Supplementary Informations : **Is Thorium a d transition metal or an actinide ? An answer from the DFT study of reaction between pyridine N-oxide and Cp2M(CH3)2 with M= Zr, Th and U**

Ahmed Yahia and Laurent Maron

Full reference 42:

Gaussian 03, Revision B.05, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

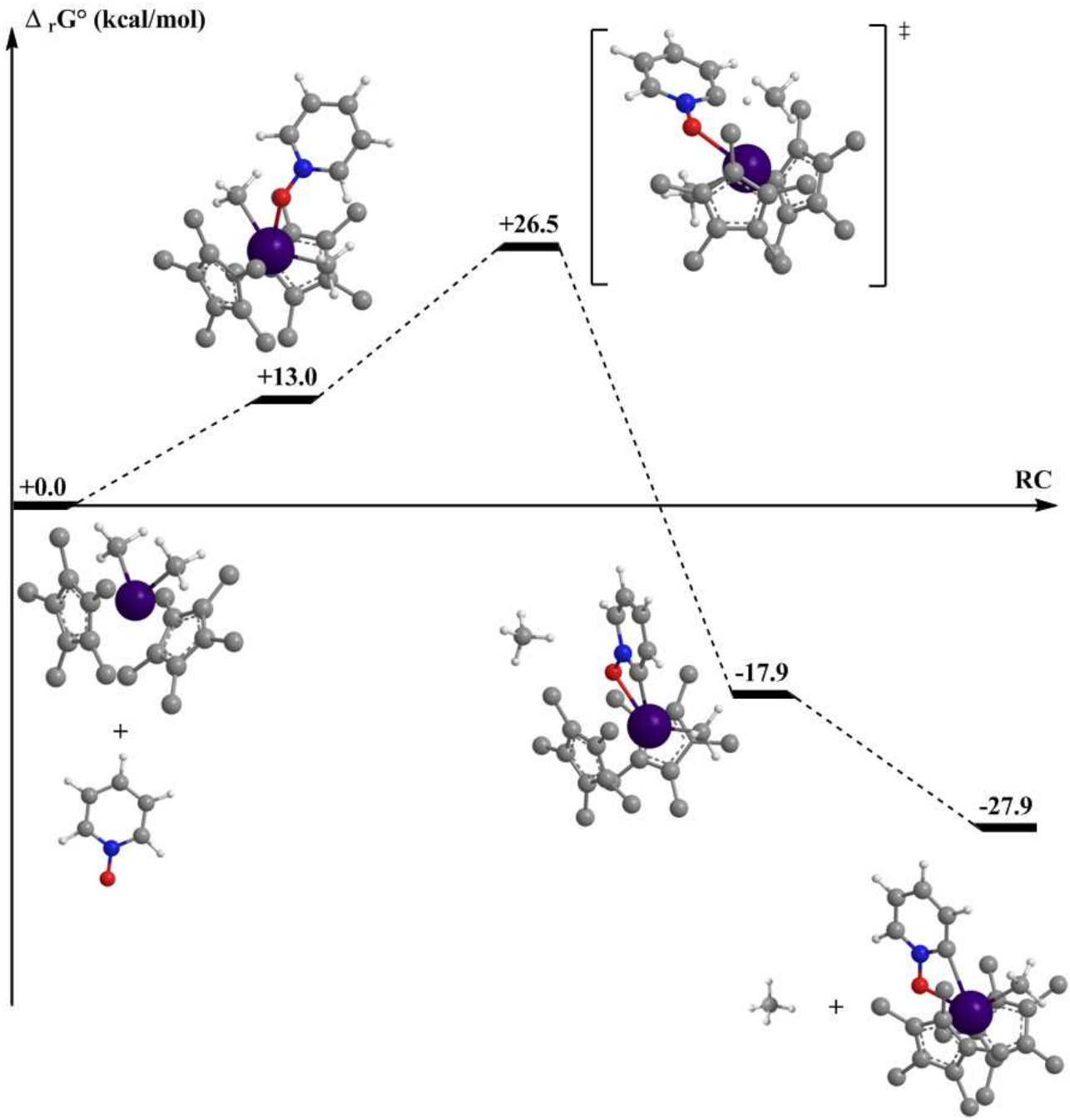

Figure 1 : Calculated free energy profile of C-H activation of pyridine N-oxide catalyzed by $Cp^*_2Th(Me)_2$. For sake of clarity, the hydrogens on the methyl groups of the Cp* rings have been omitted

****

Molecule 1 (Thorium)

HF=-502.7294712
G=-502.542788

Th	-0.435520	0.023797	-0.155605
C	0.512630	-0.016022	-2.817914
C	1.251856	1.018042	-2.195917
C	0.936453	-1.253046	-2.273988
C	2.127659	0.422346	-1.255609
C	1.932028	-0.981920	-1.304432
C	-1.443918	0.061284	2.484494

C	-0.477889	-0.972859	2.490830
C	-0.768357	1.298411	2.347284
C	0.618345	1.027307	2.256519
C	0.798788	-0.377049	2.345285
H	-0.682053	-2.032385	2.587793
H	1.749259	-0.898441	2.334654
H	1.406928	1.765525	2.161827
H	-1.230717	2.277040	2.316731
H	-2.515821	-0.071498	2.576199
H	2.843729	0.943757	-0.630521
H	2.469669	-1.720064	-0.719729
H	0.564453	-2.231627	-2.550435
H	-0.242758	0.116713	-3.583938
H	1.160248	2.077489	-2.402939
C	-1.924591	-1.925373	-0.553806
C	-1.823473	1.975507	-0.818725
H	-2.265182	-1.933655	-1.602047
H	-1.495818	-2.918721	-0.356948
H	-2.830833	-1.846666	0.068316
H	-2.763161	1.984859	-0.242717
H	-1.368350	2.968280	-0.689923
H	-2.108849	1.897287	-1.880330

****

Molecule 1 (Zirconium)

HF=-513.8954165
G=-513.696339

Zr	-0.282800	0.023643	-0.099572
C	0.397230	-0.128450	-2.570774
C	1.016349	1.036512	-2.057373
C	0.968411	-1.254045	-1.929831
C	1.960630	0.634382	-1.082081
C	1.930906	-0.785903	-1.003029
C	-1.373694	0.174890	2.219837
C	-0.570422	-0.990682	2.231889
C	-0.522039	1.299909	2.105239
C	0.811490	0.830756	2.027048
C	0.781489	-0.589543	2.105611
H	-0.929287	-2.008600	2.303260
H	1.641696	-1.246329	2.097866
H	1.698584	1.445856	1.948930
H	-0.837553	2.333694	2.063039
H	-2.454861	0.200258	2.266936
H	2.609585	1.290471	-0.516580
H	2.553273	-1.401714	-0.366775
H	0.700240	-2.287539	-2.103091
H	-0.393430	-0.153069	-3.309718
H	0.791139	2.054694	-2.344819
C	-1.701005	-1.708956	-0.514256
C	-1.626725	1.758659	-0.706070
H	-1.997930	-1.705993	-1.572000
H	-1.287250	-2.703500	-0.298384
H	-2.612262	-1.600872	0.089839
H	-2.540396	1.755947	-0.095947
H	-1.171453	2.752861	-0.600450
H	-1.925933	1.650982	-1.757703

****

Molecule 1 (Uranium)

HF=-518.2009499
G=-518.015198

U	-0.416771	0.032290	-0.149093
C	0.602696	-0.010719	-2.706321
C	1.306915	1.036475	-2.061938
C	1.031293	-1.237589	-2.145847
C	2.166811	0.456059	-1.098998
C	1.993251	-0.948294	-1.148568
C	-1.303599	0.111319	2.453353
C	-0.384591	-0.966630	2.430728
C	-0.572581	1.314437	2.303523
C	0.796922	0.979284	2.178329
C	0.913700	-0.429466	2.259522
H	-0.633387	-2.016204	2.534419
H	1.837716	-0.993917	2.220473
H	1.616125	1.680272	2.067587
H	-0.988892	2.314465	2.289572
H	-2.377211	0.029655	2.577639
H	2.853940	0.988908	-0.452755
H	2.524714	-1.676337	-0.546535
H	0.685456	-2.223375	-2.431752
H	-0.126996	0.107251	-3.498953
H	1.209347	2.094230	-2.276918
C	-1.944359	-1.781725	-0.606099
C	-1.927184	1.796393	-0.812799
H	-2.249447	-1.742672	-1.662493
H	-1.560066	-2.790022	-0.400431
H	-2.844963	-1.629905	0.008785
H	-2.839754	1.742628	-0.200770
H	-1.520596	2.813699	-0.730809
H	-2.214507	1.627810	-1.861814

****

Molecule 2

HF=-323.3314202
G=-323.266695

N	0.011654	0.000000	0.006696
C	0.032024	0.000000	1.378240
C	1.220760	0.000000	2.081254
C	2.442425	0.000000	1.410164
C	2.412759	0.000000	0.016586
C	1.209592	0.000000	-0.661433
H	-0.953203	0.000000	1.825176
H	1.174951	0.000000	3.165679
H	3.381214	0.000000	1.952148
H	3.329019	0.000000	-0.565268
H	1.103973	0.000000	-1.738131
O	-1.085274	0.000000	-0.626612

****

methane

HF=-40.508619
G=-40.483817

C	0.000000	0.000196	0.009525
H	-1.068550	-0.223519	0.002117
H	0.429931	-0.400106	0.830663
H	0.493433	-0.459374	-0.951315
H	0.145187	1.081820	0.002117

****

Molecule 6 (Thorium)

HF=-785.6075036
G=-785.376910

Th	-0.181205	0.010052	-0.014142
C	0.972854	-1.394681	-2.175848
C	0.249145	-0.345852	-2.795159
C	-1.131299	-0.597255	-2.605288
C	-1.259437	-1.805485	-1.875677
C	0.041748	-2.300249	-1.613415
H	2.051950	-1.490687	-2.142666
H	0.675858	0.495323	-3.326693
H	-1.946730	0.013685	-2.974948
H	-2.190366	-2.281140	-1.589433
H	0.282164	-3.207994	-1.075289
C	-1.433747	1.410001	2.094401
C	-2.008429	0.116612	2.134029
C	-2.819005	-0.034633	0.982809
C	-2.751881	1.168637	0.236552
C	-1.900225	2.063924	0.926867
H	-0.765100	1.831393	2.836594
H	-1.852306	-0.625974	2.905611
H	-3.407894	-0.909017	0.730293
H	-3.280208	1.376080	-0.686746
H	-1.653996	3.072975	0.621642
C	0.985147	2.283544	-0.805594
H	1.544696	-2.186280	1.220624
H	0.808864	-1.308740	2.562169
H	-0.099477	-2.586895	1.741218
C	0.597658	-1.751511	1.576328
N	2.102218	1.956424	-0.099492
C	3.232806	2.687408	-0.010931
C	3.303020	3.891262	-0.688004
C	2.203594	4.309365	-1.439420
C	1.066620	3.503354	-1.486583
O	2.039494	0.786977	0.561658
H	4.020418	2.264593	0.600491
H	4.208544	4.484232	-0.621007
H	2.238752	5.252027	-1.978435
H	0.207273	3.824117	-2.070048

****

Molecule 6 (Zirconium)

HF=-796.756565
G=-796.51.3914

Zr	-0.282800	0.023643	-0.099572

C	0.972676	-1.258401	-1.936070
C	0.394870	-0.127880	-2.562312
C	-1.012712	-0.266270	-2.498445
C	-1.302761	-1.493695	-1.839946
C	-0.072912	-2.107385	-1.500272
H	2.031600	-1.432663	-1.794307
H	0.934607	0.704411	-2.993609
H	-1.738948	0.426445	-2.903554
H	-2.288715	-1.900160	-1.655379
H	0.047851	-3.048225	-0.980397
C	-1.150086	1.321173	1.939212
C	-1.917349	0.133744	1.866132
C	-2.680370	0.180635	0.674446
C	-2.390090	1.408265	0.016416
C	-1.449205	2.113626	0.804941
H	-0.439450	1.569978	2.716953
H	-1.905258	-0.675401	2.583893
H	-3.381135	-0.572401	0.337922
H	-2.830870	1.754576	-0.909417
H	-1.017811	3.077856	0.572133
C	0.873608	1.382713	-0.335475
H	1.621036	-1.794741	0.982190
H	0.884677	-0.899810	2.326451
H	0.055320	-2.295928	1.629884
C	0.553511	-1.243608	1.202218
N	2.132007	1.345368	0.276928
C	3.031435	2.402422	0.093448
C	2.672465	3.496821	-0.702436
C	1.414066	3.534166	-1.314840
C	0.514638	2.477112	-1.131359
O	2.411234	0.494082	0.896012
H	4.010290	2.373373	0.569810
H	3.372092	4.319058	-0.845158
H	1.134839	4.385452	-1.933924
H	-0.464217	2.506161	-1.607722

****

Molecule 6 (Uranium)

HF=-801.0807347
G=-800.849744

U	-0.032267	-0.036152	0.097442
O	2.119566	0.795531	0.484303
N	2.059592	1.972326	-0.177504
C	3.155712	2.759437	-0.192149
H	4.016281	2.379836	0.344868
C	3.100824	3.959263	-0.874699
H	3.975510	4.599840	-0.893775
C	1.914633	4.312867	-1.523598
H	1.851305	5.251978	-2.066375
C	0.821412	3.452089	-1.465033
H	-0.103446	3.723461	-1.967024
C	0.869646	2.234243	-0.776136
C	0.472015	-1.894797	1.610449
H	0.723662	-1.452045	2.583156
H	-0.269847	-2.687541	1.739899

H	1.381078	-2.304796	1.145946
C	-1.348288	1.352251	2.129823
H	-0.726543	1.796831	2.898998
C	-1.906678	0.051750	2.161491
H	-1.782937	-0.675477	2.953222
C	-2.668350	-0.124634	0.982628
H	-3.231054	-1.011946	0.717680
C	-2.589712	1.069963	0.226098
H	-3.082886	1.256288	-0.720228
C	-1.782124	1.986798	0.939156
H	-1.553367	3.000988	0.639995
C	0.983123	-1.606476	-1.930796
H	1.979432	-1.997557	-1.758544
C	0.669944	-0.380935	-2.563922
H	1.380999	0.325258	-2.973623
C	-0.740437	-0.252116	-2.589904
H	-1.294861	0.575421	-3.016072
C	-1.296277	-1.403216	-1.986039
H	-2.352432	-1.612827	-1.867478
C	-0.232247	-2.239614	-1.572674
H	-0.329467	-3.200694	-1.083110

****

Transition state 4 (Thorium)

HF=-826.0610554
G=-825.786165

C	0.547634	1.660251	-2.113568
C	-0.049830	0.597410	-2.836036
C	0.603256	-0.603475	-2.472531
C	1.590248	-0.286942	-1.511385
C	1.559106	1.114348	-1.293279
Th	-0.835587	0.135183	-0.145388
C	0.260563	-1.204342	2.093026
C	1.120302	-0.098039	1.883542
C	0.408273	1.079933	2.218573
C	-0.890193	0.700325	2.636643
C	-0.980263	-0.709191	2.557441
O	-3.190000	-0.124408	0.592250
N	-3.873277	-0.196128	-0.534486
C	-3.298369	0.364957	-1.632909
C	-3.996904	0.284584	-2.835991
C	-5.224833	-0.366205	-2.908654
C	-5.760988	-0.928297	-1.747775
C	-5.062513	-0.836023	-0.558346
C	-2.005022	2.576059	-0.475535
C	-1.391641	-2.258149	-0.722432
H	-0.843895	0.692359	-3.566551
H	0.382167	-1.590532	-2.855520
H	2.265831	-0.991433	-1.040623
H	2.207908	1.671237	-0.627633
H	0.283712	2.707160	-2.187202
H	-1.681091	1.370537	2.951977
H	0.796078	2.091727	2.179324
H	2.150412	-0.145695	1.552902
H	0.508454	-2.246170	1.930241
H	-1.856024	-1.302068	2.788037

H	-2.089879	3.254628	-1.332405
H	-1.092132	2.886112	0.063529
H	-2.851447	2.761456	0.196726
H	-2.058155	-2.673676	0.048058
H	-1.884873	-2.408408	-1.693978
H	-0.488063	-2.886853	-0.733815
H	-5.383125	-1.248697	0.389710
H	-6.715374	-1.443081	-1.755993
H	-5.761491	-0.436166	-3.849698
H	-3.561558	0.743116	-3.718907
H	-2.541973	1.326544	-1.261344

****

Transition State 4 (Zirconium)

HF=-837.1814318
G=-836.896204

C	-3.076744	0.164019	-1.616023
N	-3.712606	-0.330474	-0.523837
C	-4.948770	-0.876841	-0.548237
C	-5.621540	-0.963099	-1.753136
C	-5.019018	-0.479207	-2.917561
C	-3.753088	0.095950	-2.833097
O	-3.021707	-0.261295	0.587263
Zr	-0.792180	0.134930	-0.156451
C	1.025797	-0.160515	1.626729
C	0.450534	1.118352	1.834436
C	-0.871737	0.923778	2.313339
C	-1.107066	-0.464534	2.395210
C	0.054321	-1.136775	1.950300
C	-0.236756	0.919023	-2.591473
C	0.222288	-0.407365	-2.484166
C	1.297823	-0.422320	-1.557853
C	1.525435	0.908394	-1.133071
C	0.559664	1.733521	-1.739604
C	-1.227340	-2.111763	-0.582928
C	-2.041208	2.383044	-0.355497
H	-1.046282	1.268301	-3.217057
H	-0.183802	-1.268425	-2.995584
H	1.861987	-1.296548	-1.259579
H	2.288171	1.236555	-0.440462
H	0.461354	2.802800	-1.608831
H	-1.584368	1.702067	2.553027
H	0.939786	2.072339	1.682253
H	2.033093	-0.363409	1.290910
H	0.182753	-2.208335	1.882480
H	-2.040799	-0.931505	2.671732
H	-2.114299	3.023961	-1.241457
H	-1.227474	2.783094	0.257310
H	-2.967080	2.456479	0.223351
H	-1.817858	-2.539185	0.234821
H	-1.784049	-2.272625	-1.514441
H	-0.294041	-2.684656	-0.663831
H	-5.323031	-1.229970	0.404404
H	-6.608709	-1.411893	-1.771700
H	-5.534897	-0.549710	-3.870299

H	-3.274617	0.496145	-3.722606
H	-2.356497	1.181643	-1.138787

****

Transition State 4 (Uranium)

HF=--841.5318842
G=-841.255386

C	0.236744	1.442638	-1.924620
C	-0.273953	0.300007	-2.586524
C	0.479982	-0.820512	-2.164818
C	1.446871	-0.372456	-1.235805
C	1.296996	1.026344	-1.086432
U	-0.972134	-0.083180	0.117620
C	0.213923	-1.399446	2.275350
C	1.043512	-0.277372	2.050698
C	0.309733	0.884941	2.384085
C	-0.973690	0.478902	2.825885
C	-1.032738	-0.930361	2.755875
O	-3.276541	-0.457390	0.784408
N	-3.947897	-0.287977	-0.342490
C	-3.378092	0.515379	-1.280957
C	-4.066688	0.692891	-2.478574
C	-5.287429	0.062942	-2.705117
C	-5.818812	-0.755834	-1.706540
C	-5.126054	-0.927294	-0.522461
C	-1.887030	2.447093	0.118377
C	-1.155566	-2.534545	-0.293569
H	-1.065968	0.289124	-3.325379
H	0.356393	-1.837605	-2.511715
H	2.183528	-0.993301	-0.741736
H	1.899670	1.668969	-0.456125
H	-0.107807	2.460419	-2.052993
H	-1.773460	1.133209	3.151101
H	0.677046	1.903650	2.339652
H	2.069315	-0.302692	1.705946
H	0.489420	-2.435302	2.124844
H	-1.888617	-1.542159	3.012475
H	-2.080953	3.222720	-0.631050
H	-0.878948	2.641172	0.513119
H	-2.598856	2.568927	0.943469
H	-1.753154	-2.897289	0.549723
H	-1.751613	-2.567552	-1.218411
H	-0.255877	-3.141008	-0.415832
H	-5.443861	-1.549391	0.304565
H	-6.765704	-1.267924	-1.837821
H	-5.820911	0.204216	-3.639907
H	-3.630347	1.342163	-3.231963
H	-2.560668	1.372076	-0.751266

****

Complex 3 (Zirconium)

HF=-837.2165801

G=-836.931603

C	-3.528189	-0.128174	-2.258249
N	-3.818619	-0.323782	-0.941819
C	-5.116744	-0.521972	-0.566153
C	-6.135631	-0.526647	-1.496464
C	-5.856324	-0.326563	-2.848521
C	-4.528425	-0.126540	-3.214108
O	-2.909209	-0.333835	-0.037144
Zr	-0.491080	0.170484	-0.075525
C	1.098765	-0.234056	1.859166
C	0.489520	1.030595	2.083606
C	-0.878658	0.808379	2.372942
C	-1.119343	-0.582300	2.298546
C	0.103227	-1.228451	1.987225
C	0.077439	0.894725	-2.514133
C	0.725739	-0.343688	-2.306845
C	1.701430	-0.161713	-1.298989
C	1.684954	1.209655	-0.917933
C	0.679826	1.857562	-1.660914
C	-0.928038	-2.057059	-0.682528
C	-1.773175	2.142072	-0.138316
H	-0.704200	1.101239	-3.234796
H	0.504649	-1.274632	-2.809087
H	2.365229	-0.926601	-0.917706
H	2.331029	1.674995	-0.185191
H	0.407039	2.900790	-1.591568
H	-1.613451	1.572803	2.580884
H	0.983206	1.993537	2.059215
H	2.142930	-0.406436	1.633566
H	0.243568	-2.291738	1.850832
H	-2.079095	-1.066843	2.413392
H	-2.135348	2.376912	-1.150556
H	-1.171083	3.003290	0.186891
H	-2.651138	2.089676	0.515647
H	-1.581380	-2.537648	0.055002
H	-1.429711	-2.145756	-1.658040
H	-0.003459	-2.648995	-0.748725
H	-5.248481	-0.666748	0.497646
H	-7.149965	-0.687404	-1.146844
H	-6.647658	-0.326648	-3.589586
H	-4.246506	0.033571	-4.249505
H	-2.478549	0.017479	-2.471774

****

Complex 5 (Zirconium)

HF=-837.2642517
G=-836.986946

C	-2.620376	-1.110120	-1.103830
N	-3.210027	0.093698	-0.892428
C	-4.498112	0.402862	-1.152085
C	-5.314586	-0.580239	-1.684750
C	-4.785900	-1.848624	-1.934311
C	-3.444606	-2.099194	-1.640813

O	-2.374006	0.990764	-0.380304
Zr	-0.513707	-0.428924	-0.299226
C	0.852360	-0.593702	1.823685
C	0.034267	0.564017	1.975077
C	-1.305028	0.134113	2.087863
C	-1.330136	-1.277789	1.969570
C	0.010166	-1.727599	1.833245
C	-0.124277	1.428168	-2.041507
C	-0.010998	0.193254	-2.728120
C	1.143753	-0.473036	-2.238913
C	1.713929	0.329318	-1.225523
C	0.922808	1.508356	-1.099383
C	-0.170939	-2.651525	-0.888012
C	-3.519675	4.765429	-0.608309
H	-0.917933	2.151465	-2.164301
H	-0.671559	-0.166851	-3.505788
H	1.516429	-1.429390	-2.575892
H	2.611597	0.100662	-0.665725
H	1.104525	2.330886	-0.420125
H	-2.168049	0.779395	2.172235
H	0.378278	1.589059	2.022057
H	1.931732	-0.605084	1.743389
H	0.329109	-2.755906	1.744000
H	-2.211221	-1.904993	2.002404
H	-3.719351	4.956890	-1.664989
H	-2.761125	5.465970	-0.252581
H	-4.437831	4.908436	-0.034028
H	-0.835925	-3.312939	-0.317964
H	-0.384834	-2.810153	-1.952606
H	0.861150	-2.985036	-0.705611
H	-4.803596	1.415933	-0.921221
H	-6.351759	-0.345387	-1.898646
H	-5.417328	-2.627514	-2.352227
H	-3.015943	-3.079859	-1.827316
H	-3.159492	3.742313	-0.480321

****

Complex 5 (Thorium)

HF=-826.1153245
G=-825.846463

C	0.220215	1.275353	-2.152713
C	-0.057482	0.116267	-2.919705
C	0.862887	-0.888434	-2.544655
C	1.711262	-0.353073	-1.548238
C	1.320465	0.986498	-1.310916
Th	-0.814592	-0.544567	-0.258968
C	0.414786	-1.558596	2.103103
C	1.156674	-0.396955	1.794702
C	0.317287	0.727649	1.995845
C	-0.940918	0.256336	2.442960
C	-0.884047	-1.154659	2.498987
O	-3.097599	-0.468045	0.558416
N	-3.794989	-0.413210	-0.592589
C	-3.037694	-0.305867	-1.716592

C	-3.772262	-0.243330	-2.904951
C	-5.166480	-0.285308	-2.923227
C	-5.858633	-0.401775	-1.717454
C	-5.140944	-0.467526	-0.536462
C	-2.765066	4.575619	-0.233127
C	-0.694871	-2.990490	-0.616502
H	-0.829592	0.022387	-3.671762
H	0.911007	-1.892019	-2.947320
H	2.528405	-0.874922	-1.065340
H	1.790491	1.673869	-0.618288
H	-0.301689	2.223733	-2.219265
H	-1.804795	0.864683	2.680797
H	0.600838	1.766517	1.870265
H	2.190380	-0.368047	1.473761
H	0.773194	-2.578493	2.044986
H	-1.698504	-1.809676	2.782652
H	-2.699203	5.015329	-1.230413
H	-1.767827	4.522702	0.208867
H	-3.406646	5.195418	0.396304
H	-1.321864	-3.495976	0.134623
H	-1.143161	-3.196580	-1.603013
H	0.287377	-3.479104	-0.602099
H	-5.569820	-0.560361	0.453701
H	-6.941798	-0.442144	-1.681748
H	-5.711411	-0.230935	-3.861465
H	-3.229443	-0.159773	-3.842869
H	-3.187546	3.571492	-0.303727

****

Complex 3 (Thorium)

HF=-826.074863
G=-825.201297

C	1.217007	1.664271	-1.876928
C	0.651673	0.685052	-2.729757
C	1.132855	-0.581954	-2.325614
C	1.969079	-0.391696	-1.201868
C	2.025848	1.001206	-0.929584
Th	-0.586317	0.222277	-0.211688
C	0.133429	-1.165835	2.183021
C	1.016207	-0.058938	2.121988
C	0.261570	1.116983	2.356197
C	-1.087054	0.738407	2.551033
C	-1.164419	-0.671908	2.445054
O	-3.105779	0.024767	0.201173
N	-4.031616	-0.172512	-0.689909
C	-4.106994	0.611914	-1.796149
C	-5.102596	0.408214	-2.734435
C	-6.041236	-0.604382	-2.551087
C	-5.945711	-1.393401	-1.406849
C	-4.935444	-1.165005	-0.490848
C	-1.515387	2.551120	-0.709651
C	-1.421050	-1.948559	-1.239422
H	-0.016112	0.877687	-3.562021
H	0.894720	-1.529619	-2.788926
H	2.497810	-1.169634	-0.663327

H	2.603566	1.475021	-0.144931
H	1.050483	2.731487	-1.937447
H	-1.917235	1.408948	2.737023
H	0.649290	2.129087	2.381962
H	2.085618	-0.107602	1.959346
H	0.406028	-2.206988	2.052793
H	-2.065614	-1.264997	2.532991
H	-1.666184	2.854645	-1.758973
H	-0.769667	3.262759	-0.317338
H	-2.449348	2.765328	-0.166965
H	-2.206721	-2.392755	-0.607686
H	-1.854044	-1.827266	-2.247154
H	-0.637482	-2.713498	-1.342041
H	-4.782246	-1.731236	0.417803
H	-6.647126	-2.197702	-1.213655
H	-6.826073	-0.774746	-3.279913
H	-5.130315	1.054471	-3.605073
H	-3.346126	1.382316	-1.848382

****

Complex 3 (Uranium)

HF=-841.5553779
G=--841.279131

C	-4.792927	-0.359352	-0.219856
N	-3.927776	-0.375663	-1.264267
C	-4.270215	0.181789	-2.451349
C	-5.509069	0.773799	-2.617833
C	-6.415569	0.802117	-1.560818
C	-6.039204	0.225049	-0.349770
O	-2.765803	-0.949215	-1.133868
U	-0.627258	-0.292630	-0.130371
C	-0.293346	-2.759984	-0.403656
C	-1.770065	1.928172	-0.449368
C	-1.725981	0.245132	2.399971
C	-0.468737	0.895841	2.404049
C	0.535541	-0.099597	2.424514
C	-0.096581	-1.363045	2.419300
C	-1.496737	-1.150186	2.406139
C	2.123377	-0.223309	-0.653852
C	1.571115	-0.794559	-1.821874
C	0.830259	0.208850	-2.492180
C	0.945677	1.407628	-1.746301
C	1.735813	1.138657	-0.606568
H	0.311787	0.092452	-3.438011
H	1.701411	-1.817132	-2.150828
H	2.746607	-0.735611	0.069172
H	2.011796	1.854224	0.158643
H	0.516279	2.365524	-2.008814
H	-2.690968	0.739134	2.412570
H	-0.307963	1.966824	2.409177
H	1.603670	0.076180	2.451539
H	0.399254	-2.325064	2.436493
H	-2.253157	-1.927448	2.424071
H	-1.970098	2.052056	-1.523126
H	-1.218836	2.800775	-0.088048

H	-2.720625	1.859233	0.099073
H	-1.108005	-3.199306	0.186001
H	-0.455833	-2.960429	-1.470648
H	0.667319	-3.172874	-0.086994
H	-4.415870	-0.824918	0.681341
H	-6.703961	0.222364	0.507053
H	-7.389482	1.264860	-1.676519
H	-5.748321	1.211460	-3.580714
H	-3.505607	0.117292	-3.213942

****

Complex 5 (Uranium)

HF=-841.5888537
G=--841.323703

C	-0.216526	-0.250772	-2.490382
C	0.041040	-1.579526	-2.908520
C	1.200522	-2.034403	-2.233899
C	1.648080	-0.993624	-1.386953
C	0.770060	0.106306	-1.540908
U	-0.750735	-1.852079	-0.252203
C	0.317846	-2.202250	2.281480
C	0.674048	-0.874787	1.944216
C	-0.507218	-0.099912	1.905432
C	-1.596799	-0.944134	2.231958
C	-1.086860	-2.243723	2.460119
O	-2.935636	-2.585861	-0.651831
N	-3.577501	-1.404650	-0.789441
C	-2.791507	-0.305636	-0.657100
C	-3.468205	0.912153	-0.794101
C	-4.836933	0.974102	-1.044375
C	-5.565825	-0.212038	-1.166971
C	-4.904674	-1.417654	-1.033387
C	-3.255535	8.835998	0.091312
C	-0.010128	-4.186762	-0.321447
H	-0.529127	-2.139126	-3.641691
H	1.669922	-3.001724	-2.356346
H	2.523517	-1.026216	-0.749469
H	0.853409	1.061636	-1.036621
H	-1.015212	0.385282	-2.848486
H	-2.633840	-0.642864	2.310389
H	-0.568356	0.958443	1.681642
H	1.678324	-0.512784	1.761837
H	0.999386	-3.035699	2.399222
H	-1.668239	-3.116857	2.733795
H	-2.335540	9.408740	-0.040782
H	-3.646987	9.003247	1.096660
H	-3.993909	9.158712	-0.645344
H	-0.674663	-4.632402	0.433866
H	-0.274375	-4.568535	-1.316279

H	1.030551	-4.428565	-0.090087
H	-5.361067	-2.397173	-1.106660
H	-6.632237	-0.210166	-1.363226
H	-5.338254	1.932728	-1.145624
H	-2.897220	1.831968	-0.700074
H	-3.044965	7.773415	-0.045241

****
******

Cp*2ThMe2

HF=-895.7696628
G=-895.323616

C	0.755818	-0.510392	2.588974
C	-0.599551	-0.947166	2.564189
C	-1.436050	0.202450	2.533283
C	-0.596345	1.356196	2.538042
C	0.757641	0.912889	2.575485
Th	-0.299677	0.267416	5.126347
C	1.413583	-1.436331	5.735374
C	-1.044587	-2.377422	2.463652
C	-2.931427	0.211263	2.392981
C	-1.064815	2.772010	2.356047
C	1.985053	1.773237	2.471280
C	0.468474	2.675297	6.393660
C	0.984026	1.649736	7.241117
C	-0.118548	1.007438	7.870120
C	-1.315018	1.632339	7.417027
C	-0.952430	2.661886	6.502827
C	1.295355	3.692184	5.659052
C	2.438441	1.391077	7.511086
C	-0.045971	-0.063392	8.919769
C	-2.694869	1.386429	7.952063
C	-1.908297	3.649776	5.895934
C	-2.347191	-1.046697	5.662581
H	1.194185	-2.379054	5.209863
H	2.456791	-1.181658	5.500729
H	1.373610	-1.664808	6.810967
H	-2.273205	-1.430898	6.692228
H	-3.308460	-0.518994	5.591924
H	-2.414946	-1.927695	5.006952
H	-0.487344	-3.034482	3.140429
H	-2.106338	-2.489795	2.697315
H	-0.892680	-2.763639	1.447229
C	1.962968	-1.389684	2.447550
H	1.794116	2.805186	2.778350
H	2.809203	1.392957	3.085757
H	2.355068	1.809507	1.438118
H	-0.340341	3.499011	2.735573

H	-1.218374	3.001897	1.293216
H	-2.017454	2.963323	2.860585
H	-3.381542	1.100281	2.847369
H	-3.230523	0.210325	1.336195
H	-3.391700	-0.661397	2.864089
H	-3.469100	1.589311	7.205815
H	-2.827956	0.353677	8.284952
H	-2.899864	2.035884	8.814115
H	-1.465334	4.188537	5.054265
H	-2.827958	3.173569	5.535813
H	-2.214525	4.403304	6.633429
H	0.755527	4.132343	4.814980
H	1.579764	4.521027	6.320911
H	2.225803	3.267343	5.268420
H	3.061640	1.586535	6.631945
H	2.812747	2.037659	8.316108
H	2.621252	0.356014	7.811238
H	-0.828004	-0.819947	8.793726
H	0.916696	-0.580854	8.907551
H	-0.172579	0.362372	9.923874
H	2.209166	-1.545305	1.388278
H	2.847907	-0.956973	2.923578
H	1.806317	-2.376170	2.892051

****

Cp*2ThMe2 adduct of pyridine_N-oxide

HF=-1219.105057
G=-1218.569559

C	-1.300064	-5.625940	6.222139
C	-0.053211	-5.090498	6.537954
C	0.096000	-3.724873	6.699825
N	-0.968287	-2.892090	6.553690
C	-2.193931	-3.391407	6.242271
C	-2.375109	-4.752176	6.073334
O	-0.821088	-1.618072	6.752453
Th	-0.321129	0.365356	5.165201
C	-2.817245	-0.169537	5.094606
C	-1.296768	2.585659	6.663451
C	0.019746	2.965673	6.264287
C	0.949683	2.163616	6.990620
C	0.210489	1.293170	7.832857
C	-1.177455	1.551757	7.629777
C	-2.568531	3.262428	6.239096
C	0.374009	4.193560	5.475629
C	2.441511	2.329919	6.965858
C	0.762484	0.367864	8.876709
C	-2.285755	0.935028	8.431053
C	1.833938	-0.907473	5.650358
C	0.904160	-0.348243	2.662447

C	-0.467915	-0.694484	2.505917
C	-1.223630	0.508195	2.426913
C	-0.325099	1.599821	2.575847
C	0.991311	1.070370	2.730733
C	2.063601	-1.287190	2.514093
C	-1.002628	-2.083619	2.304515
C	-2.657207	0.627408	2.005006
C	-0.691744	3.038265	2.346705
C	2.274408	1.851109	2.763037
H	1.912341	-1.911334	5.206164
H	2.714658	-0.350327	5.294183
H	1.952525	-1.020954	6.737925
H	-3.200239	-0.333437	6.112104
H	-3.400903	0.658425	4.665713
H	-3.078236	-1.058943	4.497910
H	-0.419353	-2.830421	2.855157
H	-2.043803	-2.168225	2.632439
H	-0.973456	-2.379746	1.246863
H	2.121690	2.882152	3.095151
H	3.014628	1.396542	3.430226
H	2.733868	1.903410	1.766400
H	0.113762	3.716834	2.635515
H	-0.898862	3.219765	1.283239
H	-1.590783	3.339222	2.897092
H	-3.145316	1.506407	2.436936
H	-2.728705	0.724238	0.912476
H	-3.248003	-0.244971	2.294116
H	-3.263511	1.113298	7.976090
H	-2.159327	-0.147822	8.531967
H	-2.316128	1.357022	9.444970
H	-2.535033	3.588567	5.193778
H	-3.433059	2.601278	6.342789
H	-2.765201	4.157730	6.844516
H	-0.427110	4.493111	4.795946
H	0.555901	5.042583	6.149340
H	1.284383	4.064751	4.881744
H	2.806489	2.612777	5.972827
H	2.765362	3.117201	7.660414
H	2.958896	1.409906	7.250064
H	0.271578	-0.610395	8.853585
H	1.835693	0.205181	8.746588
H	0.617005	0.784529	9.882597
H	2.363597	-1.360362	1.459351
H	2.939434	-0.961031	3.080559
H	1.820966	-2.300565	2.848054
H	-2.966893	-2.640468	6.140736
H	-1.430524	-6.695202	6.095618
H	0.818788	-5.723219	6.663655
H	1.024643	-3.221804	6.934741
H	-3.367554	-5.113525	5.826258

****

Cp*2Th C-H activation TS

HF=-1219.0857518
G=-1218.548027

C	-0.630951	-5.166622	5.757983
C	-0.236549	-4.931375	7.076657
C	-0.216939	-3.635972	7.556015
N	-0.578521	-2.619121	6.741803
C	-0.956214	-2.777623	5.445517
C	-0.995616	-4.086197	4.960254
O	-0.560250	-1.385344	7.204855
Th	-0.337212	0.152534	5.285059
C	-2.918060	-0.802718	5.308940
C	-1.275928	2.540861	6.516949
C	0.071376	2.860168	6.173611
C	0.931944	2.093177	7.010941
C	0.122795	1.326597	7.887997
C	-1.242399	1.591133	7.577579
C	-2.505728	3.223791	5.988201
C	0.524340	4.045189	5.371291
C	2.422776	2.242061	7.089483
C	0.624607	0.531707	9.055597
C	-2.425472	1.072065	8.342611
C	1.941912	-0.862425	5.633723
C	0.583865	-0.579601	2.665183
C	-0.828564	-0.734697	2.574877
C	-1.419200	0.559491	2.613655
C	-0.374235	1.516116	2.701064
C	0.864361	0.814256	2.759559
C	1.597646	-1.669109	2.472283
C	-1.551334	-1.995513	2.198398
C	-2.859845	0.877639	2.337311
C	-0.550008	2.978055	2.412366
C	2.229898	1.438170	2.714164
H	2.024054	-1.900525	5.280671
H	2.749645	-0.299985	5.142534
H	2.170991	-0.876540	6.708582
H	-3.288237	-1.094650	6.298583
H	-3.090585	0.283021	5.212089
H	-3.560993	-1.270667	4.554462
H	-0.891929	-2.864109	2.266393
H	-2.435294	-2.187355	2.815414
H	-1.896723	-1.941668	1.157348
H	2.274591	2.380209	3.270241
H	2.991498	0.776407	3.135091
H	2.530138	1.662211	1.681454
H	0.333667	3.562349	2.672433
H	-0.726134	3.124215	1.337459
H	-1.408551	3.417755	2.930136
H	-3.209618	1.751732	2.897367
H	-3.013779	1.101759	1.272270
H	-3.517872	0.042451	2.589117
H	-3.347862	1.127146	7.757095
H	-2.287018	0.028159	8.639068
H	-2.590254	1.657142	9.257360
H	-2.395733	3.520310	4.940543
H	-3.392582	2.585273	6.054902
H	-2.729749	4.136714	6.556622
H	-0.266346	4.436763	4.729598
H	0.822172	4.858881	6.046813
H	1.392771	3.830148	4.740222
H	2.863893	2.478690	6.116092

H	2.702652	3.054078	7.775196
H	2.903975	1.329752	7.451475
H	-0.107974	-0.207700	9.383864
H	1.548838	-0.004253	8.818985
H	0.838908	1.193430	9.905930
H	1.785129	-1.842295	1.403603
H	2.555266	-1.421956	2.936230
H	1.269830	-2.619957	2.903595
H	-1.758976	-1.793691	5.148994
H	-0.654648	-6.178451	5.364860
H	0.055422	-5.740841	7.736602
H	0.075649	-3.343232	8.556238
H	-1.324180	-4.249316	3.939542

****

Cp*2ThMe_pyridyl_N-oxide adduct of CH4

HF=-1219.105057
G=-1218.618773

C	0.714944	-4.698930	5.943241
C	-0.505419	-4.704651	6.619863
C	-1.209890	-3.520538	6.738341
N	-0.693868	-2.399279	6.192155
C	0.483863	-2.298532	5.523861
C	1.189447	-3.500923	5.411033
O	-1.375141	-1.248126	6.302474
Th	0.190419	0.306253	5.198123
C	-5.174420	-1.980725	5.870941
C	-0.771349	2.772567	6.367241
C	0.646294	2.907763	6.370749
C	1.176025	1.976986	7.308905
C	0.088051	1.241548	7.856426
C	-1.115012	1.731870	7.274835
C	-1.758247	3.695594	5.711745
C	1.460088	3.933802	5.635083
C	2.591879	1.959271	7.802780
C	0.170696	0.207247	8.944994
C	-2.508411	1.321802	7.657087
C	2.692660	0.205978	5.103717
C	0.409189	-0.709204	2.509083
C	-0.966878	-0.824767	2.856830
C	-1.505957	0.488156	2.956726
C	-0.457845	1.414997	2.679710
C	0.726763	0.669055	2.412924
C	1.330264	-1.830921	2.148504
C	-1.761939	-2.095674	2.940546
C	-2.958006	0.802287	3.178299
C	-0.604333	2.890501	2.442960
C	2.033800	1.243984	1.950291
H	3.112625	-0.462685	4.349535
H	3.141237	1.194683	4.941107

H	3.076575	-0.153398	6.070647
H	-5.807224	-2.224457	6.727160
H	-5.416301	-0.976235	5.517892
H	-5.359023	-2.697817	5.068147
H	-1.127898	-2.974036	3.086970
H	-2.483407	-2.073862	3.763467
H	-2.336230	-2.272900	2.021264
H	2.215700	2.238962	2.369855
H	2.878871	0.612183	2.236357
H	2.056727	1.349236	0.856805
H	0.248160	3.462268	2.823569
H	-0.672197	3.101603	1.367175
H	-1.508013	3.293915	2.903923
H	-3.117319	1.853208	3.435009
H	-3.547169	0.604204	2.272759
H	-3.394454	0.194632	3.978750
H	-3.233525	1.587773	6.881423
H	-2.582079	0.241643	7.815010
H	-2.830776	1.819534	8.581552
H	-1.292713	4.312253	4.940152
H	-2.597309	3.163588	5.251041
H	-2.191518	4.381148	6.452098
H	0.864662	4.471582	4.893117
H	1.871376	4.682958	6.324314
H	2.313922	3.487320	5.111182
H	3.310436	2.181855	7.009211
H	2.730697	2.710501	8.592476
H	2.868188	0.991071	8.230214
H	-0.642055	-0.522552	8.864451
H	1.117259	-0.343200	8.915639
H	0.100145	0.660207	9.943282
H	1.358689	-1.983959	1.061285
H	2.355369	-1.617946	2.479770
H	1.022438	-2.774918	2.605735
H	-4.123917	-2.018580	6.164329
H	1.284562	-5.618229	5.838513
H	-0.914854	-5.610286	7.054003
H	-2.162512	-3.409537	7.241150
H	2.137225	-3.482246	4.883549

****

Cp*2ThMe_pyridyl_N-oxide

HF=-1178.6447348
G=-1178.151526

C	0.683265	-4.665338	5.847462
C	-0.535438	-4.693500	6.577155
C	-1.066907	-3.372073	6.600838
C	-0.179341	-2.525975	5.878085
C	0.901858	-3.326456	5.406401
Th	1.272261	-3.152391	8.202261
C	2.085641	-5.441427	8.793396

C	-1.221372	-5.922107	7.097146
C	-2.406797	-2.962473	7.137932
C	-0.425095	-1.073569	5.583010
C	1.959615	-2.913609	4.422886
C	1.518311	-5.850687	5.460327
C	-0.487637	-3.867884	10.038165
N	-0.963037	-2.599472	10.150663
C	-1.953852	-2.191251	10.971291
C	-2.561964	-3.121851	11.794581
C	-2.131881	-4.449354	11.751901
C	-1.104183	-4.802103	10.877331
O	-0.360079	-1.701271	9.357826
C	4.069646	-2.478049	8.163790
C	3.407361	-1.271485	7.792197
C	2.684102	-0.801446	8.923379
C	2.907402	-1.711010	9.996810
C	3.777571	-2.738609	9.532378
C	3.610755	-0.511178	6.513194
C	5.030442	-3.260887	7.315232
C	4.433441	-3.784701	10.383763
C	2.416098	-1.535859	11.405626
C	1.925168	0.490809	9.013419
H	1.304039	-6.192228	8.611401
H	2.971470	-5.754839	8.218773
H	2.350106	-5.516853	9.857219
H	-2.760971	-3.648488	7.912700
H	-2.380922	-1.957925	7.570458
H	-3.163705	-2.957653	6.341888
H	2.581438	-5.597902	5.388913
H	1.428864	-6.664684	6.184002
H	1.216164	-6.245838	4.480750
H	2.940229	-3.346876	4.649216
H	1.695737	-3.250179	3.411239
H	2.079532	-1.828747	4.377143
H	0.481017	-0.564442	5.241598
H	-1.177436	-0.950096	4.792577
H	-0.796672	-0.534983	6.462161
H	1.592842	0.837761	8.029739
H	1.035800	0.391518	9.641963
H	2.548922	1.287900	9.439993
H	3.928059	-1.160356	5.693183
H	2.707467	0.016512	6.188891
H	4.392069	0.250947	6.636730
H	4.804158	-3.174407	6.247435
H	6.062284	-2.908958	7.449416
H	5.019898	-4.325783	7.567928
H	4.664933	-4.691163	9.818503
H	5.377023	-3.407244	10.800980
H	3.805125	-4.081596	11.228997
H	1.434246	-1.053778	11.430765
H	2.331018	-2.492165	11.931446
H	3.101366	-0.908430	11.991679
H	-1.900531	-6.340484	6.342066
H	-0.507006	-6.707736	7.358268
H	-1.816775	-5.711005	7.990040
H	-2.595198	-5.192646	12.394808
H	-3.358782	-2.800950	12.456815
H	-2.205143	-1.138772	10.924065
H	-0.758302	-5.831336	10.834394

****

pyridine

HF=-248.1955869

G=-248.133892

N	0.015651	0.000000	0.008986
C	0.049874	0.000000	1.344776
C	1.227724	0.000000	2.090663
C	2.442256	0.000000	1.410075
C	2.424413	0.000000	0.017927
C	1.189572	0.000000	-0.629223
H	-0.916354	0.000000	1.847446
H	1.189280	0.000000	3.175791
H	3.383281	0.000000	1.953343
H	3.344934	0.000000	-0.557943
H	1.141700	0.000000	-1.717341

****

Molecule **9 (Zirconium)**

HF=-509.3217672
G=-509.191522

C	1.416893	-2.400841	4.742418
C	0.356782	-1.514042	5.112830
C	0.894161	-0.527369	5.964085
C	2.272845	-0.822948	6.158457
C	2.601156	-1.953553	5.362878
H	3.568154	-2.434501	5.305467
H	1.333322	-3.254886	4.080557
H	-0.669439	-1.573344	4.770392
H	0.348516	0.286070	6.424831
H	2.970157	-0.240641	6.750983
Zr	1.096928	-2.834359	7.236563
C	-1.256469	-3.368762	8.124912
C	-1.200003	-1.950982	8.215819
C	-0.193159	-1.617143	9.145578
C	0.340861	-2.835178	9.673111
C	-0.333567	-3.910763	9.061937
H	-1.939981	-3.939381	7.505563
H	-1.790719	-1.254050	7.635477
H	0.095668	-0.615740	9.442423
H	1.119082	-2.920437	10.422145
H	-0.131707	-4.960667	9.225889
O	2.202558	-4.203080	7.379085

****

Molecule **9 (Thorium)**

HF=-498.1965024

G=-498.070121

C	0.131442	-0.032012	-0.039418
C	-0.049545	-0.056556	1.367250
C	1.228678	-0.095032	1.967436
C	2.202419	-0.112289	0.932041
C	1.523224	-0.086523	-0.306906
Th	1.030186	2.526489	0.875462
O	-0.112306	3.412691	2.087356
C	3.253455	4.210853	0.274894
C	2.120542	4.937908	-0.162783
C	1.597786	4.279996	-1.301353
C	2.425471	3.160865	-1.585086
C	3.448524	3.118671	-0.612001
H	1.714805	5.828055	0.302800
H	3.893048	4.475443	1.110588
H	4.253795	2.394818	-0.565438
H	2.308689	2.478155	-2.418565
H	0.744131	4.606722	-1.886117
H	-0.997821	-0.036386	1.891233
H	1.427434	-0.138153	3.032941
H	3.276026	-0.181977	1.067895
H	1.983625	-0.113977	-1.286873
H	-0.660265	-0.036307	-0.781621

****

Molecule **9 (Uranium)**

HF=-513.6941773
G=-513.568130

C	2.769061	0.430530	0.046041
C	2.395536	-0.925357	-0.133784
C	1.751813	-1.040589	-1.388769
C	1.719978	0.244406	-1.984090
C	2.348009	1.153175	-1.095197
H	3.287646	0.836718	0.906525
H	2.593266	-1.733730	0.561170
H	1.378963	-1.955812	-1.832655
H	1.322732	0.483050	-2.963040
H	2.514839	2.209823	-1.277604
O	0.020414	0.472417	2.086594
U	0.006257	0.416341	0.258693
C	-2.758799	0.443977	0.074692
C	-2.396454	-0.917758	-0.081764
C	-1.765517	-1.062344	-1.340188
C	-1.731855	0.210138	-1.961860
C	-2.344809	1.140718	-1.085235
H	-3.266570	0.870755	0.931706
H	-2.591869	-1.710482	0.631574
H	-1.403392	-1.988933	-1.769215
H	-1.343045	0.426088	-2.949380
H	-2.506204	2.194683	-1.287154

****

Transition State **8 (Zirconium)**

HF=-837.1468787
G=-836.863443

C	0.532892	-0.989362	2.262468
C	-0.614140	-0.200993	2.561606
C	-0.247469	1.155350	2.462767
C	1.105462	1.222371	2.055031
C	1.591950	-0.111957	1.953784
Zr	-0.089579	0.201196	0.033637
C	0.695442	-1.069874	-2.123091
C	0.357820	0.242471	-2.538993
C	1.292707	1.137227	-1.967151
C	2.188990	0.382269	-1.175878
C	1.822968	-0.986308	-1.275536
C	-2.482012	-0.049813	-0.296179
C	-1.003599	-2.103354	-0.004370
H	-1.594143	-0.578779	2.822937
H	0.582688	-2.069414	2.272314
H	2.601637	-0.402356	1.694122
H	1.672513	2.127053	1.877508
H	-0.906979	2.001488	2.593692
H	2.315565	-1.816836	-0.785546
H	0.184355	-1.977277	-2.412276
H	-0.458296	0.504655	-3.199721
H	1.289230	2.213643	-2.064072
H	3.016848	0.782148	-0.603983
H	-1.580103	-2.348948	-0.895491
H	-0.067683	-2.670770	0.013940
H	-1.586453	-2.298693	0.894353
H	-3.044669	-0.763423	0.303813
H	-2.737366	0.988303	-0.055177
H	-2.637476	-0.255999	-1.359425
N	-2.211901	2.914671	-0.652317
C	-2.518565	3.884979	0.214440
C	-3.056451	5.092329	-0.213041
C	-3.261328	5.296014	-1.577053
C	-2.922714	4.275902	-2.466044
C	-2.391442	3.094956	-1.964800
H	-2.318402	3.669056	1.258258
H	-3.308393	5.855186	0.516629
H	-3.670899	6.233184	-1.940932
H	-3.067987	4.387021	-3.535833
H	-2.097726	2.264882	-2.598007
O	-0.687267	2.069022	-0.234255

****

Transition State **8 (Thorium)**

HF=-826.0105951

G=-825.738639

C	0.322493	-0.955642	2.495533
C	-0.805678	-0.117553	2.668374
C	-0.375704	1.221475	2.530948
C	1.014844	1.213808	2.259869
C	1.446989	-0.133465	2.245964
Th	-0.159318	0.162465	-0.106071
C	1.131559	-1.252932	-2.247684
C	0.936363	0.054094	-2.747621
C	1.817418	0.925173	-2.053732
C	2.542083	0.159583	-1.119842
C	2.109907	-1.188041	-1.227628
C	-2.738204	0.014611	-0.607351
C	-1.007690	-2.262641	-0.124008
H	-1.817729	-0.444710	2.874412
H	0.324873	-2.037209	2.548981
H	2.461817	-0.476393	2.084387
H	1.638391	2.086156	2.101598
H	-1.004120	2.100852	2.602834
H	2.485828	-2.026616	-0.652969
H	0.618820	-2.146772	-2.579965
H	0.257245	0.338440	-3.543606
H	1.898018	1.994695	-2.202328
H	3.297111	0.533761	-0.438412
H	-1.456864	-2.520412	-1.085775
H	-0.081457	-2.827352	0.042183
H	-1.717012	-2.420800	0.690352
H	-3.272592	-0.791919	-0.101117
H	-3.148903	0.989244	-0.319890
H	-2.832581	-0.122061	-1.693557
N	-1.731868	3.523261	-1.001161
C	-1.857968	4.488244	-0.095540
C	-2.933873	5.367849	-0.147810
C	-3.886705	5.200381	-1.153033
C	-3.735491	4.165111	-2.073261
C	-2.630535	3.325055	-1.960100
H	-1.079193	4.542148	0.659322
H	-3.018261	6.163867	0.584877
H	-4.742015	5.866479	-1.213404
H	-4.459560	4.000898	-2.864492
H	-2.442532	2.491439	-2.628908
O	-0.679884	2.096647	-0.548240

****

Transition State **8 (Uranium)**

HF=-841.4935253
G=-841.222135

C	-2.839007	3.181866	-1.806711
N	-1.699357	3.355215	-1.135322
C	-1.493215	4.400625	-0.331495
C	-2.474807	5.370423	-0.182195
C	-3.679054	5.225479	-0.872896
C	-3.861421	4.116526	-1.697815

O	-0.741580	2.025072	-0.875157
U	-0.286214	0.102170	-0.279940
C	1.739781	0.983957	-2.079267
C	1.110017	-0.096737	-2.741906
C	1.457855	-1.292946	-2.062119
C	2.254307	-0.947857	-0.956976
C	2.426897	0.467655	-0.965532
C	0.004765	-0.941671	2.334083
C	-1.111807	-0.070731	2.389284
C	-0.643559	1.251753	2.213577
C	0.757196	1.200278	2.030235
C	1.156708	-0.158537	2.116375
C	-2.770953	0.058754	-0.278063
C	-0.784245	-2.319488	-0.317502
H	-2.139621	-0.363519	2.558489
H	-0.021838	-2.017395	2.446144
H	2.171901	-0.526581	2.040262
H	1.414314	2.048070	1.875918
H	-1.256395	2.144845	2.203472
H	2.679461	-1.638224	-0.239397
H	1.154298	-2.293534	-2.339766
H	0.515522	-0.028338	-3.646974
H	1.664747	2.027690	-2.353794
H	3.012372	1.040658	-0.256810
H	-1.157934	-2.503510	-1.336994
H	0.064454	-2.981387	-0.122214
H	-1.586364	-2.522132	0.398948
H	-3.213865	-0.786889	0.252811
H	-3.238779	0.995885	0.039324
H	-2.924430	-0.083146	-1.362671
H	-0.532930	4.427360	0.172390
H	-2.292616	6.223119	0.463459
H	-4.465562	5.965817	-0.766425
H	-4.781447	3.970131	-2.253883
H	-2.899573	2.290492	-2.420820

****

Complex **7 (Zirconium)**

HF=-837.2159728
G=-836.932119

C	0.459765	-1.256501	2.238352
C	-0.766635	-0.605265	2.531020
C	-0.550166	0.785686	2.464476
C	0.807325	1.006347	2.113547
C	1.433811	-0.261890	1.993430
Zr	-0.218572	-0.054673	0.063232
C	0.831760	-0.966799	-2.111522
C	0.126685	0.202025	-2.494533
C	0.794690	1.314415	-1.921915
C	1.879754	0.836458	-1.158199
C	1.904674	-0.579128	-1.278413
C	-2.522561	0.065263	-0.237779
C	-0.814822	-2.278176	-0.185150
H	-1.710799	-1.093280	2.732957

H	0.615918	-2.325636	2.200373
H	2.473302	-0.437331	1.747499
H	1.276285	1.970497	1.970976
H	-1.300477	1.552917	2.595015
H	2.622787	-1.247427	-0.820108
H	0.587026	-1.978370	-2.399742
H	-0.736604	0.232580	-3.147008
H	0.518048	2.353637	-2.031701
H	2.571890	1.443910	-0.589196
H	-1.355773	-2.420470	-1.129725
H	0.043082	-2.966921	-0.186486
H	-1.487427	-2.590546	0.622724
H	-2.967623	-0.735242	0.366479
H	-2.988061	1.004211	0.094641
H	-2.850629	-0.127362	-1.270505
N	-1.536814	3.317608	-0.440235
C	-1.687898	4.585413	0.042156
C	-2.494032	5.503777	-0.599794
C	-3.174481	5.146955	-1.763835
C	-3.012617	3.849874	-2.240459
C	-2.197030	2.950940	-1.574218
H	-1.127027	4.781048	0.946383
H	-2.581111	6.498686	-0.176126
H	-3.812049	5.857098	-2.278601
H	-3.520392	3.510624	-3.137162
H	-2.045249	1.922385	-1.868106
O	-0.759639	2.505564	0.191589

****

Complex **7 (Thorium)**

HF=-826.0756685
G=-825.801532

C	0.025256	-0.546090	2.567018
C	-1.174013	0.196396	2.459381
C	-0.837886	1.519184	2.089340
C	0.570179	1.595507	1.958878
C	1.103128	0.316862	2.258103
Th	-0.221033	-0.034555	-0.218737
C	1.012567	-0.957827	-2.597384
C	1.106593	0.451466	-2.677680
C	2.043944	0.883323	-1.707848
C	2.542847	-0.262914	-1.043238
C	1.900948	-1.398983	-1.585506
C	-2.703551	-0.128631	-0.714511
C	-0.491383	-2.499049	0.136450
H	-2.175178	-0.183605	2.622437
H	0.103267	-1.591131	2.835430
H	2.153736	0.051947	2.266080
H	1.146394	2.475137	1.694824
H	-1.542271	2.329027	1.938046
H	2.059390	-2.426554	-1.286600
H	0.382532	-1.593305	-3.209717
H	0.555550	1.092939	-3.354385
H	2.337972	1.909838	-1.524081
H	3.289568	-0.268655	-0.257797

H	-0.735027	-2.971742	-0.829648
H	0.375303	-3.040136	0.542692
H	-1.340426	-2.696928	0.807963
H	-3.097183	-1.059381	-0.279119
H	-3.334709	0.684605	-0.324261
H	-2.905155	-0.200121	-1.798843
N	-1.665521	3.203694	-1.022678
C	-1.460173	4.295624	-0.240308
C	-2.437279	5.264685	-0.109069
C	-3.648961	5.128754	-0.784147
C	-3.836247	4.002807	-1.582308
C	-2.837343	3.052063	-1.691497
H	-0.492347	4.323385	0.241948
H	-2.235161	6.121171	0.524910
H	-4.425138	5.880329	-0.690850
H	-4.759294	3.844344	-2.129198
H	-2.905414	2.145479	-2.276226
O	-0.719254	2.322378	-1.152954

****

Complex **7 (Uranium)**

HF=-841.5474199
G=--841.271929

C	-2.807761	3.173537	-1.736852
N	-1.645689	3.182061	-1.035679
C	-1.402941	4.159659	-0.124391
C	-2.334060	5.155111	0.106940
C	-3.535236	5.164737	-0.599493
C	-3.760591	4.154993	-1.531897
O	-0.743138	2.274917	-1.265851
U	-0.297059	-0.007076	-0.323392
C	1.643650	0.893491	-2.172198
C	1.074256	-0.267723	-2.753506
C	1.495174	-1.386231	-1.995580
C	2.297319	-0.915068	-0.933158
C	2.393572	0.495244	-1.047146
C	0.000268	-0.722263	2.361996
C	-1.192399	0.035997	2.316594
C	-0.848471	1.376658	2.027836
C	0.557837	1.447136	1.883703
C	1.080966	0.148157	2.095102
C	-2.753952	0.080349	-0.551421
C	-0.727115	-2.422942	-0.256638
H	-2.194460	-0.342099	2.474480
H	0.071941	-1.783746	2.561103
H	2.128104	-0.126099	2.070109
H	1.142344	2.336015	1.673781
H	-1.547702	2.200558	1.946500
H	2.767620	-1.528944	-0.174707
H	1.247329	-2.419987	-2.193937
H	0.459749	-0.297444	-3.646933
H	1.509589	1.908764	-2.521351
H	2.951968	1.150590	-0.389572
H	-1.092383	-2.733426	-1.248474
H	0.097416	-3.088049	0.025471
H	-1.548003	-2.560752	0.461220
H	-3.186144	-0.793621	-0.047918
H	-3.306409	0.967764	-0.217075

H	−2.935468	−0.052782	−1.634063
H	−0.447340	4.076686	0.375228
H	−2.104295	5.917196	0.843638
H	−4.275034	5.938823	−0.427643
H	−4.677605	4.112360	−2.109299
H	−2.905403	2.351614	−2.432124