

Supporting information

Arene C-H bond activation and methane formation by a methylplatinum(II) complex: Experimental and theoretical elucidation of mechanism

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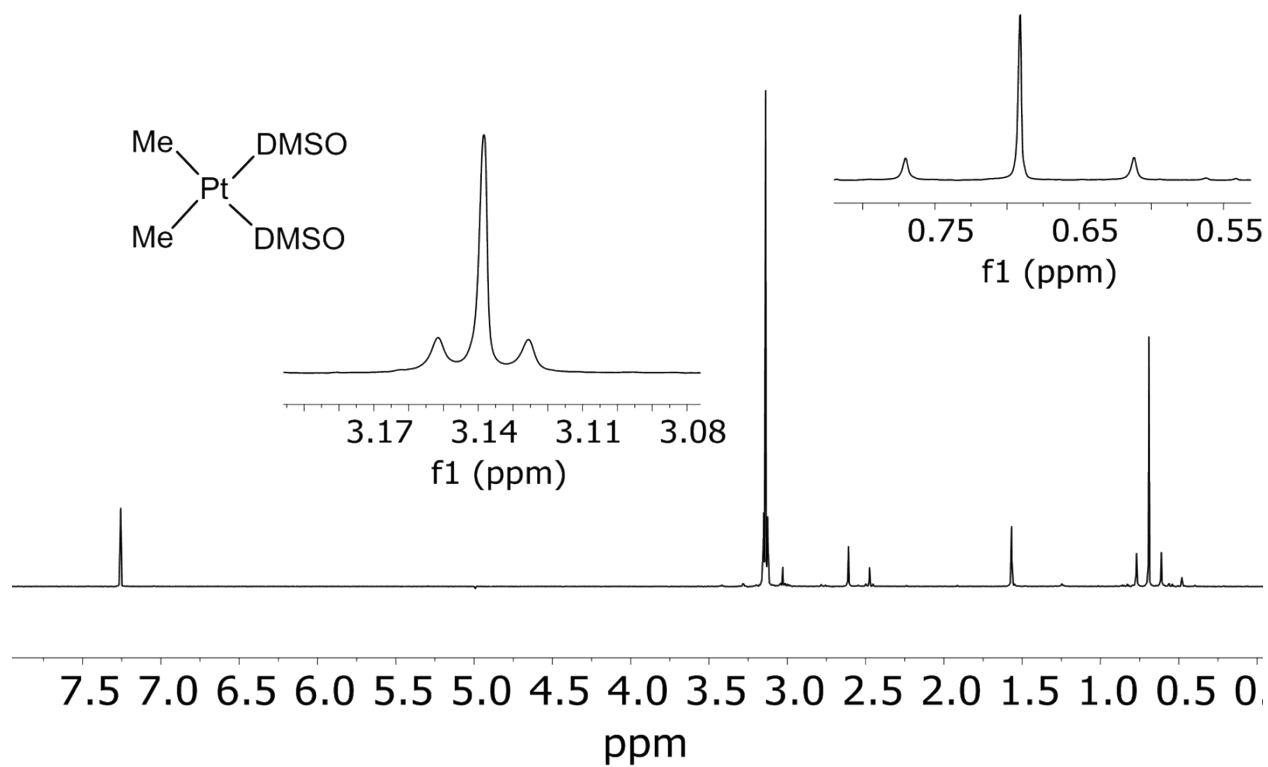


Fig. S1. The 1H NMR of complex $[PtMe_2(DMSO)_2]$, **1**, in $CDCl_3$.

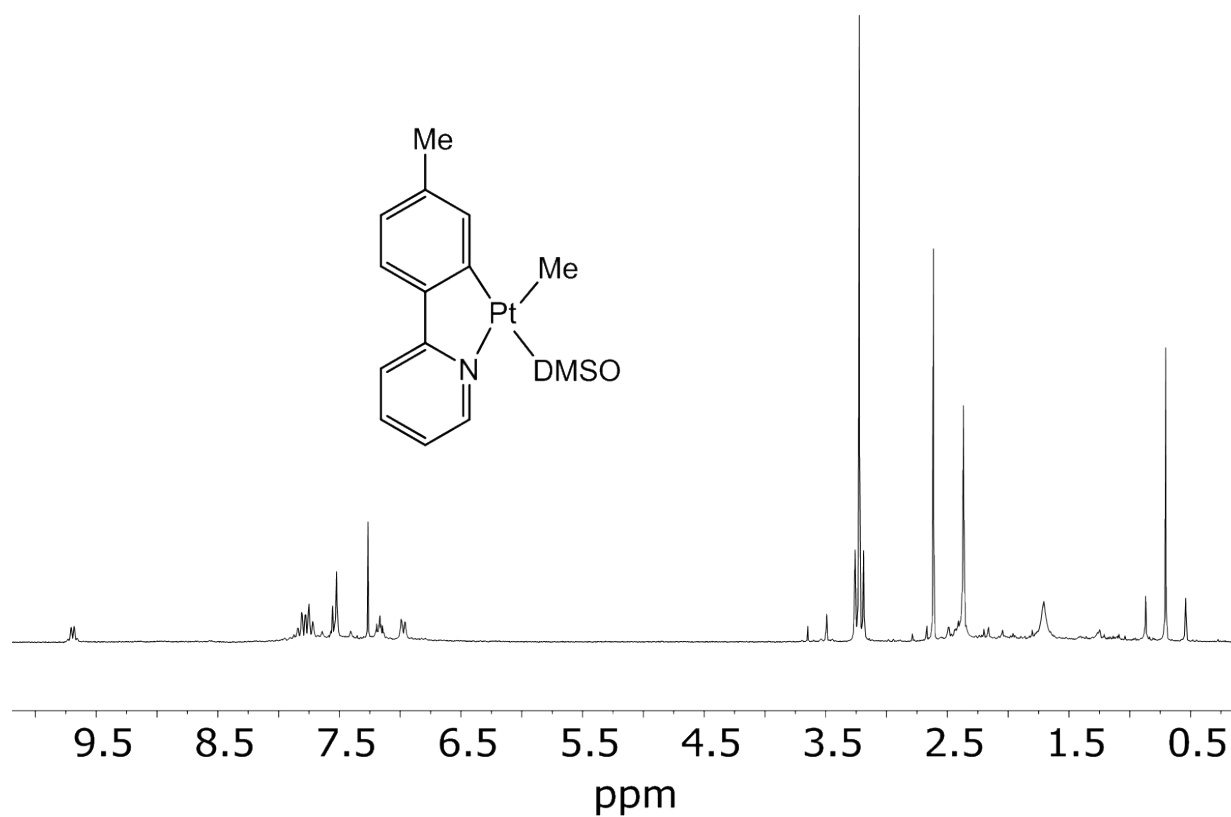


Fig. S2. The ^1H NMR of complex $[\text{PtMe}(\text{tpy})(\text{DMSO})]$, **2**, in CDCl_3 .

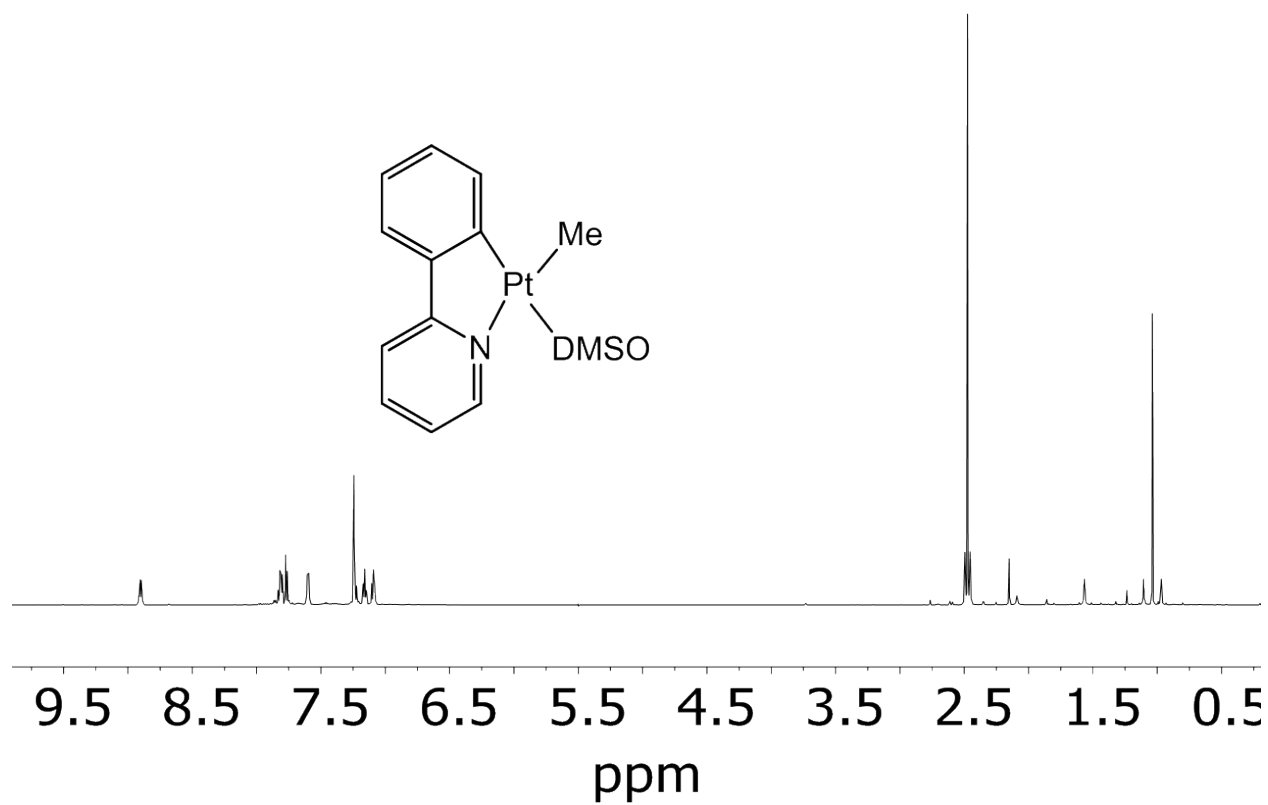


Fig. S3. The ^1H NMR of complex $[\text{PtMe}(\text{ppy})(\text{DMSO})]$, **3**, in CDCl_3 .

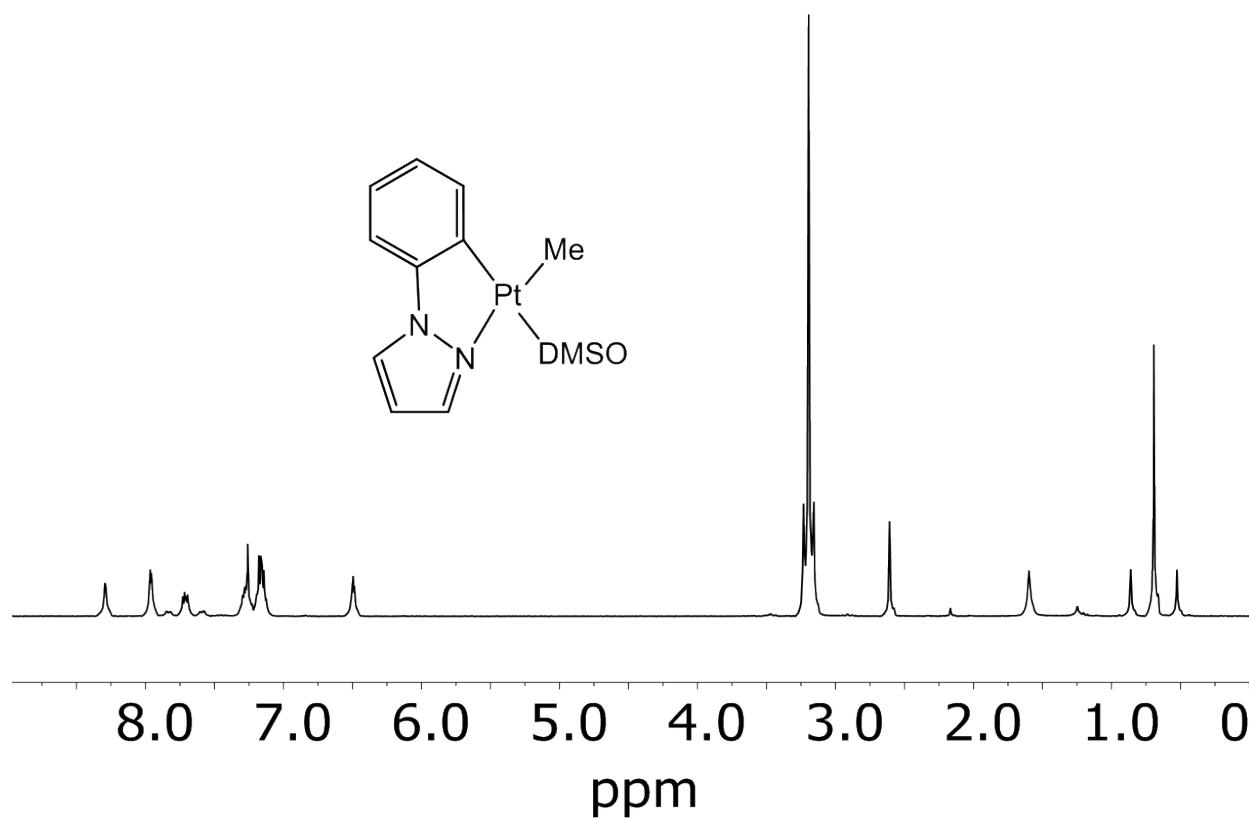


Fig. S4. The ^1H NMR of complex $[\text{PtMe}(\text{ppz})(\text{DMSO})]$, **4**, in CDCl_3 .

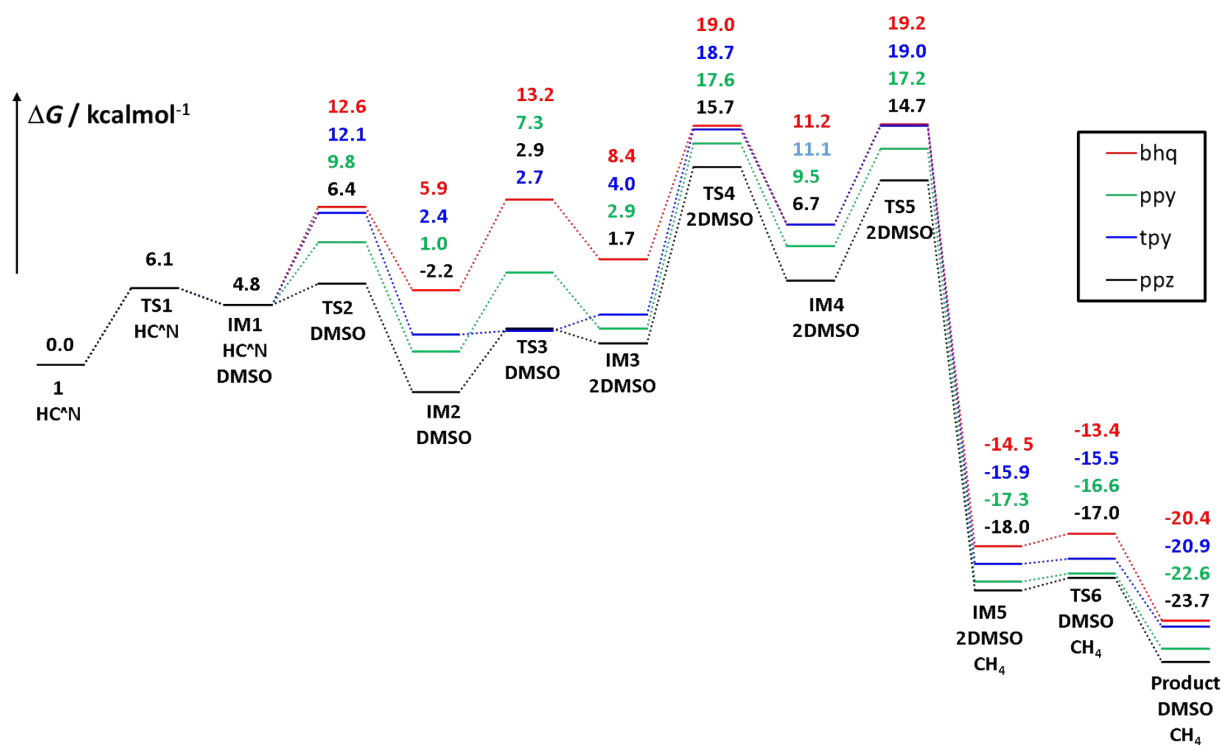
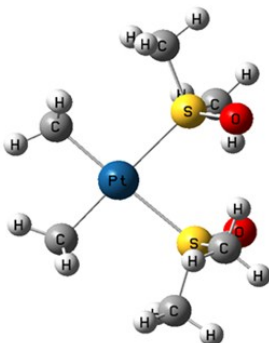


Figure S5. The free energy barriers for the cyclometalation reaction of HC^N ligand by [PtMe₂(DMSO)₂], **1**.

Optimized structures, XYZ Cartesian and their energy

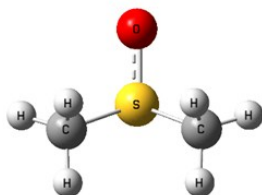
[PtMe₂(DMSO)₂], 1



Zero-point correction=	0.237951 (Hartree/Particle)
Thermal correction to Energy=	0.256744
Thermal correction to Enthalpy=	0.257688
Thermal correction to Gibbs Free Energy=	0.190695
Sum of electronic and zero-point Energies=	-1305.167090
Sum of electronic and thermal Energies=	-1305.148298
Sum of electronic and thermal Enthalpies=	-1305.147353
Sum of electronic and thermal Free Energies=	-1305.214346

Pt	-0.000004	-0.799070	0.000010	C	-1.449962	-2.266343	0.080261
S	1.694491	0.997994	-0.093961	H	-2.041083	-2.153710	0.999406
C	1.449964	-2.266327	-0.080351	H	-2.126030	-2.167379	-0.780505
H	1.030007	-3.276046	-0.067768	H	-1.030012	-3.276061	0.067378
H	2.125888	-2.167561	0.780549	S	-1.694513	0.997981	0.093980
H	2.041235	-2.153484	-0.999374	O	-1.427426	2.137642	1.058630
C	3.398665	0.436990	-0.387006	C	-1.887140	1.697499	-1.571133
H	3.674773	-0.311037	0.358454	H	-2.628171	2.500735	-1.537675
H	4.053137	1.310146	-0.329624	H	-0.901965	2.079473	-1.847334
H	3.430784	0.002953	-1.387943	H	-2.195150	0.901758	-2.254403
C	1.887428	1.697168	1.571261	C	-3.398744	0.436938	0.386624
H	0.902284	2.079016	1.847748	H	-4.053200	1.310110	0.329302
H	2.628402	2.500456	1.537814	H	-3.674729	-0.310938	-0.359033
H	2.195635	0.901300	2.254296	H	-3.431040	0.002700	1.387468
O	1.427256	2.137846	-1.058346				

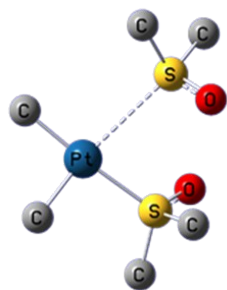
DMSO



Zero-point correction=	0.079959 (Hartree/Particle)
Thermal correction to Energy=	0.085597
Thermal correction to Enthalpy=	0.086541
Thermal correction to Gibbs Free Energy=	0.051623
Sum of electronic and zero-point Energies=	-553.116455
Sum of electronic and thermal Energies=	-553.110818
Sum of electronic and thermal Enthalpies=	-553.109874
Sum of electronic and thermal Free Energies=	-553.144791

S	-0.000001	0.230434	-0.439352	H	-1.275944	-0.929591	1.267659
O	-0.000005	1.515529	0.380163	C	1.366333	-0.814219	0.183693
C	-1.366328	-0.814227	0.183692	H	1.275950	-0.929589	1.267659
H	-2.300647	-0.303511	-0.060796	H	1.335589	-1.787150	-0.314857
H	-1.335578	-1.787160	-0.314852	H	2.300649	-0.303497	-0.060795

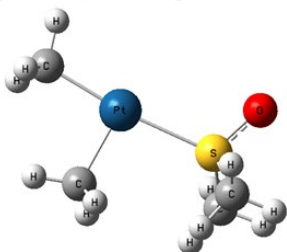
[PtMe₂(DMSO)...(DMSO)], TS1



Zero-point correction= 0.236244 (Hartree/Particle)
 Thermal correction to Energy= 0.255071
 Thermal correction to Enthalpy= 0.256015
 Thermal correction to Gibbs Free Energy= 0.187091
 Sum of electronic and zero-point Energies= -1305.155487
 Sum of electronic and thermal Energies= -1305.136660
 Sum of electronic and thermal Enthalpies= -1305.135716
 Sum of electronic and thermal Free Energies= -1305.204640

Pt	0.673545	-0.761884	-0.020077	H	-4.156875	1.460475	-1.030212
C	0.405397	-2.790035	-0.076712	H	-2.430968	1.995284	-1.122278
H	-0.674083	-2.988119	-0.158816	C	-2.973154	0.833439	1.496214
H	0.909169	-3.239642	-0.942181	H	-2.298827	1.692741	1.510373
H	0.781646	-3.276778	0.832376	H	-4.022104	1.143188	1.503892
C	2.683237	-1.070360	0.136722	H	-2.768548	0.176464	2.344894
H	3.023351	-0.705439	1.113978	C	1.721439	2.279587	-1.475659
H	2.920932	-2.134130	0.051345	H	1.099290	2.012313	-2.332047
H	3.204423	-0.524730	-0.660057	H	1.834507	3.364561	-1.406109
S	-2.627688	-0.119968	-0.018993	H	2.693461	1.786627	-1.551584
O	-3.630745	-1.260940	-0.099622	C	2.019002	2.269273	1.279383
S	0.858814	1.677653	0.008575	H	1.598185	1.990892	2.247516
O	-0.418372	2.489286	0.148501	H	2.986718	1.782994	1.137851
C	-3.123932	1.156869	-1.222787	H	2.108687	3.355398	1.197379
H	-3.042480	0.712514	-2.217612				

[PtMe₂(DMSO)], IM1

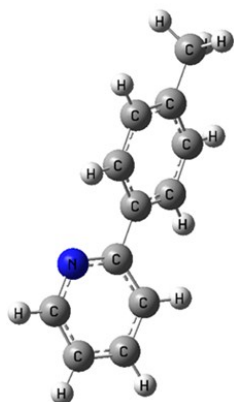


Zero-point correction= 0.151935 (Hartree/Particle)
 Thermal correction to Energy= 0.164303
 Thermal correction to Enthalpy= 0.165247
 Thermal correction to Gibbs Free Energy= 0.111706

Sum of electronic and zero-point Energies= -752.021717
 Sum of electronic and thermal Energies= -752.009349
 Sum of electronic and thermal Enthalpies= -752.008405
 Sum of electronic and thermal Free Energies= -752.061946

Pt	-0.731516	-0.152570	-0.001419	O	2.277270	-1.617441	-0.052736
C	-2.764807	-0.333961	0.001908	C	2.470937	0.739450	-1.360677
H	-3.217268	0.122043	0.892399	H	3.558725	0.659484	-1.287760
H	-3.005733	-1.409243	0.001402	H	2.116593	0.294615	-2.292758
H	-3.220424	0.123709	-0.886143	H	2.147938	1.781600	-1.296587
C	-0.870042	1.872469	0.013224	C	2.471564	0.643864	1.410645
H	-0.371233	2.261834	0.909952	H	3.558562	0.551395	1.340425
H	-0.376913	2.272958	-0.881734	H	2.165967	1.692944	1.407667
H	-1.916106	2.191457	0.018430	H	2.103002	0.148883	2.311376
S	1.715692	-0.211413	-0.005919				

Htpy

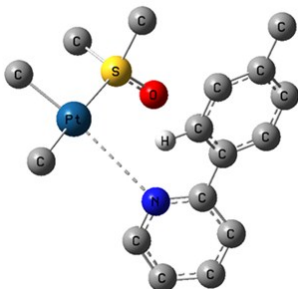


Zero-point correction= 0.197608 (Hartree/Particle)
 Thermal correction to Energy= 0.208290
 Thermal correction to Enthalpy= 0.209234
 Thermal correction to Gibbs Free Energy= 0.159788
 Sum of electronic and zero-point Energies= -518.471160
 Sum of electronic and thermal Energies= -518.460478
 Sum of electronic and thermal Enthalpies= -518.459534
 Sum of electronic and thermal Free Energies= -518.508980

C	3.993243	-0.095237	-0.014434	H	-2.872442	-2.123405	0.369449
C	3.175995	-1.206278	-0.224890	C	-3.095247	-0.011171	-0.004748
C	1.235897	0.026672	-0.002131	C	-2.387898	1.177949	-0.225394
C	1.982314	1.193884	0.237676	C	-0.993913	1.201846	-0.226546
C	3.372936	1.130572	0.225546	H	5.074012	-0.192960	-0.031741
C	-0.251496	0.029975	-0.008134	H	3.618072	-2.184839	-0.407412
C	-0.960131	-1.165944	0.199226	H	3.961969	2.024572	0.410389
C	-2.351676	-1.182983	0.202405	H	-2.935163	2.099868	-0.408097

N	1.839799	-1.159897	-0.223685	H	-4.978674	0.029843	1.059166
H	-0.401661	-2.082301	0.357261	H	-5.028666	0.815755	-0.522098
H	1.484735	2.133550	0.450728	H	-5.003250	-0.954690	-0.404488
H	-0.487803	2.141278	-0.427884				
C	-4.604978	-0.030518	0.028177				

[PtMe₂(DMSO)... (Htpy- κ^1N)], TS2



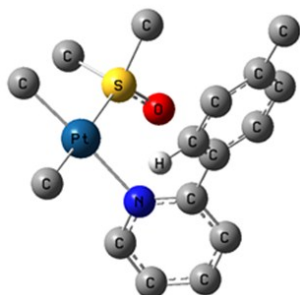
Zero-point correction=	0.353590 (Hartree/Particle)
Thermal correction to Energy=	0.377617
Thermal correction to Enthalpy=	0.378561
Thermal correction to Gibbs Free Energy=	0.296319
Sum of electronic and zero-point Energies=	-1270.501966
Sum of electronic and thermal Energies=	-1270.477940
Sum of electronic and thermal Enthalpies=	-1270.476996
Sum of electronic and thermal Free Energies=	-1270.559238

Pt	-1.725524	0.220399	-0.453196	N	1.070285	2.014442	-0.153284
C	-2.101749	1.414513	-2.071204	C	0.725270	3.281480	0.105575
H	-1.280965	2.141701	-2.153549	C	2.331491	1.616539	0.117237
H	-2.146348	0.832000	-3.001218	H	-0.302536	3.550005	-0.129385
H	-3.047233	1.962815	-1.966683	C	1.597743	4.225182	0.647889
C	-3.515757	-0.697128	-0.754471	C	3.278271	2.509337	0.648997
H	-3.372335	-1.784436	-0.805207	C	2.684834	0.205409	-0.188305
H	-4.187389	-0.458487	0.080109	H	1.261206	5.238339	0.842503
H	-3.976438	-0.359273	-1.687210	C	2.904700	3.822489	0.922468
S	-1.168189	-1.148211	1.510134	H	4.297647	2.183626	0.825334
O	-0.124246	-0.614982	2.468836	C	3.679596	-0.474690	0.533988
C	-2.635455	-1.592160	2.491714	C	2.026212	-0.490246	-1.216094
H	-3.369207	-2.086254	1.851447	H	3.626867	4.521881	1.334047
H	-2.321509	-2.248602	3.307227	C	4.005247	-1.796634	0.234674
H	-3.048703	-0.662307	2.887607	H	4.185774	0.018399	1.358896
C	-0.654036	-2.817492	1.000275	C	2.360324	-1.810356	-1.514580
H	0.257316	-2.700409	0.409974	H	1.252864	0.014406	-1.785133
H	-0.461019	-3.419766	1.892173	H	4.769928	-2.301452	0.820468
H	-1.441253	-3.263905	0.387718	C	3.358275	-2.489374	-0.798721

H	1.840965	-2.320695	-2.322786
C	3.739815	-3.909299	-1.145052
H	4.097104	-4.453659	-0.264587

H	2.893432	-4.459681	-1.569075
H	4.547038	-3.930616	-1.889585

[PtMe₂(Htpy- κ^1 N)(DMSO)], IM2



Zero-point correction=	0.354686 (Hartree/Particle)
Thermal correction to Energy=	0.378946
Thermal correction to Enthalpy=	0.379890
Thermal correction to Gibbs Free Energy=	0.298568
Sum of electronic and zero-point Energies=	-1270.518574
Sum of electronic and thermal Energies=	-1270.494314
Sum of electronic and thermal Enthalpies=	-1270.493370
Sum of electronic and thermal Free Energies=	-1270.574693

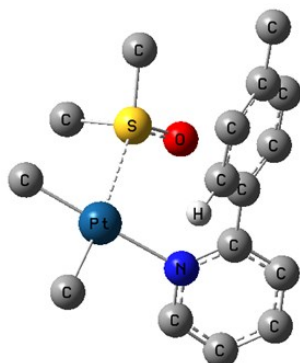
Pt	-1.226495	-0.396250	-0.612262
C	-1.639601	0.125039	-2.561653
H	-1.443517	1.192293	-2.727991
H	-1.010844	-0.454930	-3.251111
H	-2.687590	-0.081349	-2.814883
C	-2.063815	-2.236945	-1.032949
H	-1.457853	-3.065889	-0.637366
H	-3.066976	-2.315622	-0.588075
H	-2.169051	-2.396408	-2.112442
S	-0.790209	-1.024496	1.707432
O	-0.402687	0.041714	2.710862
C	-2.204833	-1.932344	2.406505
H	-2.445535	-2.780117	1.762264
H	-1.943828	-2.263291	3.414952
H	-3.045280	-1.236087	2.437964
C	0.459835	-2.345793	1.801442
H	1.401682	-1.915665	1.454834
H	0.549035	-2.677048	2.839608
H	0.159427	-3.169629	1.149776
N	-0.422825	1.651354	-0.186666

C	-1.369801	2.602261	-0.059180
C	0.861289	1.965554	0.114380
H	-2.377019	2.297440	-0.321722
C	-1.105562	3.889904	0.391846
C	1.194290	3.247020	0.579874
C	1.931090	0.953148	-0.077195
H	-1.912733	4.609235	0.477429
C	0.207796	4.215824	0.728842
H	2.231494	3.474644	0.799596
C	2.884288	0.732665	0.928571
C	2.054251	0.242173	-1.282693
H	0.461825	5.209010	1.086727
C	3.919289	-0.184272	0.739947
H	2.800196	1.260580	1.874337
C	3.097760	-0.662566	-1.468019
H	1.338360	0.413125	-2.079311
H	4.636739	-0.349909	1.540005
C	4.048549	-0.894394	-0.461882
H	3.178870	-1.194542	-2.413072
C	5.192239	-1.856509	-0.681522

H	4.880302	-2.719378	-1.279647
H	6.016775	-1.370911	-1.220434

H	5.594391	-2.223911	0.268000
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[PtMe₂(Htpy- κ^1 N)...(DMSO)], TS3



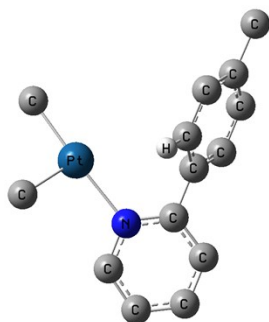
Zero-point correction=	0.352660 (Hartree/Particle)
Thermal correction to Energy=	0.377231
Thermal correction to Enthalpy=	0.378175
Thermal correction to Gibbs Free Energy=	0.293756
Sum of electronic and zero-point Energies=	-1270.505597
Sum of electronic and thermal Energies=	-1270.481026
Sum of electronic and thermal Enthalpies=	-1270.480082
Sum of electronic and thermal Free Energies=	-1270.564501

Pt	-1.304502	-0.422039	-0.745450
C	-2.809996	0.308753	-1.892798
H	-2.739028	1.402482	-1.937767
H	-2.757742	-0.097467	-2.908889
H	-3.775585	0.027707	-1.451482
C	-1.616879	-2.268582	-1.577945
H	-0.864777	-2.980672	-1.201110
H	-2.609301	-2.674465	-1.332153
H	-1.529487	-2.250020	-2.673825
S	0.442023	-1.885370	1.788993
O	0.756271	-1.065148	3.032195
C	-0.623898	-3.273057	2.307752
H	-0.787388	-3.940265	1.457088
H	-0.152919	-3.806924	3.138031
H	-1.576383	-2.844589	2.628114
C	1.930304	-2.867844	1.395340
H	2.702758	-2.163168	1.078660
H	2.255129	-3.409536	2.288326
H	1.702640	-3.560651	0.580519
N	-0.950134	1.539899	0.280184
C	-2.038830	2.127356	0.818225

C	0.271071	2.070091	0.545561
H	-2.988433	1.663930	0.576133
C	-1.978489	3.242693	1.644769
C	0.401417	3.191075	1.379361
C	1.483588	1.464589	-0.064988
H	-2.891979	3.666931	2.047216
C	-0.726692	3.782719	1.938043
H	1.389234	3.599738	1.561232
C	2.602351	1.176754	0.731854
C	1.568175	1.227731	-1.447363
H	-0.631084	4.653914	2.578948
C	3.764965	0.653470	0.164424
H	2.553440	1.339136	1.804571
C	2.737158	0.714479	-2.007558
H	0.725593	1.471412	-2.085974
H	4.617313	0.434387	0.803177
C	3.853840	0.411394	-1.213679
H	2.786149	0.555243	-3.082218
C	5.106816	-0.172089	-1.823376
H	5.040148	-1.266118	-1.891670
H	5.270903	0.205440	-2.838211

H 5.990991 0.063185 -1.222075

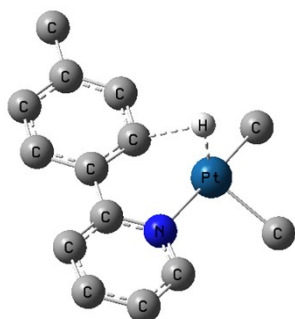
[PtMe₂(Htpy- κ^1 N)], IM3



Zero-point correction= 0.269121 (Hartree/Particle)
 Thermal correction to Energy= 0.286509
 Thermal correction to Enthalpy= 0.287453
 Thermal correction to Gibbs Free Energy= 0.220475
 Sum of electronic and zero-point Energies= -717.378764
 Sum of electronic and thermal Energies= -717.361376
 Sum of electronic and thermal Enthalpies= -717.360432
 Sum of electronic and thermal Free Energies= -717.427410

Pt	1.078107	-0.942083	-0.127592	C	0.740377	4.071650	-0.025012
C	2.932358	-1.071761	0.674467	H	-1.394302	3.750467	-0.060621
H	2.985398	-0.429325	1.563430	C	-2.536063	1.233720	-0.888642
H	3.175460	-2.099745	0.962277	C	-1.762580	0.112144	1.104164
H	3.671887	-0.730251	-0.063184	H	0.673254	5.153553	-0.086902
C	1.117305	-2.942232	-0.529900	C	-3.695223	0.459174	-0.870676
H	0.178625	-3.215439	-1.041109	H	-2.385847	1.958757	-1.684100
H	1.951513	-3.225114	-1.188200	C	-2.930523	-0.650906	1.119759
H	1.191152	-3.555030	0.380237	H	-1.022259	-0.016972	1.887323
N	0.894226	1.280753	0.132196	H	-4.438507	0.595172	-1.652568
C	2.003875	2.045609	0.136387	C	-3.914277	-0.496661	0.132465
C	-0.315202	1.896657	0.068782	H	-3.079568	-1.377236	1.915099
H	2.945058	1.511385	0.189459	C	-5.183295	-1.315837	0.161656
C	1.977054	3.433671	0.063104	H	-5.027893	-2.275991	0.664019
C	-0.412295	3.291959	-0.018811	H	-5.980778	-0.789158	0.702572
C	-1.546167	1.063438	0.092202	H	-5.554113	-1.513609	-0.849567
H	2.906943	3.991998	0.068996				

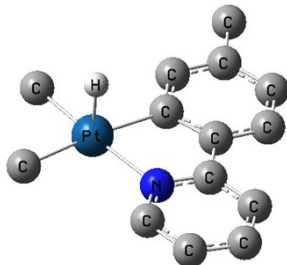
[Me₂Pt...H...tpy- κ^1 N)], TS4



Zero-point correction=	0.267645 (Hartree/Particle)
Thermal correction to Energy=	0.284388
Thermal correction to Enthalpy=	0.285332
Thermal correction to Gibbs Free Energy=	0.222292
Sum of electronic and zero-point Energies=	-717.358532
Sum of electronic and thermal Energies=	-717.341789
Sum of electronic and thermal Enthalpies=	-717.340845
Sum of electronic and thermal Free Energies=	-717.403885

Pt	1.065496	-0.236781	-0.047904	H	-3.228216	2.584666	-0.093303
C	2.882019	0.696478	0.491727	H	-1.414913	4.640374	-0.099985
H	2.980123	1.683156	0.021935	N	-1.467849	1.382184	-0.024733
H	2.843221	0.852323	1.582038	C	-1.912428	0.029936	0.002987
H	3.776689	0.106234	0.271265	C	-0.926961	-0.970907	-0.109851
C	2.128804	-2.005644	-0.043108	C	-3.265360	-0.273033	0.172512
H	2.504466	-2.178795	0.973006	C	-1.359106	-2.300393	-0.085880
H	1.502834	-2.853365	-0.339187	C	-3.661568	-1.610551	0.205657
H	2.987205	-1.948286	-0.720351	H	-4.004770	0.512968	0.289255
N	-0.128469	1.612186	-0.006256	C	-2.710319	-2.624405	0.077241
C	0.032933	2.936032	-0.034573	H	-0.633192	-3.101157	-0.194013
C	-2.150139	2.557262	-0.065029	H	-4.712288	-1.853383	0.332927
C	-1.217265	3.579485	-0.070433	H	-3.018589	-3.666126	0.100152
H	1.027780	3.357316	-0.025996	H	0.411518	-0.713177	-1.391779

[PtMe₂(H)(tpy)], IM4

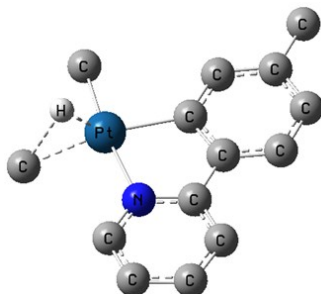


Zero-point correction=	0.268820 (Hartree/Particle)
Thermal correction to Energy=	0.285871
Thermal correction to Enthalpy=	0.286815

Thermal correction to Gibbs Free Energy= 0.223192
 Sum of electronic and zero-point Energies= -717.360638
 Sum of electronic and thermal Energies= -717.343587
 Sum of electronic and thermal Enthalpies= -717.342643
 Sum of electronic and thermal Free Energies= -717.406266

Pt	-0.619116	-1.074401	-0.00285	H	-2.196436	4.784443	0.005524
C	0.17613	-2.978088	-0.035458	C	-2.968209	2.765502	-0.01902
H	1.168553	-3.008405	0.423206	H	-3.336569	0.63333	-0.035663
H	-0.470724	-3.708959	0.456943	H	-4.016942	3.04084	-0.028861
H	0.267052	-3.24854	-1.098107	N	-1.314539	1.031787	-0.012404
C	1.214949	-0.011938	0.009715	H	0.164231	4.058172	0.023268
C	1.063789	1.401982	0.004035	H	2.088985	3.321147	-0.002879
C	2.522615	-0.513424	0.013026	C	5.051097	-0.284213	-0.028521
C	2.193634	2.239612	-0.001349	H	5.05313	-1.31779	0.332939
C	-0.307648	1.948739	0.001203	H	5.456974	-0.293939	-1.049396
C	3.661112	0.307668	0.000544	H	5.748135	0.29582	0.586999
H	2.680295	-1.591112	0.025173	H	-0.598427	-1.211435	1.514617
C	3.475134	1.698315	-0.001786	C	-2.574782	-1.929339	-0.037597
C	-0.625746	3.317132	0.009477	H	-3.220019	-1.503496	0.743041
H	4.338496	2.359917	-0.002585	H	-3.035916	-1.696172	-1.011071
C	-1.954335	3.72577	-0.000583	H	-2.581229	-3.018483	0.085222
C	-2.5972	1.426523	-0.023562				

[Me(tpy)Pt...Me...H], TS5

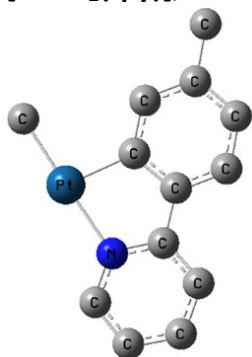


Zero-point correction= 0.268295 (Hartree/Particle)
 Thermal correction to Energy= 0.284937
 Thermal correction to Enthalpy= 0.285881
 Thermal correction to Gibbs Free Energy= 0.223044
 Sum of electronic and zero-point Energies= -717.358145
 Sum of electronic and thermal Energies= -717.341504
 Sum of electronic and thermal Enthalpies= -717.340560
 Sum of electronic and thermal Free Energies= -717.403397

Pt	-0.588597	-1.087203	-0.044599	H	0.921167	-3.018797	0.879698
C	0.373686	-2.914144	-0.066409	H	-0.323586	-3.751446	-0.166196

H	1.096462	-2.955039	-0.888644	H	-3.367985	0.548524	-0.070765
C	1.203054	0.022474	-0.030769	H	-4.109286	2.931679	-0.045568
C	1.011253	1.430509	0.012313	N	-1.354769	0.993070	-0.029351
C	2.522511	-0.447456	-0.022157	H	0.042332	4.058701	0.045394
C	2.117835	2.295847	0.056538	H	1.986080	3.373756	0.085296
C	-0.375233	1.939119	0.001722	H	-1.419403	-1.600338	-1.254706
C	3.638398	0.402473	0.026491	C	5.043270	-0.152279	0.063711
H	2.703676	-1.520383	-0.054758	H	5.425024	-0.195459	1.092966
C	3.412991	1.786514	0.061829	H	5.082222	-1.168809	-0.341164
C	-0.728089	3.297718	0.019152	H	5.737631	0.472427	-0.509386
H	4.257917	2.470727	0.094238	C	-2.455972	-2.034554	0.453383
C	-2.067077	3.672490	0.003497	H	-3.348424	-1.600941	-0.007707
C	-2.646039	1.356801	-0.046388	H	-2.449444	-3.110322	0.261980
H	-2.337039	4.724238	0.017916	H	-2.486622	-1.854745	1.536409
C	-3.053380	2.685579	-0.031387				

[PtMe₂(tpy)], IM5



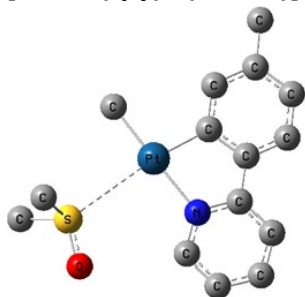
Zero-point correction=	0.221873 (Hartree/Particle)
Thermal correction to Energy=	0.235780
Thermal correction to Enthalpy=	0.236725
Thermal correction to Gibbs Free Energy=	0.179283
Sum of electronic and zero-point Energies=	-676.925653
Sum of electronic and thermal Energies=	-676.911745
Sum of electronic and thermal Enthalpies=	-676.910801
Sum of electronic and thermal Free Energies=	-676.968243

Pt	0.214942	-1.308666	-0.000386	C	1.154713	1.517241	0.000082
C	-1.230386	-2.774210	-0.000983	C	-3.132249	1.401941	-0.006354
H	-1.873015	-2.734797	-0.890692	H	-2.879066	-0.726449	-0.008109
H	-0.727878	-3.757399	0.000712	C	-2.471126	2.640949	-0.010019
H	-1.875692	-2.733131	0.886692	C	1.982676	2.648147	0.001901
C	-0.963600	0.259982	-0.001619	H	-3.049197	3.561663	-0.016499
C	-0.312594	1.524422	-0.001695	C	3.365068	2.491094	0.003811
C	-2.365289	0.228592	-0.005158	C	3.036360	0.122034	0.002541
C	-1.082180	2.699464	-0.006654	H	4.011007	3.363956	0.005208

C	3.909671	1.204401	0.004010
H	3.399360	-0.901436	0.002901
H	4.981426	1.039835	0.005436
N	1.702792	0.271428	0.000694
H	1.548078	3.641076	0.002161
H	-0.596402	3.671342	-0.011493

C	-4.641734	1.334219	0.015000
H	-5.001273	0.334872	-0.249517
H	-5.033799	1.573095	1.012630
H	-5.084536	2.053661	-0.683345
Pt	0.214942	-1.308666	-0.000386

[PtMe₂(tpy)...(DMSO)], TS6

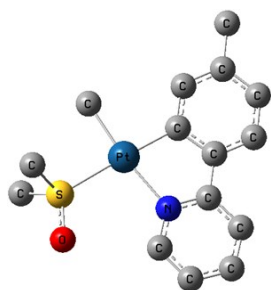


Zero-point correction=	0.305327 (Hartree/Particle)
Thermal correction to Energy=	0.326380
Thermal correction to Enthalpy=	0.327324
Thermal correction to Gibbs Free Energy=	0.250547
Sum of electronic and zero-point Energies	-1230.057624
Sum of electronic and thermal Energies=	-1230.036571
Sum of electronic and thermal Enthalpies=	-1230.035627
Sum of electronic and thermal Free Energies=	-1230.112404

Pt	1.065496	-0.236781	-0.047904
C	2.882019	0.696478	0.491727
H	2.980123	1.683156	0.021935
H	2.843221	0.852323	1.582038
H	3.776689	0.106234	0.271265
C	2.128804	-2.005644	-0.043108
H	2.504466	-2.178795	0.973006
H	1.502834	-2.853365	-0.339187
H	2.987205	-1.948286	-0.720351
N	-0.128469	1.612186	-0.006256
C	0.032933	2.936032	-0.034573
C	-2.150139	2.557262	-0.065029
C	-1.217265	3.579485	-0.070433
H	1.027780	3.357316	-0.025996

H	-3.228216	2.584666	-0.093303
H	-1.414913	4.640374	-0.099985
N	-1.467849	1.382184	-0.024733
C	-1.912428	0.029936	0.002987
C	-0.926961	-0.970907	-0.109851
C	-3.265360	-0.273033	0.172512
C	-1.359106	-2.300393	-0.085880
C	-3.661568	-1.610551	0.205657
H	-4.004770	0.512968	0.289255
C	-2.710319	-2.624405	0.077241
H	-0.633192	-3.101157	-0.194013
H	-4.712288	-1.853383	0.332927
H	-3.018589	-3.666126	0.100152
H	0.411518	-0.713177	-1.391779

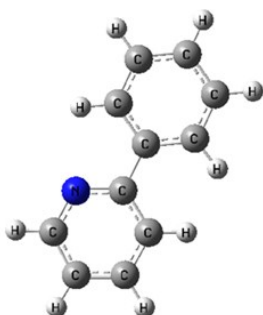
[PtMe₂(tpy)(DMSO)], 2



Zero-point correction= 0.307562 (Hartree/Particle)
 Thermal correction to Energy= 0.328465
 Thermal correction to Enthalpy= 0.329409
 Thermal correction to Gibbs Free Energy= 0.256344
 Sum of electronic and zero-point Energies= -1230.069750
 Sum of electronic and thermal Energies= -1230.048847
 Sum of electronic and thermal Enthalpies= -1230.047903
 Sum of electronic and thermal Free Energies= -1230.120968

Pt	-0.423325	-0.494263	0.007610	H	-1.996042	2.322696	-0.064070
C	-0.499932	-2.565535	0.090336	H	-1.384738	4.748963	-0.024401
H	0.050774	-2.924593	0.968820	N	-0.042454	1.659269	-0.026667
H	-1.510338	-2.989425	0.152171	H	2.747617	3.553867	0.057272
H	-0.026464	-2.996707	-0.801439	H	4.047205	1.931491	0.015935
C	1.597437	-0.482454	0.004492	S	-2.872949	-0.411259	-0.020240
C	2.190472	0.809574	0.006955	O	-3.579260	0.929057	-0.098232
C	2.459828	-1.587837	-0.004731	C	-3.572011	-1.292163	1.408769
C	3.588808	0.946746	0.008299	H	-4.660525	-1.300165	1.311228
C	1.284614	1.967082	0.003992	H	-3.170778	-2.306236	1.451644
C	3.856826	-1.461105	-0.010719	H	-3.269726	-0.731479	2.295418
H	2.044478	-2.590624	-0.006175	C	-3.521547	-1.430240	-1.379384
C	4.412330	-0.173156	0.001448	H	-4.612355	-1.445514	-1.313531
C	1.692692	3.308383	0.028753	H	-3.199321	-0.949956	-2.305355
H	5.492617	-0.048354	0.004530	H	-3.105606	-2.437161	-1.315148
C	0.743947	4.324939	0.019912	C	4.746055	-2.682394	-0.051618
C	-0.959307	2.643688	-0.037369	H	4.208348	-3.580779	0.268163
H	1.058956	5.364090	0.040751	H	5.118166	-2.867060	-1.068568
C	-0.609986	3.989980	-0.015349	H	5.624195	-2.560764	0.592778

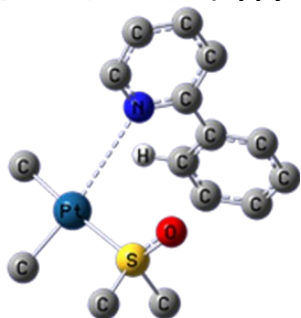
Hppy



Zero-point correction= 0.170107 (Hartree/Particle)
 Thermal correction to Energy= 0.178033
 Thermal correction to Enthalpy= 0.178977
 Thermal correction to Gibbs Free Energy= 0.136911
 Sum of electronic and zero-point Energies= -479.180016
 Sum of electronic and thermal Energies= -479.172090
 Sum of electronic and thermal Enthalpies= -479.171145
 Sum of electronic and thermal Free Energies= -479.213212

C	-3.526767	-0.098931	-0.000354	C	1.480510	1.220036	0.000200
C	-2.703268	-1.225179	-0.000264	H	-4.607067	-0.202427	-0.000461
C	-0.765415	0.036599	-0.000083	H	-3.138950	-2.223430	-0.000302
C	-1.520077	1.222876	-0.000168	H	-3.501968	2.062770	-0.000372
C	-2.910395	1.151543	-0.000304	H	4.635781	-0.064912	0.000467
C	0.726262	0.033133	0.000074	H	3.433335	2.116398	0.000438
C	1.420510	-1.190135	0.000098	N	-1.368519	-1.170839	-0.000131
C	2.813315	-1.225753	0.000237	H	0.848015	-2.110523	0.000000
H	3.325264	-2.184506	0.000249	H	-1.037907	2.193354	-0.000135
C	3.549569	-0.038267	0.000360	H	0.989473	2.187529	0.000195
C	2.874698	1.184347	0.000342				

[PtMe₂(DMSO)... (Hppy- κ^1 N)], TS2

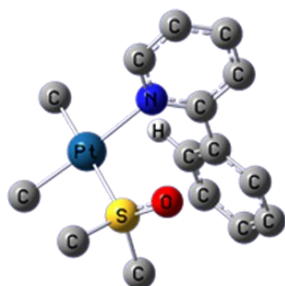


Zero-point correction= 0.326088 (Hartree/Particle)
 Thermal correction to Energy= 0.348381
 Thermal correction to Enthalpy= 0.349325
 Thermal correction to Gibbs Free Energy= 0.270506
 Sum of electronic and zero-point Energies= -1231.211616

Sum of electronic and thermal Energies= -1231.189324
 Sum of electronic and thermal Enthalpies= -1231.188379
 Sum of electronic and thermal Free Energies= -1231.267198

Pt	1.473427	-0.539243	-0.441139	C	-1.771343	-2.699970	0.482358
C	1.411251	-1.881990	-1.982147	C	-2.811652	-0.666048	0.124205
H	0.397103	-2.304643	-2.020233	H	-0.851339	-3.275635	0.405457
H	1.627302	-1.401911	-2.946156	C	-2.928040	-3.278336	1.005824
H	2.128637	-2.701411	-1.842386	C	-4.022164	-1.174597	0.624831
C	3.461694	-0.281141	-0.782573	C	-2.703838	0.732031	-0.371921
H	3.687976	0.788532	-0.881400	H	-2.923723	-4.310008	1.342308
H	4.027790	-0.694574	0.061998	C	-4.077568	-2.491459	1.074308
H	3.769940	-0.792101	-1.699245	H	-4.911254	-0.553650	0.639667
S	1.418604	1.029543	1.446658	C	-3.503475	1.759522	0.156852
O	0.256953	0.925000	2.412372	C	-1.791798	1.048226	-1.393277
C	2.951488	0.995764	2.427340	H	-5.007243	-2.898234	1.461967
H	3.808082	1.176350	1.774246	C	-3.394380	3.065570	-0.322419
H	2.883848	1.759345	3.206470	H	-4.196549	1.546431	0.965462
H	3.022910	0.001604	2.873007	C	-1.686238	2.353368	-1.875153
C	1.496332	2.750554	0.858698	H	-1.172475	0.258849	-1.805529
H	0.598458	2.920553	0.260657	H	-4.013973	3.848542	0.106059
H	1.516798	3.421881	1.721464	C	-2.487273	3.367759	-1.341403
H	2.387433	2.879734	0.239283	H	-0.983309	2.576852	-2.673348
N	-1.704283	-1.433994	0.053833	H	-2.404993	4.384218	-1.716375

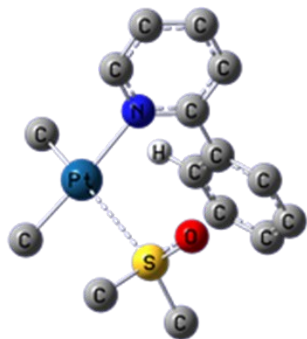
[PtMe₂(Hppy- κ^1N)(DMSO)], IM2



Zero-point correction= 0.327396 (Hartree/Particle)
 Thermal correction to Energy= 0.349660
 Thermal correction to Enthalpy= 0.350604
 Thermal correction to Gibbs Free Energy= 0.274598
 Sum of electronic and zero-point Energies= -1231.228306
 Sum of electronic and thermal Energies= -1231.206042
 Sum of electronic and thermal Enthalpies= -1231.205098
 Sum of electronic and thermal Free Energies= -1231.281104

Pt	-1.162661	0.255984	-0.518385	C	0.334214	2.761339	0.382307
C	-1.388600	1.311411	-2.274155	C	1.901706	1.059758	0.140863
H	-0.707621	2.171764	-2.297920	H	-0.701866	3.056633	0.258088
H	-1.161985	0.666809	-3.134835	C	1.276240	3.644318	0.896442
H	-2.417277	1.674940	-2.393207	C	2.900194	1.899667	0.656645
C	-2.867665	-0.785105	-1.040987	C	2.253021	-0.315360	-0.300926
H	-2.772765	-1.862872	-0.840654	H	0.979904	4.650243	1.173161
H	-3.734870	-0.416305	-0.473120	C	2.589367	3.198982	1.043699
H	-3.098629	-0.670168	-2.106404	H	3.916580	1.528491	0.727287
S	-0.951824	-0.977411	1.580431	C	3.018481	-1.145103	0.533953
O	0.022272	-0.500249	2.637372	C	1.878402	-0.785682	-1.570727
C	-2.577878	-1.139918	2.382799	H	3.359458	3.854065	1.439603
H	-3.287389	-1.583519	1.681205	C	3.386215	-2.425986	0.117030
H	-2.465791	-1.757977	3.277311	H	3.303896	-0.794835	1.521670
H	-2.899831	-0.131933	2.652204	C	2.256068	-2.062311	-1.989383
C	-0.610771	-2.740737	1.280047	H	1.307136	-0.143216	-2.231727
H	0.387892	-2.799610	0.842601	H	3.967521	-3.061475	0.779171
H	-0.642972	-3.275085	2.233406	C	3.005520	-2.887643	-1.145758
H	-1.352492	-3.136629	0.582565	H	1.968571	-2.410579	-2.977572
N	0.624143	1.495967	0.019559	H	3.295001	-3.882503	-1.472707

[PtMe₂(Hppy- κ^1 N)...(DMSO)], TS3



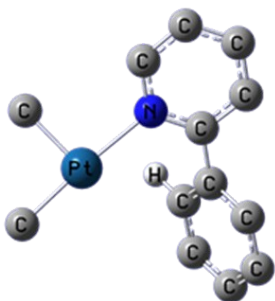
Zero-point correction=	0.325312 (Hartree/Particle)
Thermal correction to Energy=	0.347809
Thermal correction to Enthalpy=	0.348754
Thermal correction to Gibbs Free Energy=	0.269793
Sum of electronic and zero-point Energies=	-1231.215574
Sum of electronic and thermal Energies=	-1231.193076
Sum of electronic and thermal Enthalpies=	-1231.192132
Sum of electronic and thermal Free Energies=	-1231.271093

Pt	-1.359613	-0.145432	-0.508943	H	-3.517947	0.544015	-1.851419
C	-3.031181	0.917128	-0.943939	H	-3.739489	0.834763	-0.107925
H	-2.764864	1.972307	-1.085820	C	-2.240155	-1.813702	-1.310101

H	-1.547416	-2.667645	-1.231987
H	-3.169621	-2.090814	-0.791438
H	-2.482156	-1.680414	-2.374529
S	0.758522	-1.962865	1.490072
O	1.672693	-1.286069	2.503457
C	-0.492557	-2.899454	2.433359
H	-1.101722	-3.485175	1.739480
H	0.004924	-3.547883	3.160178
H	-1.121614	-2.168952	2.947220
C	1.660405	-3.402660	0.816592
H	2.499975	-3.011627	0.237242
H	2.025377	-4.025787	1.638078
H	0.992479	-3.970890	0.162984
N	-0.323018	1.584684	0.457262
C	-1.028487	2.300629	1.356665
C	1.016233	1.790669	0.371854
H	-2.093912	2.102109	1.383195
C	-0.452863	3.227005	2.218275

C	1.660551	2.701995	1.220367
C	1.806222	1.050141	-0.649191
H	-1.074864	3.768862	2.922483
C	0.926229	3.424149	2.155817
H	2.730736	2.847300	1.122240
C	2.971977	0.363717	-0.272930
C	1.436431	1.075125	-2.004473
H	1.419010	4.133491	2.813736
C	3.744954	-0.295463	-1.231483
H	3.244436	0.311422	0.776517
C	2.217368	0.424967	-2.961415
H	0.549427	1.622329	-2.306869
H	4.638621	-0.832313	-0.925308
C	3.371195	-0.264422	-2.577520
H	1.927091	0.462812	-4.007717
H	3.976612	-0.771520	-3.323712

[PtMe₂(Hppy- κ^1 N)], IM3



Zero-point correction=	0.241728 (Hartree/Particle)
Thermal correction to Energy=	0.257185
Thermal correction to Enthalpy=	0.258129
Thermal correction to Gibbs Free Energy=	0.196381
Sum of electronic and zero-point Energies=	-678.088084
Sum of electronic and thermal Energies=	-678.072628
Sum of electronic and thermal Enthalpies=	-678.071683
Sum of electronic and thermal Free Energies=	-678.133432

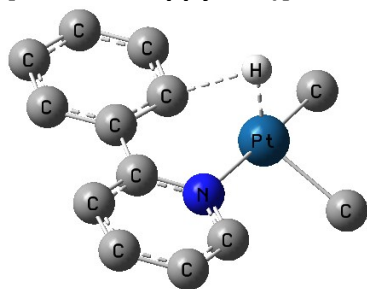
Pt	1.243322	-0.43253	-0.13607
C	2.87185	0.410435	0.72315
H	2.556499	1.008525	1.588133
H	3.58596	-0.34947	1.056422
H	3.371559	1.063424	-0.00596
C	2.341294	-2.11257	-0.52316

H	1.705358	-2.83281	-1.06541
H	3.222641	-1.90829	-1.14794
H	2.692039	-2.60602	0.394814
N	-0.05761	1.363016	0.123507
C	0.503298	2.588963	0.113597
C	-1.41104	1.271347	0.068196

H	1.585431	2.613566	0.159426
C	-0.23142	3.766145	0.034304
C	-2.21049	2.418931	-0.02299
C	-2.04445	-0.07439	0.108266
H	0.281501	4.721835	0.027473
C	-1.62064	3.6793	-0.04425
H	-3.28892	2.3096	-0.05645
C	-3.00876	-0.42222	-0.85195
C	-1.73992	-0.9904	1.130855

H	-2.23314	4.573221	-0.11099
C	-3.64245	-1.66484	-0.80277
H	-3.24985	0.277591	-1.64737
C	-2.38224	-2.22898	1.182285
H	-1.01554	-0.72052	1.892331
H	-4.37807	-1.92435	-1.5588
C	-3.33103	-2.57043	0.214852
H	-2.14657	-2.92301	1.984144
H	-3.82872	-3.53523	0.256696

[Me₂Pt...H...ppy- κ^1 N)], TS4

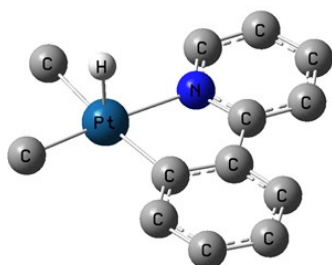


Zero-point correction=	0.240478 (Hartree/Particle)
Thermal correction to Energy=	0.255180
Thermal correction to Enthalpy=	0.256125
Thermal correction to Gibbs Free Energy=	0.198490
Sum of electronic and zero-point Energies=	-678.067869
Sum of electronic and thermal Energies=	-678.053167
Sum of electronic and thermal Enthalpies=	-678.052223
Sum of electronic and thermal Free Energies=	-678.109857

Pt	-1.13371	-0.1876	-0.05212
C	-2.26361	-1.89171	0.54241
H	-1.87596	-2.22319	1.51912
H	-3.33907	-1.71568	0.64624
H	-2.118	-2.721	-0.16286
C	-2.92712	0.841246	-0.05124
H	-2.81974	1.843701	-0.477
H	-3.69573	0.298328	-0.61015
H	-3.25925	0.929901	0.991194
N	0.820242	-1.24188	-0.00915
C	0.993371	-2.57226	-0.02708
C	1.896267	-0.41053	-0.01257
H	0.088515	-3.16936	-0.01539
C	2.252088	-3.16194	-0.05145
C	3.191764	-0.9474	-0.04028

C	1.583021	1.031291	0.009512
H	2.346358	-4.24204	-0.06549
C	3.370598	-2.32651	-0.0595
H	4.052841	-0.29014	-0.05604
C	2.576261	2.010695	0.183778
C	0.223756	1.414063	-0.11481
H	4.372505	-2.7443	-0.08372
C	2.239577	3.362258	0.215046
H	3.61657	1.726086	0.311528
C	-0.08991	2.776507	-0.10038
H	3.015451	4.110295	0.350852
C	0.903849	3.745912	0.070406
H	-1.12158	3.097012	-0.21535
H	0.63554	4.799458	0.087723
H	-0.91002	0.397377	-1.47417

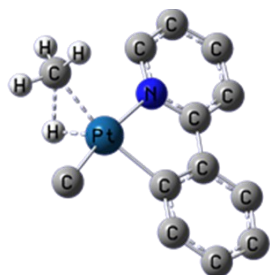
[PtMe₂(H)(ppy)], IM4



Zero-point correction=	0.241386 (Hartree/Particle)
Thermal correction to Energy=	0.256542
Thermal correction to Enthalpy=	0.257487
Thermal correction to Gibbs Free Energy=	0.198583
Sum of electronic and zero-point Energies=	-678.070413
Sum of electronic and thermal Energies=	-678.055257
Sum of electronic and thermal Enthalpies=	-678.054313
Sum of electronic and thermal Free Energies=	-678.113216

Pt	-1.156646	-0.057597	-0.001306	C	1.696269	0.850522	0.002170
C	-2.542568	-1.676639	-0.037908	H	1.824941	-4.488554	-0.024927
H	-2.300487	-2.444798	0.709660	C	3.067063	-2.705681	0.002758
H	-3.581566	-1.369984	0.129279	H	3.987000	-0.769277	0.025864
H	-2.487533	-2.153638	-1.030259	C	2.825289	1.689753	-0.012854
C	-2.722623	1.279723	-0.050276	C	0.380730	1.392490	0.009259
H	-2.504092	2.176286	0.537025	H	4.013651	-3.237895	0.009795
H	-2.838115	1.568896	-1.105523	C	2.674603	3.074553	-0.019447
H	-3.660687	0.841217	0.300324	H	3.829655	1.276026	-0.022275
N	0.665376	-1.327067	-0.009863	C	0.269963	2.790535	0.005618
C	0.680149	-2.668800	-0.020195	H	-1.297949	-0.001978	1.515093
C	1.830422	-0.622454	0.002149	H	3.551822	3.715745	-0.031404
H	-0.289827	-3.152994	-0.031755	C	1.390869	3.626962	-0.011448
C	1.858855	-3.404825	-0.015626	H	-0.715974	3.250803	0.012968
C	3.051765	-1.315379	0.011596	H	1.265206	4.707600	-0.017727

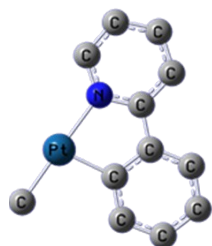
[Me(ppy)Pt...Me...H], TS5



Zero-point correction=	0.240780 (Hartree/Particle)
Thermal correction to Energy=	0.255597
Thermal correction to Enthalpy=	0.256541
Thermal correction to Gibbs Free Energy=	0.198128
Sum of electronic and zero-point Energies=	-678.067908
Sum of electronic and thermal Energies=	-678.053091
Sum of electronic and thermal Enthalpies=	-678.052147
Sum of electronic and thermal Free Energies=	-678.110559

Pt	1.143432	-0.137301	-0.043300	H	-3.266393	3.949299	0.116890
C	2.749740	1.157314	-0.050442	C	-3.251613	-2.490652	-0.004443
H	2.735936	1.720074	0.892299	C	-0.867906	-2.622246	-0.050720
H	3.706361	0.632460	-0.134441	H	-4.233738	-2.953714	0.006239
H	2.664622	1.869805	-0.878241	C	-2.096547	-3.272650	-0.039197
C	-0.279838	1.404482	-0.012455	H	0.061806	-3.179166	-0.075616
C	-1.629517	0.956723	0.021728	H	-2.139190	-4.355960	-0.056517
C	-0.063807	2.790089	0.004810	N	-0.754152	-1.285908	-0.029610
C	-2.692205	1.876039	0.067553	H	-4.027845	-0.491532	0.042946
C	-1.868037	-0.503137	0.003665	H	-3.724115	1.538346	0.094852
C	-1.119524	3.705907	0.049826	H	1.809288	-0.876699	-1.241225
H	0.953653	3.173165	-0.016749	C	2.443636	-1.793681	0.424649
C	-2.438541	3.246364	0.080892	H	2.166534	-2.757136	-0.013079
C	-3.135448	-1.104738	0.016368	H	3.493515	-1.593133	0.198833
H	-0.916125	4.774301	0.062007	H	2.304729	-1.838160	1.513051

[PtMe₂(ppy)], IM5

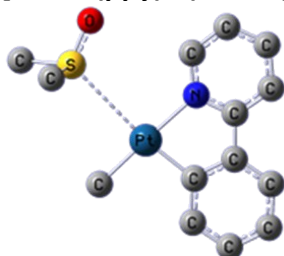


Zero-point correction=	0.194409 (Hartree/Particle)
Thermal correction to Energy=	0.206356
Thermal correction to Enthalpy=	0.207300
Thermal correction to Gibbs Free Energy=	0.155030

Sum of electronic and zero-point Energies= -637.635325
 Sum of electronic and thermal Energies= -637.623378
 Sum of electronic and thermal Enthalpies= -637.622434
 Sum of electronic and thermal Free Energies= -637.674704

Pt	0.763960	-0.985540	-0.000020	C	-3.028490	1.112907	0.000103
C	2.797489	-1.287838	0.000111	H	2.681869	3.797982	0.000198
H	3.287839	-0.869163	0.889139	H	0.433727	4.874645	-0.000093
H	2.985531	-2.375894	-0.000022	C	-4.039450	0.156611	0.000148
H	3.287962	-0.868927	-0.888733	C	-2.352806	-1.539334	-0.000054
C	0.762329	0.974425	-0.000029	H	-5.080225	0.466228	0.000235
C	-0.518325	1.596652	-0.000075	C	-3.701398	-1.198635	0.000061
C	1.901911	1.793308	0.000130	H	-2.027985	-2.575510	-0.000141
C	-0.619671	2.997422	-0.000146	H	-4.459251	-1.974143	0.000061
C	-1.687813	0.706276	-0.000042	N	-1.376946	-0.618426	-0.000102
C	1.783366	3.185616	0.000091	H	-3.278406	2.167536	0.000175
H	2.888984	1.345768	0.000284	H	-1.595677	3.474273	-0.000232
C	0.523753	3.792304	-0.000068				

[PtMe₂(ppy)...(DMSO)], TS6

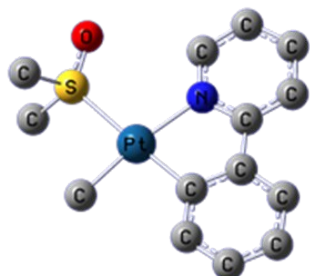


Zero-point correction= 0.277634 (Hartree/Particle)
 Thermal correction to Energy= 0.296871
 Thermal correction to Enthalpy= 0.297815
 Thermal correction to Gibbs Free Energy= 0.226827
 Sum of electronic and zero-point Energies= -1190.767666
 Sum of electronic and thermal Energies= -1190.748429
 Sum of electronic and thermal Enthalpies= -1190.747485
 Sum of electronic and thermal Free Energies= -1190.818473

Pt	0.076011	-0.704998	0.192383	C	-1.808209	1.598647	-0.019689
C	0.517100	-2.713989	0.317287	C	-3.974720	-2.065017	-0.317070
H	0.307971	-3.249092	-0.619465	H	-2.063474	-3.018188	-0.103239
H	1.590950	-2.834968	0.534926	C	-4.678458	-0.859017	-0.381326
H	-0.039681	-3.213127	1.121592	C	-2.329896	2.898530	-0.049915
C	-1.869093	-0.869085	-0.045883	H	-4.507281	-3.009719	-0.396112
C	-2.590215	0.356898	-0.117508	H	-5.757037	-0.855720	-0.509370
C	-2.586785	-2.070088	-0.151199	C	-1.470557	3.988841	0.049975
C	-3.984799	0.344327	-0.282596	C	0.363237	2.455262	0.201049

H	-1.868956	4.998811	0.028710	C	3.894149	-0.314812	-1.838428
C	-0.097927	3.768236	0.176245	H	4.912239	0.034658	-2.031381
H	1.423605	2.229988	0.288238	H	3.821661	-1.398158	-1.968130
H	0.605405	4.590235	0.253601	H	3.190186	0.184504	-2.507890
N	-0.468434	1.403906	0.107986	C	4.747761	-0.776461	0.730254
H	-3.397480	3.056393	-0.148815	H	5.716782	-0.407151	0.383063
H	-4.536429	1.278499	-0.337281	H	4.629779	-0.579499	1.798141
S	3.411132	0.117258	-0.133403	H	4.646518	-1.847989	0.537135
O	3.663472	1.609159	0.052717				

[PtMe₂(ppy)(DMSO)], 3



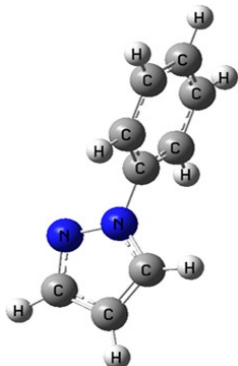
Zero-point correction=	0.280229 (Hartree/Particle)
Thermal correction to Energy=	0.299168
Thermal correction to Enthalpy=	0.300113
Thermal correction to Gibbs Free Energy=	0.231636
Sum of electronic and zero-point Energies=	-1190.779453
Sum of electronic and thermal Energies=	-1190.760514
Sum of electronic and thermal Enthalpies=	-1190.759570
Sum of electronic and thermal Free Energies=	-1190.828046

Pt	-0.401040	-0.509489	0.000468	C	2.088921	3.776288	0.000971
C	-1.064145	-2.476927	0.003191	C	-0.021891	2.647085	-0.000693
H	-0.681492	-2.999578	0.889145	H	2.686156	4.683289	0.001680
H	-2.154562	-2.600190	0.006453	C	0.695492	3.839013	0.000117
H	-0.686529	-3.000573	-0.884385	H	-1.107411	2.631359	-0.001520
C	1.538511	-1.074829	0.000160	H	0.167813	4.786614	0.000096
C	2.479141	-0.007235	-0.000106	N	0.578914	1.443746	-0.000657
C	2.050239	-2.381551	-0.000434	H	3.792182	2.468830	0.001576
C	3.860431	-0.265724	-0.000851	H	4.574645	0.552509	-0.001162
C	1.938486	1.362198	0.000071	S	-2.722344	0.264951	-0.001151
C	3.425486	-2.633199	-0.001197	O	-3.018081	1.753018	-0.005198
H	1.371288	-3.227575	-0.000376	C	-3.636656	-0.451985	1.397476
C	4.336343	-1.574084	-0.001370	H	-4.685213	-0.154848	1.316398
C	2.710615	2.531944	0.000903	H	-3.530299	-1.538105	1.389321
H	3.785355	-3.659516	-0.001696	H	-3.188934	-0.038396	2.303220
H	5.406026	-1.763990	-0.001989	C	-3.636609	-0.459516	-1.395950

H	-4.685268	-0.162436	-1.316141
H	-3.189256	-0.050217	-2.303822

H	-3.529779	-1.545526	-1.382389
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Hppz

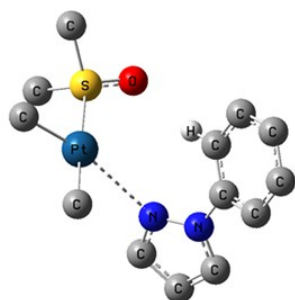


Zero-point correction=	0.151852 (Hartree/Particle)
Thermal correction to Energy=	0.159184
Thermal correction to Enthalpy=	0.160128
Thermal correction to Gibbs Free Energy=	0.119180
Sum of electronic and zero-point Energies=	-457.102694
Sum of electronic and thermal Energies=	-457.095363
Sum of electronic and thermal Enthalpies=	-457.094418
Sum of electronic and thermal Free Energies=	-457.135367

C	2.498057	-1.210584	-0.007312
C	1.102270	-1.214295	0.004898
C	0.412458	-0.000018	0.012763
C	1.102244	1.214284	0.006048
C	2.498027	1.210617	-0.006170
C	3.195615	0.000025	-0.012425
H	3.038725	-2.152525	-0.013021
H	0.545886	-2.146489	0.006751
H	0.545832	2.146460	0.008792
H	3.038679	2.152572	-0.010980

H	4.281855	0.000046	-0.021605
N	-1.020863	-0.000038	0.025162
C	-1.836990	-0.001052	1.116001
C	-3.001017	0.000458	-0.759179
C	-3.136294	-0.000359	0.646054
H	-1.429890	-0.001955	2.116864
H	-3.780830	0.001007	-1.510524
H	-4.044212	-0.000689	1.231726
N	-1.722318	0.001054	-1.141173

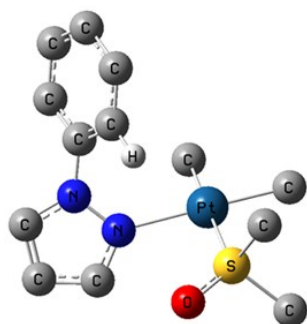
[PtMe₂(DMSO)... (Hppz- κ^1N)], TS2



Zero-point correction=	0.308357 (Hartree/Particle)
Thermal correction to Energy=	0.329770
Thermal correction to Enthalpy=	0.330714
Thermal correction to Gibbs Free Energy=	0.254144
Sum of electronic and zero-point Energies=	-1209.140432
Sum of electronic and thermal Energies=	-1209.119019
Sum of electronic and thermal Enthalpies=	-1209.118075
Sum of electronic and thermal Free Energies=	-1209.194644

Pt	1.107585	-0.223359	-0.763730	N	-1.445491	-1.522191	0.641104
C	0.241891	-0.830856	-2.514141	C	-1.627805	-2.819118	0.886605
H	-0.797704	-1.117510	-2.301852	C	-3.653846	-1.956230	0.727380
H	0.239280	-0.033169	-3.268638	C	-2.998679	-3.149952	0.953343
H	0.763818	-1.699112	-2.938705	H	-0.767722	-3.465666	1.001966
C	2.797438	0.239883	-1.798545	H	-4.704829	-1.709571	0.714273
H	2.959243	1.324573	-1.757822	H	-3.444922	-4.114309	1.147021
H	3.658748	-0.272423	-1.349883	N	-2.696530	-1.000236	0.541162
H	2.712368	-0.065946	-2.845187	C	-2.891528	0.386315	0.285055
S	2.055417	0.463752	1.394088	C	-1.979570	1.321473	0.789500
O	1.083071	0.783461	2.514265	C	-3.997544	0.800972	-0.465408
C	3.215608	-0.791449	2.019884	C	-2.187649	2.678037	0.534849
H	3.984728	-0.981561	1.267191	H	-1.127852	0.991403	1.375137
H	3.657683	-0.435487	2.954254	C	-4.199059	2.162063	-0.698926
H	2.633037	-1.698282	2.193914	H	-4.682766	0.068320	-0.879597
C	3.199812	1.872505	1.254706	C	-3.295367	3.104761	-0.202924
H	2.611523	2.724554	0.908438	H	-1.482501	3.404888	0.928220
H	3.622806	2.076206	2.241614	H	-5.057868	2.480814	-1.282543
H	3.983946	1.640318	0.531320	H	-3.451965	4.162779	-0.391877

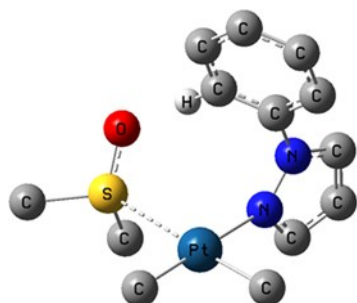
[PtMe₂(Hppz- κ^1 N)(DMSO)], IM2



Zero-point correction= 0.309097 (Hartree/Particle)
 Thermal correction to Energy= 0.330888
 Thermal correction to Enthalpy= 0.331832
 Thermal correction to Gibbs Free Energy= 0.255661
 Sum of electronic and zero-point Energies= -1209.154920
 Sum of electronic and thermal Energies= -1209.133129
 Sum of electronic and thermal Enthalpies= -1209.132185
 Sum of electronic and thermal Free Energies= -1209.208356

Pt	-0.747818	-0.330074	-0.696791	N	0.541830	1.404162	-0.191658
C	0.467865	-0.798776	-2.294049	C	0.209146	2.683011	-0.387851
H	1.242675	-0.034876	-2.430633	C	2.364837	2.677420	0.086016
H	0.959299	-1.766489	-2.126812	C	1.321473	3.527070	-0.226710
H	-0.117328	-0.875611	-3.219432	H	-0.811177	2.931453	-0.640485
C	-1.945298	-1.896965	-1.302966	H	3.399714	2.868827	0.327448
H	-2.336040	-2.481028	-0.456394	H	1.356935	4.602303	-0.316667
H	-2.808675	-1.517620	-1.869996	N	1.873685	1.407965	0.101045
H	-1.403888	-2.590904	-1.956214	C	2.599931	0.223132	0.431302
S	-2.254136	0.229130	1.142792	C	2.118027	-0.640404	1.419510
O	-2.042880	1.505775	1.929354	C	3.812631	-0.031191	-0.214634
C	-3.977074	0.233088	0.555364	C	2.855683	-1.777413	1.750067
H	-4.195155	-0.719568	0.068438	H	1.186593	-0.411820	1.924341
H	-4.639515	0.403910	1.407802	C	4.549527	-1.164512	0.134673
H	-4.062973	1.048768	-0.165407	H	4.165659	0.642739	-0.988944
C	-2.375380	-1.133903	2.345838	C	4.071101	-2.040901	1.111468
H	-1.398358	-1.225690	2.824443	H	2.485060	-2.450493	2.517525
H	-3.139907	-0.883463	3.086026	H	5.491531	-1.365320	-0.366835
H	-2.622687	-2.059664	1.821710	H	4.643826	-2.924811	1.376390

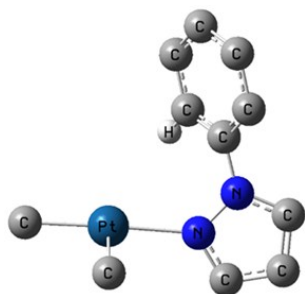
[PtMe₂(Hppz- κ^1 N)...(DMSO)], TS3



Zero-point correction=	0.307281 (Hartree/Particle)
Thermal correction to Energy=	0.329261
Thermal correction to Enthalpy=	0.330205
Thermal correction to Gibbs Free Energy=	0.251129
Sum of electronic and zero-point Energies=	-1209.144218
Sum of electronic and thermal Energies=	-1209.122239
Sum of electronic and thermal Enthalpies=	-1209.121295
Sum of electronic and thermal Free Energies=	-1209.200370

Pt	0.482077	-1.239779	-0.236697	N	-0.444670	-0.085907	1.418718
C	-0.599735	-2.876249	0.271270	C	-0.116326	-0.148459	2.714689
H	-0.505273	-3.040623	1.352411	C	-2.008310	0.985115	2.615432
H	-1.654359	-2.686954	0.030471	C	-1.067519	0.511442	3.511406
H	-0.262894	-3.770082	-0.263457	H	0.779483	-0.676450	3.009627
C	1.383689	-2.305420	-1.726842	H	-2.907236	1.566641	2.757053
H	2.081872	-1.656547	-2.281010	H	-1.066992	0.630507	4.584447
H	1.960317	-3.157659	-1.337939	N	-1.612180	0.616386	1.368787
H	0.655255	-2.702610	-2.448946	C	-2.283066	0.896851	0.135311
S	2.354769	1.658490	-0.253959	C	-1.640642	1.657508	-0.846488
O	1.490344	2.915458	-0.256682	C	-3.584806	0.424381	-0.047644
C	3.256890	1.629430	1.331715	C	-2.318195	1.928401	-2.036701
H	3.975447	0.805179	1.323490	H	-0.641089	2.047019	-0.668314
H	3.762711	2.587576	1.480505	C	-4.253974	0.712400	-1.239030
H	2.516538	1.467242	2.118041	H	-4.058748	-0.169640	0.727713
C	3.789867	1.990422	-1.332992	C	-3.620087	1.458402	-2.235513
H	3.411656	2.085214	-2.353392	H	-1.829618	2.519370	-2.806058
H	4.269978	2.922251	-1.021248	H	-5.265119	0.345619	-1.388668
H	4.488875	1.151746	-1.272190	H	-4.140607	1.676786	-3.163543

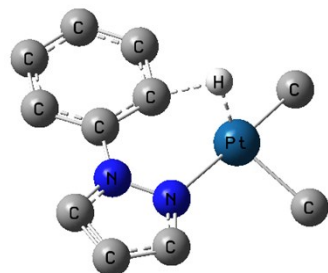
[PtMe₂(Hppz- κ^1 N)], IM3



Zero-point correction= 0.223494 (Hartree/Particle)
 Thermal correction to Energy= 0.237537
 Thermal correction to Enthalpy= 0.238481
 Thermal correction to Gibbs Free Energy= 0.180073
 Sum of electronic and zero-point Energies= -656.014031
 Sum of electronic and thermal Energies= -655.999988
 Sum of electronic and thermal Enthalpies= -655.999044
 Sum of electronic and thermal Free Energies= -656.057452

Pt	1.360111	-0.318473	-0.098153	H	-3.002706	2.788975	-0.153472
C	2.074101	0.369570	1.664775	H	-0.912386	4.569408	-0.374510
H	2.244095	1.451262	1.585029	N	-1.432714	1.356378	-0.155211
H	1.320599	0.185225	2.442497	C	-2.182296	0.144779	-0.057352
H	3.009299	-0.124456	1.946638	C	-1.981698	-0.883335	-0.984453
C	2.728328	-1.828976	-0.082833	C	-3.142017	0.022543	0.951222
H	2.573950	-2.462872	-0.972836	C	-2.742424	-2.048754	-0.886222
H	3.761013	-1.452372	-0.118497	H	-1.250940	-0.761187	-1.777342
H	2.642221	-2.474239	0.803567	C	-3.908418	-1.141772	1.029939
N	-0.071075	1.376049	-0.247287	H	-3.275489	0.824110	1.670933
C	0.264873	2.666943	-0.343148	C	-3.707356	-2.179422	0.116808
C	-1.936797	2.620231	-0.190126	H	-2.588835	-2.849015	-1.603979
C	-0.872213	3.492490	-0.310055	H	-4.653914	-1.239009	1.813471
H	1.307564	2.938508	-0.424194	H	-4.301069	-3.086184	0.184812

[Me₂Pt...H...ppz- κ^1 N)], TS4

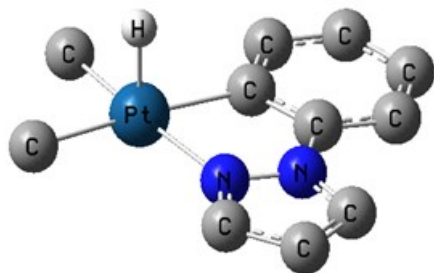


Zero-point correction= 0.222193 (Hartree/Particle)
 Thermal correction to Energy= 0.236374
 Thermal correction to Enthalpy= 0.237319
 Thermal correction to Gibbs Free Energy= 0.180384

Sum of electronic and zero-point Energies= -655.993260
 Sum of electronic and thermal Energies= -655.979079
 Sum of electronic and thermal Enthalpies= -655.978135
 Sum of electronic and thermal Free Energies= -656.035069

Pt	1.065496	-0.236781	-0.047904	H	-3.228216	2.584666	-0.093303
C	2.882019	0.696478	0.491727	H	-1.414913	4.640374	-0.099985
H	2.980123	1.683156	0.021935	N	-1.467849	1.382184	-0.024733
H	2.843221	0.852323	1.582038	C	-1.912428	0.029936	0.002987
H	3.776689	0.106234	0.271265	C	-0.926961	-0.970907	-0.109851
C	2.128804	-2.005644	-0.043108	C	-3.265360	-0.273033	0.172512
H	2.504466	-2.178795	0.973006	C	-1.359106	-2.300393	-0.085880
H	1.502834	-2.853365	-0.339187	C	-3.661568	-1.610551	0.205657
H	2.987205	-1.948286	-0.720351	H	-4.004770	0.512968	0.289255
N	-0.128469	1.612186	-0.006256	C	-2.710319	-2.624405	0.077241
C	0.032933	2.936032	-0.034573	H	-0.633192	-3.101157	-0.194013
C	-2.150139	2.557262	-0.065029	H	-4.712288	-1.853383	0.332927
C	-1.217265	3.579485	-0.070433	H	-3.018589	-3.666126	0.100152
H	1.027780	3.357316	-0.025996	H	0.411518	-0.713177	-1.391779

[PtMe₂(H)(ppz)], IM4

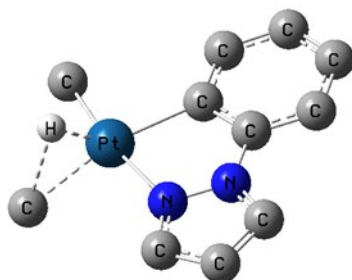


Zero-point correction= 0.223404 (Hartree/Particle)
 Thermal correction to Energy= 0.237851
 Thermal correction to Enthalpy= 0.238795
 Thermal correction to Gibbs Free Energy= 0.181425
 Sum of electronic and zero-point Energies= -655.997798
 Sum of electronic and thermal Energies= -655.983351
 Sum of electronic and thermal Enthalpies= -655.982407
 Sum of electronic and thermal Free Energies= -656.039777

Pt	-1.066666	-0.254460	-0.001048	N	0.097293	1.613751	-0.020288
C	-1.956016	-2.111451	-0.062237	C	-0.091005	2.935869	-0.018936
H	-1.431424	-2.827000	0.577987	C	2.096511	2.596108	0.007014
H	-3.010427	-2.075637	0.224095	C	1.144603	3.603099	-0.003164
H	-1.876393	-2.448787	-1.105580	H	-1.094535	3.336287	-0.027415

H	3.173826	2.648371	0.021797	C	2.804751	-2.559653	-0.001168
H	1.323202	4.667808	0.001359	H	0.731433	-3.102983	0.021015
N	1.440861	1.407571	-0.004227	H	4.801193	-1.728551	-0.024204
C	1.919965	0.056842	-0.002528	H	3.146151	-3.592073	-0.000864
C	0.941855	-0.959658	0.007717	H	-1.208953	-0.361374	1.513155
C	3.294897	-0.194363	-0.015544	C	-3.002935	0.625570	-0.030917
C	1.434919	-2.272624	0.011129	H	-2.971835	1.689218	0.238697
C	3.735436	-1.518467	-0.014203	H	-3.393622	0.546347	-1.057254
H	4.020571	0.613321	-0.028777	H	-3.714178	0.126044	0.636364

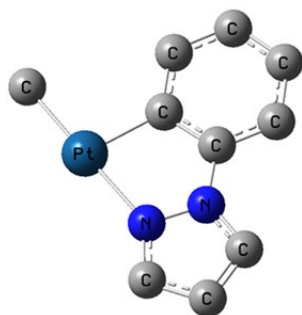
[Me(ppz)Pt...Me...H], TS5



Zero-point correction=	0.222985 (Hartree/Particle)
Thermal correction to Energy=	0.237007
Thermal correction to Enthalpy=	0.237951
Thermal correction to Gibbs Free Energy=	0.181552
Sum of electronic and zero-point Energies=	-655.995330
Sum of electronic and thermal Energies=	-655.981308
Sum of electronic and thermal Enthalpies=	-655.980364
Sum of electronic and thermal Free Energies=	-656.036763

Pt	-1.056547	-0.264767	-0.049453	C	0.938441	-0.949191	-0.004094
C	-1.861110	-2.162605	-0.066893	C	3.281682	-0.165020	0.072692
H	-1.570512	-2.663823	0.865517	C	1.437634	-2.259725	0.019744
H	-2.953337	-2.146737	-0.135075	C	3.729309	-1.486721	0.090868
H	-1.462037	-2.740510	-0.907860	H	4.002054	0.646786	0.097793
N	0.070805	1.612174	-0.013709	C	2.808275	-2.536247	0.064502
C	-0.130568	2.931545	-0.038832	H	0.737951	-3.092213	0.001775
C	2.060933	2.617302	-0.016083	H	4.795991	-1.688871	0.127535
C	1.098542	3.612704	-0.040583	H	3.158127	-3.565384	0.080375
H	-1.137544	3.323008	-0.055496	H	-2.031939	0.073698	-1.219687
H	3.137720	2.680643	-0.010774	C	-2.961833	0.600953	0.454195
H	1.264962	4.679193	-0.058352	H	-2.898634	0.547851	1.548496
N	1.416750	1.421617	0.000466	H	-3.061843	1.643463	0.140670
C	1.906559	0.077830	0.024765	H	-3.830398	0.033247	0.113427

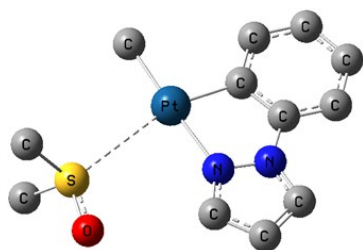
[PtMe₂(ppz)], IM5



Zero-point correction= 0.176055 (Hartree/Particle)
 Thermal correction to Energy= 0.187404
 Thermal correction to Enthalpy= 0.188349
 Thermal correction to Gibbs Free Energy= 0.137405
 Sum of electronic and zero-point Energies= -615.559295
 Sum of electronic and thermal Energies= -615.547946
 Sum of electronic and thermal Enthalpies= -615.547001
 Sum of electronic and thermal Free Energies= -615.597945

Pt	-1.140729	-0.361682	-0.000135	N	1.786956	-0.691549	0.000053
C	-2.864777	0.737539	-0.000155	C	1.539201	0.706173	0.000040
H	-2.971807	1.374967	-0.888151	C	0.176555	1.095864	0.000053
H	-3.706676	0.022586	-0.001293	C	2.582725	1.632151	0.000049
H	-2.972847	1.373443	0.888839	C	-0.087687	2.473537	0.000269
N	0.697298	-1.501538	0.000637	C	2.282997	2.994849	0.000170
C	1.154109	-2.755861	0.000554	H	3.617059	1.302244	-0.000028
C	2.930137	-1.427254	-0.000373	C	0.950317	3.411372	0.000327
C	2.561717	-2.761527	-0.000019	H	-1.115348	2.819146	0.000383
H	0.460252	-3.584567	0.000883	H	3.089605	3.721702	0.000169
H	3.903421	-0.961720	-0.000884	H	0.712641	4.471883	0.000505
H	3.219041	-3.617932	-0.000196				

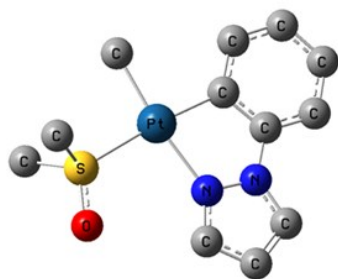
[PtMe₂(ppz)...(DMSO)], TS6



Zero-point correction= 0.259987 (Hartree/Particle)
 Thermal correction to Energy= 0.278345
 Thermal correction to Enthalpy= 0.279289
 Thermal correction to Gibbs Free Energy= 0.210383
 Sum of electronic and zero-point Energies= -1168.691581
 Sum of electronic and thermal Energies= -1168.673222
 Sum of electronic and thermal Enthalpies= -1168.672278
 Sum of electronic and thermal Free Energies= -1168.741185

Pt	-0.047434	-0.682932	-0.066397	C	4.727595	-0.220095	0.142145
C	-0.245060	-2.728011	-0.084335	H	4.286218	1.888564	0.102437
H	0.153287	-3.194892	0.826574	C	4.192275	-1.509538	0.130983
H	-1.316017	-2.982699	-0.146556	H	2.414242	-2.713213	0.061754
H	0.254800	-3.189141	-0.946732	H	5.801600	-0.067340	0.189965
N	0.266243	1.461413	-0.052301	H	4.852155	-2.372209	0.170490
C	-0.398367	2.619470	-0.079369	S	-3.260278	0.215117	0.073586
C	1.766431	3.115971	-0.017549	O	-3.531198	1.714295	0.064640
C	0.510733	3.695725	-0.059491	C	-4.275483	-0.533723	-1.243531
H	-1.481912	2.612509	-0.101545	H	-5.318558	-0.230550	-1.118032
H	2.750377	3.557618	0.009979	H	-3.887260	-0.166867	-2.196314
H	0.283694	4.751267	-0.072991	H	-4.176305	-1.621740	-1.197239
N	1.589286	1.767706	-0.013689	C	-4.143948	-0.494686	1.501906
C	2.496689	0.677870	0.032069	H	-5.196919	-0.202920	1.461196
C	1.921933	-0.617347	0.018201	H	-4.038612	-1.582894	1.481794
C	3.875797	0.883560	0.092645	H	-3.675411	-0.093618	2.403312
C	2.808041	-1.703066	0.069377				

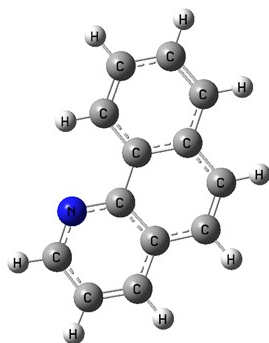
[PtMe₂(ppz)(DMSO)], 4



Zero-point correction= 0.261749 (Hartree/Particle)
 Thermal correction to Energy= 0.279187
 Thermal correction to Enthalpy= 0.280131
 Thermal correction to Gibbs Free Energy= 0.216292
 Sum of electronic and zero-point Energies= -1168.706385
 Sum of electronic and thermal Energies= -1168.688947
 Sum of electronic and thermal Enthalpies= -1168.688003
 Sum of electronic and thermal Free Energies= -1168.751842

Pt	-0.347681	-0.442079	-0.000028	C	4.484759	-0.993954	0.000016
C	-0.835482	-2.451874	0.000012	H	4.469943	1.159146	0.000022
H	-0.413563	-2.943365	0.886291	C	3.704168	-2.151319	0.000007
H	-1.913907	-2.658485	0.000435	H	1.726686	-2.976904	0.000001
H	-0.414258	-2.943254	-0.886668	H	5.569047	-1.057008	0.000007
N	0.444875	1.558785	-0.000082	H	4.181325	-3.128081	-0.000017
C	0.038475	2.831098	-0.000017	S	-2.671800	0.228599	-0.000124
C	2.257440	2.858719	0.000206	O	-2.973607	1.711896	-0.000881
C	1.151654	3.691780	0.000158	C	-3.572237	-0.514487	-1.393388
H	-1.021415	3.042459	-0.000119	H	-4.627043	-0.238589	-1.317080
H	3.312538	3.083767	0.000337	H	-3.131592	-0.102300	-2.303210
H	1.152488	4.771463	0.000236	H	-3.444015	-1.598686	-1.372614
N	1.803058	1.578110	0.000059	C	-3.571845	-0.512991	1.394183
C	2.471628	0.321386	0.000046	H	-4.626686	-0.237224	1.317862
C	1.643104	-0.825402	0.000043	H	-3.443571	-1.597204	1.374548
C	3.866493	0.256652	0.000031	H	-3.130969	-0.099798	2.303437
C	2.307886	-2.060405	0.000019				

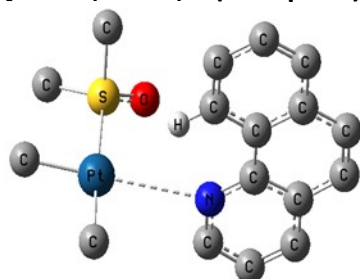
Hbhq



Zero-point correction= 0.183197 (Hartree/Particle)
 Thermal correction to Energy= 0.192438
 Thermal correction to Enthalpy= 0.193382
 Thermal correction to Gibbs Free Energy= 0.148560
 Sum of electronic and zero-point Energies= -555.402140
 Sum of electronic and thermal Energies= -555.392900
 Sum of electronic and thermal Enthalpies= -555.391956
 Sum of electronic and thermal Free Energies= -555.436778

C	3.499993	-0.384385	-0.000006	C	-2.838698	-1.540961	0.000011
C	2.852663	0.835033	0.000036	C	-1.455623	-1.568131	0.000012
C	1.440665	0.874028	0.000020	H	1.259628	3.041210	0.000010
C	0.742822	-0.367085	0.000024	H	4.583100	-0.452433	-0.000018
C	2.717016	-1.555516	-0.000044	H	3.412901	1.766753	0.000018
C	0.704732	2.106436	-0.000002	H	3.202300	-2.530923	-0.000090
C	-0.710577	-0.367862	0.000003	H	-1.207461	3.043342	-0.000042
C	-1.403307	0.877668	-0.000013	H	-4.613044	-0.296476	-0.000001
C	-0.657042	2.105945	-0.000014	H	-3.398419	-2.472224	0.000034
C	-2.818715	0.877491	-0.000014	H	-0.917138	-2.509307	0.000020
H	-3.342512	1.830247	-0.000031	N	1.391024	-1.559485	0.000007
C	-3.526684	-0.309959	-0.000004				

[PtMe₂(DMSO)... (Hbhq- κ^1 N)], TS2

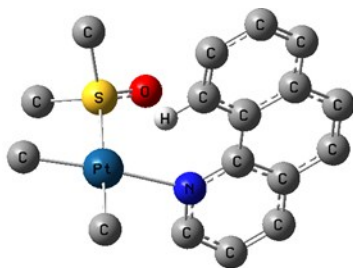


Zero-point correction= 0.339082 (Hartree/Particle)
 Thermal correction to Energy= 0.361834
 Thermal correction to Enthalpy= 0.362778
 Thermal correction to Gibbs Free Energy= 0.284040

Sum of electronic and zero-point Energies= -1307.431271
 Sum of electronic and thermal Energies= -1307.408519
 Sum of electronic and thermal Enthalpies= -1307.407575
 Sum of electronic and thermal Free Energies= -1307.486313

Pt	1.809279	-0.226916	-0.643422	C	-2.697857	0.634659	-0.245700
C	1.654277	-0.853270	-2.583634	C	-3.490426	-1.631326	0.396044
H	0.707635	-1.402085	-2.690776	C	-1.910691	-3.455011	0.457176
H	1.647906	-0.005919	-3.282179	H	0.106714	-2.862768	-0.069435
H	2.480280	-1.520033	-2.863663	C	-4.029071	1.117510	-0.069618
C	3.656288	0.510446	-1.069519	C	-1.695147	1.544185	-0.653319
H	3.699068	1.570871	-0.788300	C	-4.814515	-1.102706	0.557589
H	4.408988	-0.048824	-0.499835	C	-3.200850	-2.994743	0.623037
H	3.877777	0.418687	-2.136511	H	-1.651267	-4.495456	0.623361
S	1.892739	0.479855	1.724307	C	-4.305500	2.486588	-0.301238
O	0.983851	-0.217021	2.714541	C	-5.070780	0.215505	0.335869
C	3.578670	0.433657	2.409511	C	-1.992227	2.878569	-0.873785
H	4.249178	1.022187	1.779752	H	-0.682689	1.182483	-0.796083
H	3.548879	0.829681	3.427786	H	-5.607802	-1.780196	0.862513
H	3.892720	-0.612019	2.416739	H	-4.000796	-3.665098	0.927168
C	1.588784	2.269576	1.855366	C	-3.306344	3.356288	-0.696040
H	0.571174	2.445919	1.500840	H	-5.323062	2.843808	-0.163970
H	1.688383	2.573667	2.900898	H	-6.075555	0.610748	0.461272
H	2.302063	2.801629	1.220884	H	-1.206907	3.560345	-1.188844
C	-2.422479	-0.774155	-0.002435	H	-3.532241	4.404447	-0.871096
C	-0.921639	-2.534379	0.064507	N	-1.157402	-1.246074	-0.158812

[PtMe₂(Hbhq- κ^1 N)(DMSO)], IM2



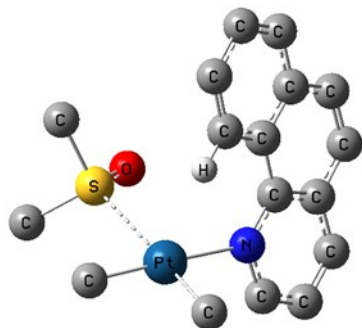
Zero-point correction= 0.339935 (Hartree/Particle)
 Thermal correction to Energy= 0.362998
 Thermal correction to Enthalpy= 0.363942
 Thermal correction to Gibbs Free Energy= 0.285755
 Sum of electronic and zero-point Energies= -1307.442689
 Sum of electronic and thermal Energies= -1307.419627

Sum of electronic and thermal Enthalpies= -1307.418683

Sum of electronic and thermal Free Energies= -1307.496870

Pt	-1.478938	0.186197	-0.584970	C	2.206941	-0.539452	-0.351464
C	-1.588096	0.911715	-2.510387	C	2.805253	1.743880	0.414225
H	-0.767737	1.615903	-2.698506	C	1.174369	3.516269	0.378021
H	-1.512800	0.089843	-3.235123	H	-0.784359	2.860369	-0.242750
H	-2.540858	1.426732	-2.687030	C	3.548946	-0.943064	-0.060923
C	-3.344538	-0.631054	-0.890686	C	1.344606	-1.498343	-0.932405
H	-3.412926	-1.650384	-0.484508	C	4.140235	1.292055	0.679256
H	-4.113819	-0.018946	-0.397986	C	2.460290	3.092883	0.632990
H	-3.592539	-0.682556	-1.956701	H	0.867809	4.546708	0.520166
S	-1.386525	-0.645941	1.715034	C	3.951129	-2.275630	-0.316898
O	-0.297851	-0.153039	2.644345	C	4.493316	-0.001872	0.466818
C	-2.978433	-0.387794	2.560379	C	1.764094	-2.794580	-1.180691
H	-3.783624	-0.813569	1.957950	H	0.329642	-1.207102	-1.189910
H	-2.932044	-0.855777	3.547091	H	4.858398	2.013360	1.059035
H	-3.114458	0.691325	2.656237	H	3.218342	3.781706	0.995707
C	-1.346013	-2.466427	1.744887	C	3.075874	-3.194173	-0.863240
H	-0.415016	-2.769735	1.261685	H	4.972552	-2.562320	-0.080479
H	-1.367195	-2.801991	2.785182	H	5.503301	-0.343497	0.676665
H	-2.200982	-2.858412	1.188993	H	1.074324	-3.503277	-1.630767
C	1.809978	0.836787	-0.066712	H	3.399921	-4.212851	-1.056515
C	0.243171	2.566841	-0.058752	N	0.524529	1.274607	-0.260371

[PtMe₂(Hbhq- κ^1 N)...(DMSO)], TS3



Zero-point correction=

0.338270 (Hartree/Particle)

Thermal correction to Energy=

0.361414

Thermal correction to Enthalpy=

0.362359

Thermal correction to Gibbs Free Energy=

0.282165

Sum of electronic and zero-point Energies=

-1307.429233

Sum of electronic and thermal Energies=

-1307.406088

Sum of electronic and thermal Enthalpies=

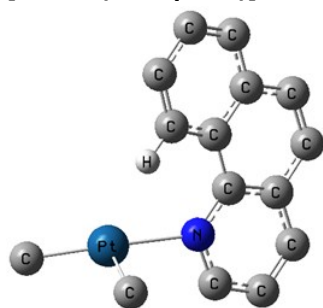
-1307.405144

Sum of electronic and thermal Free Energies=

-1307.485337

Pt	1.591892	-0.565422	-0.497095	C	-2.090881	0.131109	-0.695953
C	2.004775	-2.198624	-1.629162	C	-2.710122	-1.536574	1.034233
H	1.329080	-3.016299	-1.349593	C	-1.077080	-3.095683	1.874836
H	1.851822	-1.953219	-2.687816	H	0.898050	-2.781467	1.066677
H	3.042544	-2.519860	-1.487407	C	-3.438511	0.611282	-0.656223
C	3.417943	0.190099	-1.020821	C	-1.211231	0.720005	-1.633836
H	3.485677	1.243653	-0.707121	C	-4.050882	-1.027448	1.027119
H	4.239327	-0.357780	-0.537219	C	-2.370216	-2.620278	1.869199
H	3.585048	0.152258	-2.106136	H	-0.773740	-3.932361	2.494509
S	0.895185	2.010509	1.602109	C	-3.830800	1.670182	-1.509339
O	-0.293377	1.918421	2.545929	C	-4.396946	0.014196	0.227481
C	2.352850	2.476032	2.597220	C	-1.620730	1.750906	-2.462887
H	3.208554	2.627950	1.933567	H	-0.190381	0.349048	-1.703142
H	2.133693	3.384033	3.165959	H	-4.779112	-1.494982	1.683921
H	2.556225	1.646323	3.278185	H	-3.137140	-3.067284	2.495839
C	0.737658	3.570817	0.668877	C	-2.939073	2.240044	-2.397467
H	-0.116335	3.459045	-0.003128	H	-4.857089	2.024229	-1.456844
H	0.566980	4.395332	1.366867	H	-5.411263	0.403976	0.231827
H	1.647718	3.735992	0.085576	H	-0.917962	2.177900	-3.173219
C	-1.703230	-0.951233	0.204734	H	-3.255018	3.051078	-3.047488
C	-0.134994	-2.452310	1.063603	N	-0.411630	-1.413617	0.265535

[PtMe₂(Hbhq- κ^1 N)], IM3

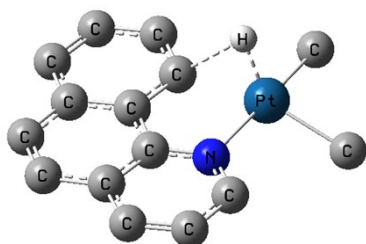


Zero-point correction=	0.254325 (Hartree/Particle)
Thermal correction to Energy=	0.270454
Thermal correction to Enthalpy=	0.271398
Thermal correction to Gibbs Free Energy=	0.208692
Sum of electronic and zero-point Energies=	-754.302576
Sum of electronic and thermal Energies=	-754.286446
Sum of electronic and thermal Enthalpies=	-754.285502
Sum of electronic and thermal Free Energies=	-754.348209

Pt	1.790789	-0.157715	-0.191978	C	2.530860	0.189548	1.659859
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H	2.167875	1.160847	2.019583	C	-3.801526	1.544751	-0.252308
H	2.174074	-0.596584	2.338362	C	-1.974793	3.186529	-0.040160
H	3.625867	0.190361	1.661979	H	-0.257184	4.478203	0.167486
C	3.493518	-1.138661	-0.722377	C	-3.810470	-2.159978	-0.061747
H	3.401300	-1.442744	-1.778848	C	-4.237805	0.258854	-0.276968
H	4.389107	-0.508550	-0.631831	C	-1.594056	-2.983988	0.395179
H	3.658832	-2.046442	-0.124697	H	-0.034836	-1.528332	0.550496
C	-1.450647	0.796627	0.071344	H	-4.493737	2.373160	-0.374586
C	0.253750	2.384559	0.214150	H	-2.704942	3.984500	-0.144530
C	-1.929720	-0.582031	0.111825	C	-2.961911	-3.225655	0.168284
C	-2.411056	1.846252	-0.071497	H	-4.872673	-2.326394	-0.221178
C	-0.635075	3.462556	0.126013	H	-5.290425	0.033180	-0.425039
H	1.318727	2.566622	0.302720	H	-0.922976	-3.814125	0.597936
C	-3.325606	-0.830701	-0.083423	H	-3.348712	-4.240622	0.185546
C	-1.093467	-1.693403	0.369724	N	-0.114827	1.098165	0.171930

[Me₂Pt...H...bhq- κ^1 N)], TS4

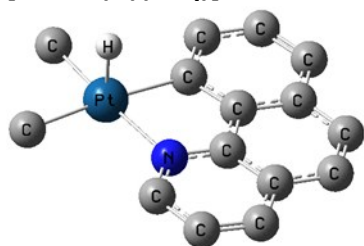


Zero-point correction=	0.253098 (Hartree/Particle)
Thermal correction to Energy=	0.268613
Thermal correction to Enthalpy=	0.269557
Thermal correction to Gibbs Free Energy=	0.209736
Sum of electronic and zero-point Energies=	-754.287875
Sum of electronic and thermal Energies=	-754.272359
Sum of electronic and thermal Enthalpies=	-754.271415
Sum of electronic and thermal Free Energies=	-754.331237

Pt	-1.452095	-0.030044	-0.051376	C	1.502311	-0.682323	-0.039919
C	-2.808838	-1.548138	0.549020	C	0.367939	-2.713819	-0.106444
H	-2.531753	-1.836294	1.576313	C	1.406714	0.750445	-0.030489
H	-3.860243	-1.243812	0.557631	C	2.761349	-1.333656	0.004174
H	-2.710491	-2.445091	-0.076677	C	1.572506	-3.435589	-0.091715
C	-3.057612	1.265863	0.037777	H	-0.590110	-3.221509	-0.133192
H	-2.789932	2.265197	-0.318584	C	2.600249	1.515787	0.081228
H	-3.898297	0.890349	-0.554184	C	0.127752	1.364984	-0.112143
H	-3.378177	1.334143	1.085037	C	3.947287	-0.528232	0.093167

C	2.769805	-2.744218	-0.030439	C	1.246944	3.525041	0.049781
H	1.546526	-4.519363	-0.119688	H	3.393277	3.525886	0.211743
C	2.492037	2.924641	0.125181	H	4.769947	1.430575	0.221325
C	3.865293	0.833116	0.140784	H	-0.881927	3.266291	-0.164796
C	0.071697	2.751813	-0.084368	H	1.169500	4.609066	0.080440
H	4.911544	-1.027281	0.131949	N	0.333272	-1.383367	-0.079736
H	3.717158	-3.276080	-0.006044	H	-1.129117	0.600623	-1.439351

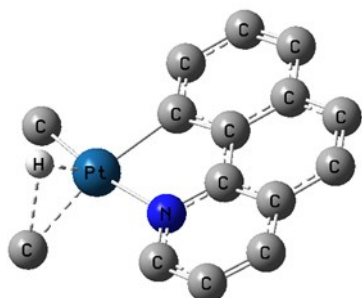
[PtMe₂(H)(bhq)], IM4



Zero-point correction=	0.254303 (Hartree/Particle)
Thermal correction to Energy=	0.270049
Thermal correction to Enthalpy=	0.270993
Thermal correction to Gibbs Free Energy=	0.211156
Sum of electronic and zero-point Energies=	-754.290870
Sum of electronic and thermal Energies=	-754.275125
Sum of electronic and thermal Enthalpies=	-754.274180
Sum of electronic and thermal Free Energies=	-754.334017

Pt	1.457622	-0.000242	-0.003378	H	-3.526621	3.440410	-0.007512
C	2.952158	1.413581	-0.052688	C	-3.940610	-0.626553	0.001972
H	2.641215	2.342637	0.433264	H	-4.827560	1.307792	0.000128
H	3.878774	1.058547	0.406064	C	-2.696442	-2.804764	-0.004703
H	3.139232	1.614958	-1.118013	C	-0.297661	-2.712073	-0.013335
C	-0.155269	1.377196	-0.000610	H	-4.889572	-1.155866	0.002999
C	-1.429531	0.734594	0.000223	H	-3.630459	-3.360496	-0.003392
C	-0.169168	2.769575	-0.002385	C	-1.481193	-3.466801	-0.012183
C	-2.656410	1.457389	-0.001546	H	0.675155	-3.191835	-0.018647
C	-1.486172	-0.703996	-0.001474	H	-1.426233	-4.549869	-0.017385
C	-1.373237	3.509273	-0.008616	N	-0.300011	-1.380772	-0.006852
H	0.767602	3.323880	-0.000510	C	2.926272	-1.541631	-0.021087
C	-2.601161	2.869796	-0.006020	H	2.704859	-2.329857	0.711404
C	-3.901780	0.737217	0.000432	H	2.920334	-2.007456	-1.019918
C	-2.726948	-1.394286	-0.000180	H	3.942189	-1.180251	0.176097
H	-1.334182	4.596474	-0.013398	H	1.593757	0.064101	1.513461

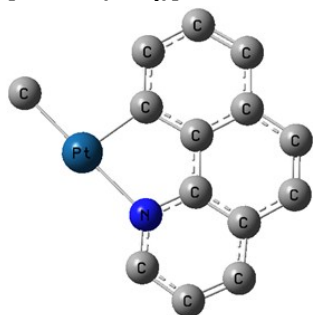
[Me(bhq)Pt...Me...H], TS5



Zero-point correction= 0.253726 (Hartree/Particle)
 Thermal correction to Energy= 0.269089
 Thermal correction to Enthalpy= 0.270033
 Thermal correction to Gibbs Free Energy= 0.211036
 Sum of electronic and zero-point Energies= -754.288340
 Sum of electronic and thermal Energies= -754.272977
 Sum of electronic and thermal Enthalpies= -754.272033
 Sum of electronic and thermal Free Energies= -754.331030

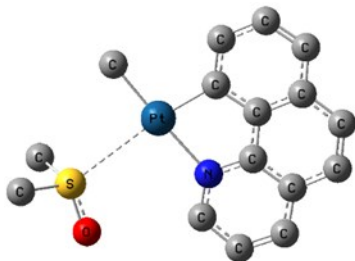
Pt	1.451389	-0.018333	-0.039811	H	-3.461498	3.483082	0.073296
C	2.896859	1.449932	-0.038265	C	-3.944466	-0.575547	0.032548
H	2.820193	1.999533	0.909146	H	-4.799886	1.372926	0.071021
H	3.906281	1.036582	-0.127820	C	-2.737487	-2.774122	-0.015105
H	2.727492	2.154218	-0.860016	C	-0.337532	-2.717994	-0.050846
C	-0.131100	1.367368	-0.005700	H	-4.901631	-1.089645	0.041683
C	-1.413497	0.742631	0.009544	H	-3.680367	-3.314504	-0.007011
C	-0.117482	2.759472	0.014003	C	-1.533407	-3.454112	-0.042405
C	-2.626602	1.485869	0.037458	H	0.624158	-3.218954	-0.070651
C	-1.492043	-0.694509	-0.007343	H	-1.494755	-4.537790	-0.056388
C	-1.308606	3.518755	0.041842	N	-0.314711	-1.387472	-0.033509
H	0.830693	3.292748	0.006167	H	2.202611	-0.668651	-1.239868
C	-2.545707	2.897476	0.052442	C	2.919568	-1.534342	0.405629
C	-3.883962	0.787290	0.048999	H	2.708192	-2.523846	-0.009804
C	-2.743741	-1.362942	0.002903	H	3.940595	-1.248848	0.142188
H	-1.252768	4.604866	0.055059	H	2.820522	-1.570773	1.498594

[PtMe₂(bhq)], IM5



Zero-point correction=	0.207420 (Hartree/Particle)		
Thermal correction to Energy=	0.219995		
Thermal correction to Enthalpy=	0.220939		
Thermal correction to Gibbs Free Energy=	0.167667		
Sum of electronic and zero-point Energies=	-713.854013		
Sum of electronic and thermal Energies=	-713.841438		
Sum of electronic and thermal Enthalpies=	-713.840494		
Sum of electronic and thermal Free Energies=	-713.893766		
Pt	1.486568	-0.461702	-0.000001
C	3.321299	0.464958	0.000122
H	3.477839	1.089345	0.889527
H	4.098940	-0.318334	-0.000032
H	3.477677	1.089449	-0.889257
C	0.382771	1.160231	-0.000065
C	-1.021348	0.911917	-0.000054
C	0.803090	2.488399	-0.000003
C	-1.974893	1.964148	-0.000027
C	-1.476317	-0.444510	-0.000096
C	-0.138902	3.540587	0.000038
H	1.860059	2.730104	0.000044
C	-1.502844	3.296005	0.000015
C	-3.373796	1.623736	-0.000024
C	-2.856540	-0.759240	0.000037
H	0.222175	4.566213	0.000115
H	-2.213994	4.117638	-0.000032
C	-3.799144	0.325870	0.000026
H	-4.099594	2.433194	-0.000079
C	-3.210339	-2.125650	0.000140
C	-0.868484	-2.686968	-0.000052
H	-4.860374	0.092757	0.000055
H	-4.258944	-2.411059	0.000360
C	-2.215485	-3.089076	0.000009
H	-0.065080	-3.417574	-0.000098
H	-2.456657	-4.146474	0.000137
N	-0.506963	-1.404994	-0.000144

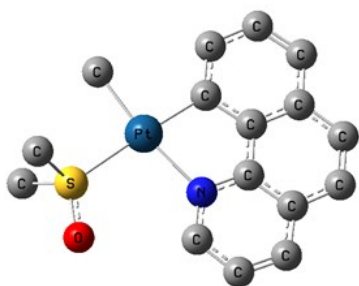
[PtMe₂(bhq)...(DMSO)], TS6



Zero-point correction=	0.290829 (Hartree/Particle)		
Thermal correction to Energy=	0.310544		
Thermal correction to Enthalpy=	0.311489		
Thermal correction to Gibbs Free Energy=	0.240133		
Sum of electronic and zero-point Energies=	-1266.986248		
Sum of electronic and thermal Energies=	-1266.966533		
Sum of electronic and thermal Enthalpies=	-1266.965589		
Sum of electronic and thermal Free Energies=	-1267.036944		
Pt	-0.479942	-0.761752	-0.094998
C	-1.239591	-2.668712	-0.097719
H	-0.996437	-3.212450	0.825524
H	-2.337738	-2.627385	-0.177892
H	-0.869675	-3.263155	-0.944208
C	1.421442	-1.271269	0.004973

C	2.319422	-0.163045	0.029326	H	2.578478	4.469837	-0.024915
C	1.975794	-2.547748	0.056882	C	0.594895	3.635442	-0.104721
C	3.727431	-0.329635	0.105117	H	-1.246321	2.466953	-0.159683
C	1.775728	1.159231	-0.019363	H	0.082175	4.590802	-0.138172
C	3.375756	-2.723313	0.131587	N	0.417079	1.246115	-0.084986
H	1.338828	-3.425173	0.041243	S	-3.581387	0.556628	0.104561
C	4.244061	-1.644084	0.155929	O	-3.567075	2.080162	0.088989
C	4.558659	0.845998	0.128232	C	-4.762415	0.005326	-1.171714
C	2.607829	2.303316	0.005598	H	-5.726357	0.496479	-1.012247
H	3.775500	-3.733767	0.170961	H	-4.346784	0.294480	-2.139573
H	5.318475	-1.796784	0.214182	H	-4.865429	-1.082139	-1.122698
C	4.029077	2.104248	0.080625	C	-4.534986	0.028822	1.566651
H	5.636034	0.712341	0.186266	H	-5.513089	0.517754	1.558228
C	1.976272	3.565280	-0.041445	H	-4.642236	-1.059187	1.552183
C	-0.159100	2.447974	-0.123112	H	-3.968129	0.333670	2.449101
H	4.675755	2.977243	0.100456				

[PtMe₂(bhq)(DMSO)], 5

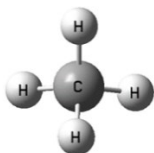


Zero-point correction=	0.293081 (Hartree/Particle)
Thermal correction to Energy=	0.312613
Thermal correction to Enthalpy=	0.313557
Thermal correction to Gibbs Free Energy=	0.244581
Sum of electronic and zero-point Energies=	-1266.999537
Sum of electronic and thermal Energies=	-1266.980005
Sum of electronic and thermal Enthalpies=	-1266.979061
Sum of electronic and thermal Free Energies=	-1267.048038

Pt	-0.754057	-0.509669	-0.011017	C	1.450420	-2.700110	-0.001382
C	-1.671154	-2.368047	-0.022271	C	3.519782	-0.789241	0.011347
H	-1.386197	-2.931303	0.875562	C	1.823429	0.988818	-0.002741
H	-2.767480	-2.338880	-0.051061	C	2.805614	-3.099053	0.010483
H	-1.341562	-2.941044	-0.898014	H	0.689826	-3.473958	-0.005198
C	1.086005	-1.355871	-0.007046	C	3.829701	-2.167859	0.016606
C	2.150512	-0.406538	0.000184	C	4.530458	0.234714	0.017338

C	2.833754	1.982321	0.001498	S	-2.919063	0.600967	0.018602
H	3.044586	-4.160044	0.015198	O	-2.982024	2.115296	0.054507
H	4.869829	-2.483585	0.025809	C	-3.943958	0.062339	-1.384085
C	4.206812	1.560629	0.012064	H	-4.928580	0.527907	-1.292622
H	5.573851	-0.071069	0.026186	H	-3.438369	0.408703	-2.287639
C	2.425357	3.332975	-0.004436	H	-4.019920	-1.026584	-1.390635
C	0.134181	2.591790	-0.014458	C	-3.925569	-0.003714	1.406994
H	4.982954	2.321093	0.016326	H	-4.915641	0.454792	1.343717
H	3.173703	4.121135	-0.001951	H	-3.989841	-1.092632	1.369334
C	1.075827	3.635339	-0.013192	H	-3.414541	0.310642	2.319114
H	-0.933531	2.789022	-0.017587				
H	0.728613	4.663008	-0.018035				
N	0.494708	1.306887	-0.009187				

CH₄



Zero-point correction=	0.045071 (Hartree/Particle)
Thermal correction to Energy=	0.047937
Thermal correction to Enthalpy=	0.048881
Thermal correction to Gibbs Free Energy=	0.027747
Sum of electronic and zero-point Energies=	-40.473479
Sum of electronic and thermal Energies=	-40.470613
Sum of electronic and thermal Enthalpies=	-40.469669
Sum of electronic and thermal Free Energies=	-40.490803

C	0.000000	0.000000	0.000000	H	-0.631282	0.631282	-0.631282
H	0.631282	0.631282	0.631282	H	0.631282	-0.631282	-0.631282
H	-0.631282	-0.631282	0.631282				