1.360536
C	-3.282368	-3.221922	0.798808	C	-4.906561	-0.175463	-0.261751
C	-3.633375	-4.663341	1.213763	C	-4.323358	0.650704	0.684329
H	-3.499164	-5.364695	0.360734	C	-2.927822	1.017734	0.580797
H	-2.980346	-5.014614	2.041287	H	-4.616218	-1.305702	-2.132272
H	-4.687851	-4.747101	1.555719	H	-4.888133	1.052784	1.536876
C	-1.797176	-3.111583	0.435864	C	-6.353782	-0.591070	-0.135844
H	-1.558577	-3.844995	-0.373827	F	-6.462730	-1.938900	0.041557
H	0.830770	-0.826763	3.079420	F	-6.986292	-0.001717	0.905628
H	-1.163097	-3.373207	1.313843	F	-7.061024	-0.290617	-1.258320
O	-0.668688	0.614130	-1.126270	C	-1.949744	-0.804909	-2.594792
H	-5.243467	-3.074859	-0.179501	H	-0.968617	-1.184008	-2.240773
C	-3.093807	1.350710	0.877353	H	-2.463858	-1.594171	-3.175431
H	-4.167678	1.422659	1.145042	H	-1.732535	0.043641	-3.279636
H	-2.643216	0.545602	1.493792	O	-2.341474	1.788257	1.385105
C	-2.365836	2.639496	1.160970	N	-2.229864	0.442083	-0.491832
C	-1.061600	2.597244	1.705510	C	2.034963	-1.420764	-0.439010
C	-2.916599	3.897351	0.830230	O	1.282931	-1.626840	-1.444426

C	2.817742	-0.067383	-0.454664	C	-0.172923	1.043077	2.737809
H	3.182251	0.080394	-1.490134	O	-0.706150	0.188007	1.949895
N	1.884964	1.057993	-0.179135	O	0.359605	2.142716	2.350140
H	1.692757	1.159806	0.887733	C	-2.352191	-1.990767	-0.431386
C	2.237975	2.312750	-0.755472	C	-3.463738	-2.836267	-0.397067
O	3.174756	2.449004	-1.530171	C	-4.691164	-2.319008	0.091373
C	-0.489557	2.580541	-1.909789	C	-4.786894	-1.012333	0.541563
H	-0.072295	1.483697	-2.004539	C	-3.629497	-0.145216	0.524816
H	-1.586482	2.580960	-2.021095	H	-3.370663	-3.875126	-0.741498
H	-0.037027	2.862526	-2.890026	H	-5.725640	-0.595796	0.932292
O	2.185627	-2.188889	0.552233	C	-5.892853	-3.234843	0.121031
C	4.001175	-0.011505	0.530798	F	-5.678561	-4.310522	0.928428
H	4.349701	1.041098	0.593348	F	-7.016006	-2.622181	0.565238
H	3.639341	-0.309494	1.534771	F	-6.170371	-3.730470	-1.116647
C	5.149130	-0.891120	0.088431	C	-1.010054	-2.457018	-0.919932
C	5.450049	-2.102707	0.745997	H	-0.231419	-2.277234	-0.149036
C	5.932037	-0.514581	-1.026505	H	-1.033825	-3.535661	-1.166633
C	6.509060	-2.916066	0.304779	H	-0.700279	-1.894920	-1.825510
H	4.843084	-2.408815	1.612753	O	-3.630517	1.042058	0.948767
C	6.988285	-1.326578	-1.471837	N	-2.460377	-0.701765	-0.004957
H	5.706534	0.432367	-1.545661	C	1.940370	-0.254140	-0.359141
C	7.280464	-2.532102	-0.806627	O	1.883207	-0.788794	-1.510633
H	6.732532	-3.857028	0.833429	C	2.079244	1.299502	-0.328516
H	7.590050	-1.015654	-2.341257	H	2.418853	1.613638	-1.334522
H	8.109750	-3.169622	-1.153174	N	0.740236	1.909749	-0.120380
Cs	-0.762094	-3.371755	0.311967	H	0.515877	2.123671	1.138334
C	-0.005842	3.504181	-0.819854	C	0.505896	3.087715	-0.845065
C	1.323028	3.425035	-0.328611	O	1.404258	3.737495	-1.386782
C	1.757625	4.351888	0.629588	C	-1.532085	1.356620	-2.194721
C	0.921602	5.355533	1.128147	H	-0.694537	0.629683	-1.789431
C	-0.394529	5.4235	0.641801	H	-2.412248	0.744850	-2.455557
C	-0.856279	4.51045	-0.320938	H	-0.947015	1.557491	-3.122620
H	1.300888	6.051016	1.891323	O	1.925231	-0.867485	0.751867
H	-1.073119	6.200093	1.027269	C	3.108906	1.769349	0.719996
H	-1.890612	4.571766	-0.691565	H	3.234355	2.867581	0.603567
F	3.017859	4.230698	1.109288	H	2.714163	1.583442	1.737530
E = -2112.011855 Hartree				C	4.434465	1.058193	0.551556
TS2b				C	4.957304	0.254195	1.588614
Pd	-0.896691	0.584129	-0.056340	C	5.147497	1.128543	-0.667316
C	-0.141420	0.706232	4.200980	C	6.159193	-0.456587	1.418232
H	-0.148713	1.632270	4.806267	H	4.406063	0.181563	2.540415
H	-0.985691	0.046663	4.473827	C	6.345723	0.414169	-0.844490
H	0.808550	0.166099	4.404565	H	4.760341	1.753513	-1.488814
				C	6.856097	-0.383292	0.197442

H	6.550678	-1.075460	2.242140	H	1.897334	2.844976	3.694329
H	6.886950	0.483104	-1.802138	H	0.287114	3.265388	3.007960
H	7.795923	-0.941935	0.059536	O	-1.195089	-0.444255	0.913325
Cs	3.708006	-3.092111	-0.543963	C	-2.650502	1.697221	-1.194087
C	-2.672272	5.165937	-0.420338	H	-2.593546	2.747766	-1.548654
C	-3.624694	4.330121	-1.025335	H	-1.961295	1.092271	-1.819353
C	-3.249937	3.091945	-1.572091	C	-4.056784	1.162838	-1.309658
C	-1.909857	2.658320	-1.520978	C	-4.300975	-0.086171	-1.921059
C	-0.936041	3.498352	-0.913110	C	-5.150036	1.867345	-0.756849
C	-1.342502	4.734588	-0.384383	C	-5.600513	-0.622719	-1.976126
H	-2.942235	6.133363	0.028403	H	-3.455493	-0.644925	-2.356799
H	-4.678018	4.648261	-1.063839	C	-6.448322	1.333974	-0.807422
H	-4.005126	2.443293	-2.041024	H	-4.977525	2.845266	-0.277736
F	-0.414222	5.513357	0.218250	C	-6.678702	0.084142	-1.414038
E = -1883.09418 Hartree				H	-5.770870	-1.598286	-2.460442
IM2b				H	-7.288867	1.897137	-0.370428
Pd	0.493009	0.394548	0.187098	H	-7.697655	-0.333260	-1.454044
C	2.059672	-2.436665	0.261481	Cs	-3.178946	-3.041711	0.620584
C	3.326633	-2.981599	-0.001716	C	1.869124	4.076102	-0.733518
C	4.350276	-2.138715	-0.495817	C	1.195893	3.576177	0.390379
C	4.129811	-0.777772	-0.729428	C	1.931895	3.344808	1.581493
C	2.833688	-0.286015	-0.446263	C	3.314337	3.626860	1.586170
H	3.508698	-4.050370	0.177844	C	3.962114	4.122072	0.441237
H	4.909462	-0.104271	-1.109037	C	3.239832	4.350146	-0.741527
C	5.708087	-2.748043	-0.767414	H	3.892363	3.449253	2.507284
F	5.628784	-3.746649	-1.688079	H	5.043615	4.329607	0.466217
F	6.604502	-1.846123	-1.232071	H	3.717932	4.725266	-1.658869
F	6.237896	-3.298410	0.358242	F	1.157566	4.257859	-1.879324
C	0.899521	-3.241624	0.764894	E = -1883.066971 Hartree			
H	0.114901	-3.297663	-0.019772	TS3b			
H	1.205927	-4.271319	1.028063	Pd	-0.588194	0.944419	-0.071773
H	0.444531	-2.757090	1.653318	C	2.190673	1.495198	1.070258
O	2.391691	0.940498	-0.576637	C	3.588903	1.484667	0.996433
N	1.858193	-1.119212	0.032828	C	4.200552	1.261803	-0.259557
C	-2.254167	0.337751	0.914512	C	3.435591	1.107478	-1.411737
O	-3.340839	-0.049225	1.378102	C	2.008380	1.137691	-1.308539
C	-2.080048	1.704876	0.260310	H	4.185554	1.644801	1.904694
H	-2.641886	2.456111	0.854635	H	3.889004	0.951484	-2.400002
N	-0.657253	2.030665	0.246077	C	5.704874	1.125268	-0.324917
C	-0.290831	3.322525	0.307917	F	6.096319	-0.112072	0.101762
O	-1.098681	4.288130	0.319439	F	6.192232	1.280579	-1.578261
C	1.253688	2.762810	2.796579	F	6.333861	2.026878	0.470404
H	1.024784	1.685654	2.631510	C	1.456444	1.720692	2.360088

H	0.877123	0.817495	2.643149	IM3b			
H	2.159403	1.968503	3.177513	Pd	0.970468	-0.678317	-0.056218
H	0.724914	2.548625	2.247573	C	-1.277621	-2.623887	0.564758
O	1.217334	1.015571	-2.313964	C	-2.591248	-3.104250	0.465120
N	1.444970	1.288357	-0.051701	C	-3.446959	-2.562606	-0.513364
C	-1.573794	-1.396623	1.214724	C	-2.987475	-1.574138	-1.388319
O	-1.637772	-2.465836	1.841371	C	-1.660021	-1.133604	-1.230307
C	-2.679023	-0.964388	0.230977	H	-2.937101	-3.887913	1.152500
H	-3.667113	-1.168432	0.696934	H	-3.620431	-1.128597	-2.167483
N	-2.520721	0.458127	-0.009989	C	-4.896146	-2.994715	-0.568416
C	-3.577510	1.274264	-0.202733	F	-5.655946	-2.239898	0.276506
O	-4.766621	0.876459	-0.286104	F	-5.426547	-2.855179	-1.806234
C	-1.179408	2.309997	-1.714839	F	-5.057915	-4.286436	-0.196546
H	-0.508351	2.946787	-2.327810	C	-0.305299	-3.131753	1.584573
H	-0.101118	1.479577	-1.682432	H	0.040627	-2.297631	2.231883
H	-1.816218	1.709781	-2.395253	H	-0.761149	-3.917007	2.216260
O	-0.533382	-0.592919	1.317075	H	0.597939	-3.545203	1.088094
C	-2.581406	-1.763997	-1.106507	O	-1.174812	-0.164219	-2.018603
H	-3.459351	-1.453222	-1.711590	N	-0.841316	-1.639696	-0.274340
H	-1.669940	-1.416565	-1.637467	C	0.963622	1.950762	1.148821
C	-2.545579	-3.263905	-0.945537	O	0.731597	2.999552	1.785609
C	-1.377961	-3.992842	-1.258646	C	2.227016	1.837778	0.267575
C	-3.659969	-3.966863	-0.434037	H	3.036942	2.433421	0.739504
C	-1.318071	-5.384580	-1.061993	N	2.618345	0.434272	0.177529
H	-0.502882	-3.456944	-1.664263	C	3.896416	0.124190	-0.139237
C	-3.604371	-5.355907	-0.235860	O	4.797095	0.981312	-0.345863
H	-4.581508	-3.414660	-0.186236	C	2.007778	-1.926537	-1.276138
C	-2.431135	-6.070819	-0.545123	H	1.406532	-2.806181	-1.581678
H	-0.396574	-5.934487	-1.314206	H	-0.226118	0.004748	-1.699608
H	-4.483250	-5.886987	0.164386	H	2.201546	-1.292628	-2.170587
H	-2.388007	-7.160461	-0.387567	O	0.154284	0.928637	1.136413
Cs	1.865157	-2.512584	0.648623	C	1.951246	2.423987	-1.164039
C	-1.644262	4.567378	-0.697281	H	2.938730	2.660520	-1.610067
C	-2.008928	3.210993	-0.835379	H	1.502408	1.601732	-1.759899
C	-3.204303	2.740225	-0.212242	C	1.031294	3.617520	-1.194961
C	-3.980034	3.668379	0.505721	C	-0.332477	3.446525	-1.523315
C	-3.620644	5.016299	0.649293	C	1.479884	4.906927	-0.831884
C	-2.436735	5.460154	0.043924	C	-1.225900	4.532717	-1.490782
H	-0.727430	4.924704	-1.192435	H	-0.693866	2.443615	-1.806091
H	-4.265533	5.684863	1.238998	C	0.590150	5.993569	-0.795861
H	-2.133610	6.514265	0.143804	H	2.540559	5.056358	-0.570874
F	-5.104827	3.252927	1.136690	C	-0.767405	5.810828	-1.122662
				H	-2.285030	4.380163	-1.756725
				H	0.957537	6.992856	-0.510867

E = -1883.103586 Hartree

H	-1.463761	6.664408	-1.096327	C	3.280023	-2.334755	-0.613887
Cs	-2.775791	1.810776	1.291479	C	4.206245	-1.355420	-0.134357
C	5.415896	-1.812876	0.425339	H	6.688197	-3.457085	1.024945
C	5.733629	-3.171538	0.557900	H	5.030864	-5.196225	0.208209
C	4.805239	-4.122559	0.107731	H	2.875541	-4.455764	-0.837762
C	3.595376	-3.706732	-0.470425	F	6.310731	-0.918998	0.914641