Supporting information

The Bond Between CO and Cp'_3U in $Cp'_3U(CO)$ involves Backbonding from the Cp'_3U Ligand-based Orbitals of π-Symmetry, where Cp' Represents a Substituted Cyclopentadienyl Ligand.

Laurent Maron,[a] Odile Eisenstein,[b]* Richard A. Andersen[c]

a) LPCNO, Université de Toulouse, INSA, UPS, LPCNO, 135 avenue de Rangueil, F-31077 Toulouse, France, and CNRS, LPCNO, F-31077 Toulouse, France b) Institut Charles Gerhardt, Université Montpellier 2, UMR 5253 CNRS-UM2-ENSCM-UM1, Place E. Bataillon, F-34095 Montpellier France, and CNRS, Institut Charles Gerhardt, F-34095 Montpellier France, c) Department of Chemistry and Chemical Sciences Division of Lawrence Berkeley National Laboratory, University of California, Berkeley, California 94720-1460

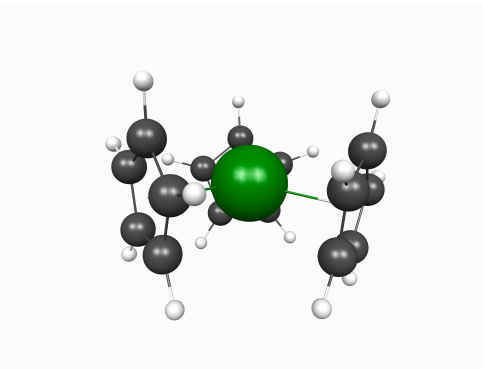
List of coordinates for all optimized species with the 32 electron ECP for uranium. E in au. Unscaled ν_{CO} in cm^{-1} for the CO adducts.

Cn is the center of the cyclopentadienyl rings. The coordinates of Cn are obtained from the calculated coordinates of the carbon atoms of each ring. Drawings are added.

CO
E =-113.294338, ν_{CO} = 2173 cm^{-1}
C 0.000000 0.000000 -0.013444
O 0.000000 0.000000 1.1334444

Base free species

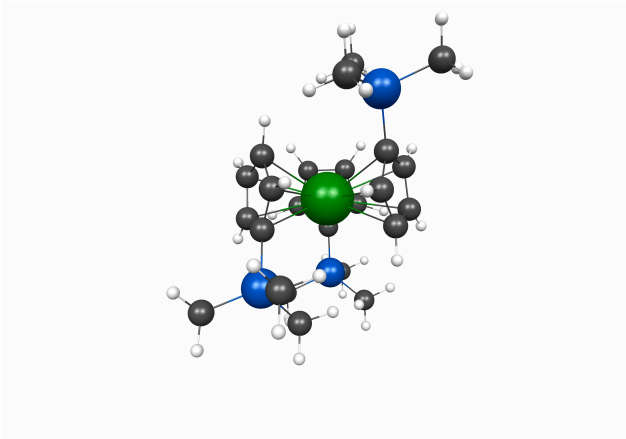
$(C_5H_5)_3U$
E = -1057.5304183



31 (and 3 Cn)

C	0.094559	2.521204	-1.222589
C	-1.253549	2.104699	-1.376479
C	-1.850781	2.072561	-0.093815
C	-0.869034	2.446106	0.855363
C	0.329820	2.736188	0.155692
U	0.001505	0.000077	-0.108548
C	-2.228431	-1.183719	-1.220438
C	-1.193896	-2.143525	-1.373179
C	-0.866612	-2.641970	-0.089876
C	-1.680413	-1.976711	0.858578
C	-2.531975	-1.085442	0.157730
C	2.145576	-1.338356	-1.217020
C	2.460109	0.037901	-1.363931
C	2.724269	0.565990	-0.077912
C	2.551389	-0.474597	0.866559
C	2.207102	-1.654870	0.160364
H	2.536699	0.577668	-2.300421
H	1.936050	-2.033547	-2.020570
H	-3.302767	-0.467389	0.599423
H	0.806854	2.683971	-2.022033
H	3.031493	1.579703	0.141109
H	-1.692999	-2.161249	1.927804
H	-2.883273	1.830833	0.119718
H	-2.727317	-0.651318	-2.020879
H	-1.023515	2.549973	1.924392
H	-0.765434	-2.474449	-2.311829
H	-1.753315	1.898922	-2.315657
H	2.713114	-0.397070	1.936736
H	2.057250	-2.633242	0.597932
H	-0.142003	-3.415810	0.124595
H	1.249953	3.095300	0.597999
Cn	-0.709797	2.3761516	-0.3363656
Cn	-1.7002654	-1.8062734	-0.333437
Cn	2.417689	-0.5727864	-0.326388

$(C_5H_4(SiMe_3)_3U$
E -1426.6783313

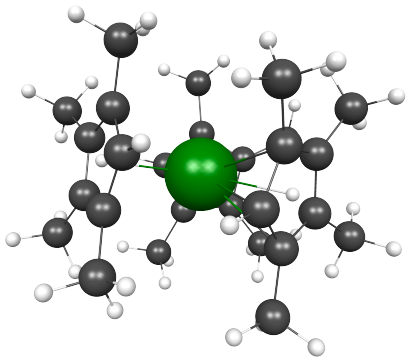


67

C	1.917446	1.114273	1.808513
C	0.739343	1.010646	2.581865
C	0.507494	-0.366767	2.836571
C	1.535024	-1.097972	2.205620
C	2.427060	-0.192957	1.549030
U	0.026302	-0.049898	0.126635
C	-1.438975	-2.245918	0.964067
C	-2.374594	-1.472210	0.210301
C	-1.936585	-1.536770	-1.147111
C	-0.759831	-2.314681	-1.219351
C	-0.452086	-2.757830	0.094387
C	-0.723801	1.430734	-2.099865
C	-0.073763	2.375689	-1.241749
C	1.306830	2.019787	-1.243956
C	1.494144	0.881718	-2.060660
C	0.233784	0.528757	-2.605553
Si	-0.804015	3.956196	-0.517282
H	-1.777709	1.431780	-2.355450
H	0.369673	-3.407662	0.370555
H	2.377827	2.041307	1.492915
H	2.092204	2.557459	-0.730223
H	-0.213728	-2.568215	-2.120450
H	-0.297301	-0.776621	3.434323
H	-1.494351	-2.439444	2.028409
H	1.647995	-2.175097	2.245301
Si	-4.029315	-0.818431	0.831039
H	0.152698	1.837881	2.967048
H	2.441611	0.406721	-2.287403
H	0.042421	-0.280722	-3.298768
H	-2.438875	-1.080770	-1.991315
Si	4.102239	-0.651599	0.815160
C	-4.803761	0.305553	-0.485457
C	-5.192925	-2.281917	1.153040
C	-3.804598	0.134596	2.458080
H	-6.169531	-1.937740	1.511080
H	-5.349968	-2.862710	0.238618
H	-4.773421	-2.955377	1.907364

H	-5.760882	0.705805	-0.134460
H	-4.157384	1.153379	-0.733300
H	-4.995833	-0.250949	-1.408711
H	-4.773484	0.465545	2.847926
H	-3.340759	-0.498371	3.222151
H	-3.179093	1.024346	2.332429
C	5.238010	-1.239886	2.217852
C	3.922692	-2.070981	-0.434849
C	4.903302	0.852499	-0.014714
H	4.903112	-2.370020	-0.821724
H	3.470921	-2.951859	0.033724
H	3.299072	-1.787995	-1.289102
H	5.898326	0.587832	-0.388818
H	4.317201	1.224799	-0.859765
H	5.027563	1.673242	0.699471
H	6.223858	-1.524113	1.833175
H	5.377272	-0.447789	2.960511
H	4.812803	-2.107460	2.732817
C	-2.130888	3.589096	0.794541
C	0.580806	4.968851	0.287318
C	-1.605519	4.959452	-1.912302
H	0.184758	5.912854	0.676834
H	1.039832	4.431589	1.123438
H	1.367021	5.209312	-0.435344
H	-2.550934	4.522191	1.186282
H	-2.960299	3.005946	0.381340
H	-1.713875	3.037563	1.644539
H	-2.030700	5.894805	-1.532220
H	-0.868158	5.207325	-2.682288
H	-2.410998	4.393979	-2.392116

$(C_5HMe_4)_3U$
E = -1529.1613162

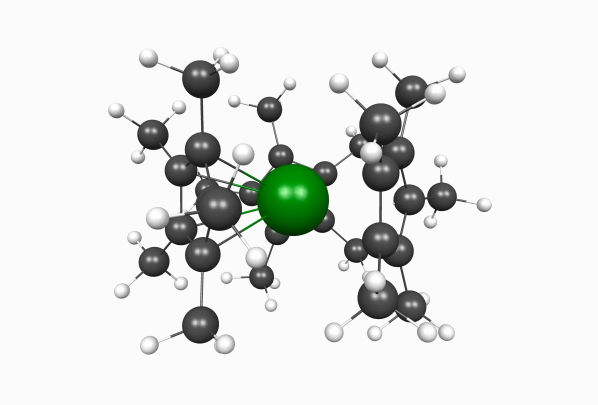


67 (and 3 Cn)

C	2.289313	0.461004	1.040606
C	1.182581	0.794604	1.860597
C	0.616182	-0.396253	2.380970
C	1.413394	-1.483711	1.918835
C	2.435265	-0.957237	1.082429
U	-0.017736	-0.356647	-0.325386
C	-1.182414	-2.842484	-0.603126
C	0.218349	-3.061496	-0.666730
C	0.703744	-2.569855	-1.902226
C	-0.414426	-2.077616	-2.636448
C	-1.578517	-2.250312	-1.839287
C	-0.106900	2.415326	-0.450433
C	-1.385464	2.063812	0.046354
C	-2.114464	1.482657	-1.031283
C	-1.282358	1.492522	-2.185478
C	-0.021341	2.041826	-1.814085
H	0.851906	1.797705	2.095075
C	1.118735	2.348903	-2.744553
H	0.809663	-3.565076	0.084840
C	1.346335	-2.874560	2.477495
H	0.669737	2.922979	0.106849
C	-3.003795	-2.116609	-2.288323
C	-1.739234	1.301082	-3.600397
C	-0.356261	-1.736030	-4.096265
C	-2.115922	-3.319352	0.475472
C	3.617244	-1.708632	0.545290
C	3.270646	1.415988	0.422937
C	-1.967737	2.422515	1.383609
C	2.082793	-2.746576	-2.472070
C	-0.494677	-0.492952	3.389659
C	-3.580851	1.162490	-0.986435
H	2.529988	-1.810557	-2.831053
H	2.766308	-3.176387	-1.737251
H	2.061579	-3.427384	-3.333830
H	0.433412	-1.013349	-4.331986
H	-0.141623	-2.636302	-4.689198
H	-1.298728	-1.327492	-4.464147
H	-3.123606	-1.391893	-3.097309
H	-3.380368	-3.078515	-2.663843
H	-3.669695	-1.815628	-1.473596
H	-2.903325	-2.592169	0.711429
H	-2.630024	-4.243794	0.179227
H	-1.578701	-3.537733	1.403113
H	2.033973	2.574031	-2.189025
H	1.341918	1.522635	-3.430486

H	0.898966	3.223735	-3.371247
H	-0.920041	1.018464	-4.265627
H	-2.523641	0.546363	-3.697611
H	-2.155461	2.241061	-3.990028
H	-4.182611	2.082001	-0.990628
H	-3.896834	0.566683	-1.845162
H	-3.863991	0.611275	-0.081389
H	-1.196314	2.744603	2.088071
H	-2.681014	3.252564	1.288843
H	-2.517645	1.595363	1.849292
H	1.928243	-3.590166	1.890033
H	1.759109	-2.894482	3.495678
H	0.323171	-3.258477	2.547251
H	-1.019317	0.460614	3.495309
H	-1.240557	-1.256614	3.134391
H	-0.107516	-0.760216	4.382074
H	3.947769	-1.325501	-0.425486
H	4.475189	-1.625951	1.227287
H	3.408653	-2.775232	0.424112
H	3.551472	1.136401	-0.599672
H	2.873361	2.434099	0.389039
H	4.202884	1.453869	1.002887
Cn	1.587347	-0.3163186	1.6566874
Cn	-0.45065	-2.56035	-1.529563
Cn	-0.982105	1.899229	-1.086985

$(C_5Me_5)_3U$
E = -1647.0318812 au



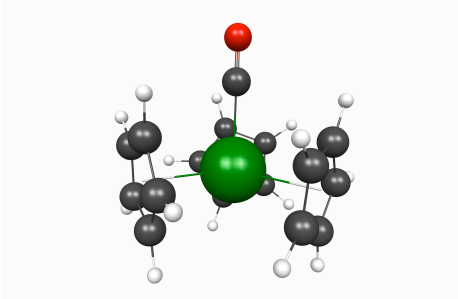
76

C	1.480754	0.841546	1.861644
C	0.421624	0.090222	2.440507
C	0.714251	-1.295888	2.272275
C	1.915967	-1.398923	1.521154
C	2.367557	-0.075571	1.234755
U	0.008098	-0.348578	-0.345122
C	-1.751007	-2.603951	-0.466227
C	-0.464257	-3.210487	-0.410287
C	0.206528	-2.908535	-1.628337
C	-0.706841	-2.217632	-2.480938
C	-1.917551	-2.032331	-1.764302
C	0.636963	2.272189	-1.250059
C	-0.552292	2.433257	-0.490856
C	-1.614466	1.789957	-1.199235
C	-1.094124	1.302105	-2.428595
C	0.309163	1.528738	-2.425656
C	-0.656552	0.607884	3.351068
C	1.249760	1.344056	-3.583677
C	-0.095026	-4.341539	0.503349
C	2.785769	-2.608486	1.327248
C	1.933900	3.016996	-1.111546
C	-3.267175	-1.669303	-2.312543
C	-1.909091	1.028666	-3.656805
C	-0.474788	-2.068042	-3.956931
C	-2.880604	-2.797808	0.507112
C	3.713371	0.240644	0.644557
C	1.834886	2.247889	2.244834
C	-0.806727	3.399683	0.629374
C	1.514555	-3.485190	-2.094426
C	0.044090	-2.358394	3.094415
C	-3.063309	1.917346	-0.818742
H	2.231891	-2.726749	-2.434084
H	2.001149	-4.066058	-1.307362
H	1.363960	-4.164957	-2.944790
H	0.309962	-1.348978	-4.215276
H	-0.165176	-3.030636	-4.385246
H	-1.384019	-1.768299	-4.482309
H	-3.224902	-1.414476	-3.372715
H	-3.948516	-2.525287	-2.215440
H	-3.744806	-0.833767	-1.789754
H	-3.510124	-1.904976	0.597077
H	-3.545071	-3.614561	0.189420
H	-2.527410	-3.051235	1.510137
H	2.207218	0.895372	-3.290771
H	0.817058	0.714803	-4.364898
H	1.493932	2.308165	-4.052758
H	-1.462700	0.286095	-4.318593
H	-2.923704	0.706287	-3.422495
H	-1.998677	1.957863	-4.237210
H	-3.246305	1.672806	0.234728

H	-3.423429	2.946061	-0.963570
H	-3.705588	1.269768	-1.420658
H	0.101015	3.924444	0.929591
H	-1.527701	4.162461	0.305443
H	-1.230247	2.933988	1.525517
H	2.890198	-2.923853	0.283595
H	3.800165	-2.402919	1.693151
H	2.416172	-3.465431	1.895065
H	-1.022270	-2.478989	2.874469
H	0.517473	-3.332994	2.969154
H	0.113749	-2.101796	4.160120
H	3.896696	1.317051	0.612693
H	4.520140	-0.201602	1.245757
H	3.846751	-0.145845	-0.374457
H	2.312961	2.814830	1.445564
H	0.968726	2.814478	2.588317
H	2.544904	2.219604	3.083445
H	2.799632	2.374546	-0.921745
H	2.148849	3.564377	-2.038678
H	1.890738	3.760139	-0.312605
H	0.962995	-4.368990	0.765209
H	-0.671263	-4.331693	1.428881
H	-0.323299	-5.292559	0.001500
H	-0.843380	1.675394	3.208537
H	-1.610412	0.086310	3.208522
H	-0.384955	0.471232	4.407908

CO adducts

$(C_5H_5)_3U(CO)$
E = -1170.8260277 ν_{co} = 1995 cm^{-1}

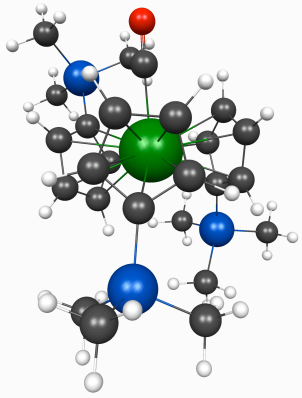


33 (and 3 Cn)

C	0.277209	2.605737	-1.045820
C	-0.988932	2.159595	-1.507847
C	-1.846706	2.046555	-0.384509
C	-1.104981	2.387515	0.768101
C	0.210830	2.735101	0.355992
U	-0.001011	-0.001159	-0.149842
C	-0.032943	0.013319	2.225946
O	-0.050919	0.017254	3.380977
C	-2.424392	-1.062385	-0.971122
C	-1.417772	-1.919445	-1.488565
C	-0.842455	-2.621860	-0.398675
C	-1.464130	-2.174575	0.786941
C	-2.445000	-1.207341	0.430444
C	2.146020	-1.537847	-0.995522
C	2.405757	-0.216451	-1.444741
C	2.699495	0.579269	-0.308880
C	2.590231	-0.237992	0.837953
C	2.247701	-1.550311	0.410218
H	2.435916	0.110557	-2.478314
H	1.918739	-2.386998	-1.627747
H	-3.109198	-0.695241	1.115681
H	1.139742	2.814436	-1.666277
H	2.981614	1.623442	-0.318731
H	-1.278133	-2.551008	1.784947
H	-2.892735	1.772253	-0.405993
H	-3.066935	-0.417445	-1.556847
H	-1.489681	2.446170	1.778446
H	-1.180374	-2.062660	-2.537090
H	-1.268021	1.996590	-2.543103
H	2.801557	0.062460	1.856387

H	2.113712	-2.411956	1.052519
H	-0.078701	-3.384849	-0.464723
H	1.011063	3.067671	1.005538
Cn	-0.690516	2.3869006	-0.3628166
Cn	-1.7187498	-1.7971212	-0.3281954
Cn	2.4178408	-0.5926664	-0.3001944

$(C_5H_4(SiMe_3))_3U(CO)$
E = -1539.9606517
ν_{co} = 1980 cm^{-1}

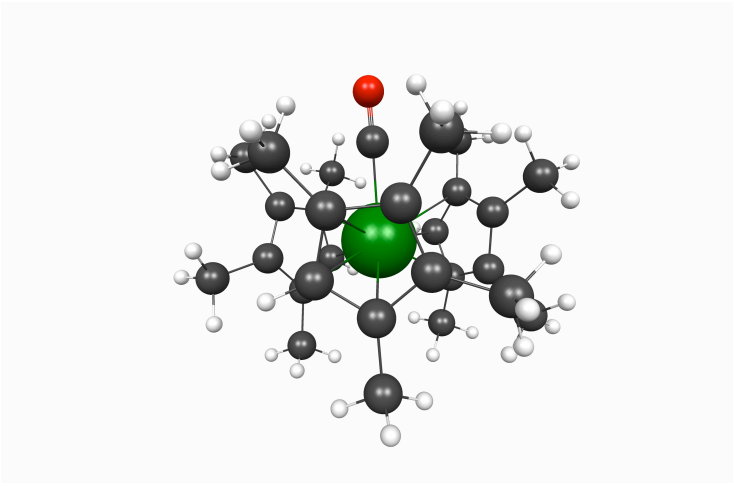


69

C	1.631954	0.759129	1.603021
C	0.411731	0.393353	2.223552
C	0.370029	-1.022058	2.285735
C	1.541292	-1.516848	1.680003
C	2.356763	-0.416269	1.256976
U	0.075693	-0.341127	-0.396230
C	1.790105	-1.435570	-1.685484
O	2.547953	-1.989793	-2.357291
C	-1.247398	-2.754421	0.121425
C	-2.297301	-1.828508	-0.155042
C	-2.168537	-1.495008	-1.539008
C	-1.068765	-2.184030	-2.088375
C	-0.494387	-2.973992	-1.048309
C	-1.222182	1.655557	-1.804284
C	-0.416590	2.374717	-0.864014
C	0.934738	2.159825	-1.267248
C	0.959118	1.336896	-2.415592
C	-0.385462	1.026838	-2.750385
Si	-1.030842	3.751068	0.273913
H	-2.305994	1.636621	-1.814151

H	0.323482	-3.675661	-1.156349
H	1.977367	1.774085	1.457935
H	1.807678	2.589713	-0.792385
H	-0.753187	-2.168608	-3.124234
H	-0.422750	-1.611706	2.725695
H	-1.072621	-3.241451	1.072743
H	1.805108	-2.563733	1.583972
Si	-3.836220	-1.515520	0.895305
H	-0.325497	1.071430	2.638063
H	1.838569	1.056294	-2.981393
H	-0.709800	0.430827	-3.593936
H	-2.833941	-0.839930	-2.087346
Si	4.202040	-0.482529	0.843076
C	-4.863128	-0.130062	0.111313
C	-4.862258	-3.112073	0.911811
C	-3.415597	-1.066216	2.689198
H	-5.778027	-2.984061	1.499545
H	-5.146708	-3.402730	-0.104398
H	-4.292947	-3.939482	1.347606
H	-5.773867	0.044085	0.694285
H	-4.307468	0.811258	0.072444
H	-5.166935	-0.390447	-0.907724
H	-4.337194	-0.912672	3.261658
H	-2.855172	-1.867819	3.181581
H	-2.824037	-0.148335	2.756176
C	5.138934	0.151002	2.368437
C	4.733058	-2.270200	0.509511
C	4.651059	0.629618	-0.626217
H	5.816145	-2.311886	0.350486
H	4.500957	-2.911690	1.366016
H	4.249341	-2.690948	-0.375775
H	5.737522	0.646267	-0.766932
H	4.198381	0.277729	-1.557068
H	4.325323	1.661378	-0.457181
H	6.221524	0.127257	2.200941
H	4.855808	1.181883	2.604899
H	4.916663	-0.464700	3.245811
C	-2.620251	3.249055	1.178152
C	0.293862	4.260429	1.530754
C	-1.422250	5.254805	-0.816823
H	-0.025383	5.169837	2.051631
H	0.473824	3.490815	2.286571
H	1.245908	4.484170	1.038077
H	-2.976662	4.074710	1.803864
H	-3.418171	3.009489	0.467683
H	-2.471295	2.379656	1.825666
H	-1.799251	6.089175	-0.214911
H	-0.526086	5.594224	-1.346063
H	-2.178925	5.008945	-1.568774

$(C_5HMe_4)_3U(CO)$
E = -1642.4470617
ν_{co} = 1934 cm^{-1}

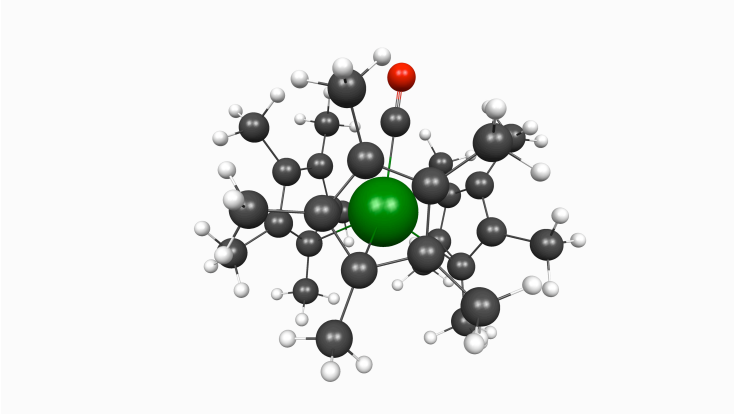


69

C	2.335974	0.633082	0.957219
C	1.232450	0.743962	1.831716
C	0.834927	-0.554097	2.251128
C	1.736600	-1.484194	1.656130
C	2.642810	-0.758368	0.836299
U	0.060467	-0.345754	-0.401466
C	1.725741	-0.191827	-2.036629
O	2.559890	-0.137254	-2.841332
C	-1.580958	-2.561161	-0.481972
C	-0.258998	-3.058481	-0.325774
C	0.444323	-2.900956	-1.540992
C	-0.456307	-2.301699	-2.477176
C	-1.710066	-2.125310	-1.834355
C	-0.222241	2.401823	-0.301550
C	-1.486000	1.887889	0.075697
C	-2.110795	1.384653	-1.108593
C	-1.207338	1.555690	-2.188843
C	-0.026643	2.189723	-1.685794
H	0.792361	1.669196	2.180735
C	1.040765	2.826362	-2.529547
H	0.116694	-3.550486	0.559517
C	1.914846	-2.908316	2.092087
H	0.461916	2.928890	0.349578
C	-3.013785	-1.906216	-2.541578
C	-1.492388	1.379008	-3.650729
C	-0.201911	-2.173716	-3.950203
C	-2.696030	-2.710404	0.515904

C	3.893708	-1.306796	0.214166
C	3.198256	1.753113	0.453870
C	-2.164770	2.054615	1.405679
C	1.772600	-3.509443	-1.886378
C	-0.192807	-0.862029	3.303671
C	-3.572484	1.053417	-1.182876
H	2.422756	-2.835426	-2.452008
H	2.313020	-3.818535	-0.988209
H	1.630817	-4.408709	-2.500935
H	0.828222	-1.877730	-4.169490
H	-0.375241	-3.132858	-4.458269
H	-0.864807	-1.440591	-4.416495
H	-2.949986	-1.165358	-3.342033
H	-3.340068	-2.846449	-3.008085
H	-3.808852	-1.599564	-1.859529
H	-3.338487	-1.824366	0.579929
H	-3.350328	-3.553277	0.255971
H	-2.305886	-2.907705	1.519225
H	1.944526	3.030347	-1.949233
H	1.329865	2.213231	-3.387526
H	0.685066	3.787027	-2.926281
H	-0.657327	0.912946	-4.182940
H	-2.380938	0.769731	-3.829491
H	-1.670496	2.351941	-4.129032
H	-4.167292	1.952264	-0.970448
H	-3.868231	0.699700	-2.171415
H	-3.882733	0.297214	-0.452831
H	-1.454295	2.345090	2.184550
H	-2.930748	2.840901	1.359341
H	-2.675426	1.144736	1.743976
H	2.244052	-3.567035	1.283198
H	2.679029	-2.966693	2.879499
H	0.997223	-3.329374	2.514300
H	-0.892536	-0.030902	3.433419
H	-0.780264	-1.757555	3.072252
H	0.279709	-1.038702	4.279218
H	4.179389	-0.765284	-0.691918
H	4.737031	-1.230192	0.914692
H	3.793480	-2.361655	-0.052486
H	3.535221	1.597819	-0.575979
H	2.678065	2.713844	0.494158
H	4.100066	1.851109	1.073288

$(C_5Me_5)U(CO)$
E = -1760.330572 ν_{CO} = 1954 cm^{-1}



78

C	1.431271	0.823432	1.863947
C	0.372282	0.029154	2.384883
C	0.736399	-1.346803	2.231463
C	1.965446	-1.396976	1.530716
C	2.384105	-0.050499	1.278625
U	0.061748	-0.377685	-0.387991
C	2.033599	-0.638133	-1.621434
O	3.009961	-0.767651	-2.232765
C	-1.731989	-2.548950	-0.479733
C	-0.481130	-3.221857	-0.392969
C	0.224728	-2.985641	-1.601559
C	-0.634018	-2.252076	-2.482413
C	-1.847886	-2.002221	-1.798261
C	0.656812	2.291859	-1.333762
C	-0.477346	2.444305	-0.500246
C	-1.580445	1.785219	-1.131226
C	-1.142040	1.315685	-2.400753
C	0.251232	1.568159	-2.501142
C	-0.752111	0.501665	3.264104
C	1.050392	1.496479	-3.770408
C	-0.178604	-4.366708	0.527669
C	2.876724	-2.574040	1.340733
C	1.974020	3.005881	-1.246101
C	-3.177900	-1.633205	-2.387432
C	-2.027870	1.088784	-3.589402
C	-0.346410	-2.100578	-3.947781
C	-2.888307	-2.678131	0.472311
C	3.776096	0.340800	0.873692
C	1.747398	2.225660	2.292309
C	-0.676709	3.434179	0.609909
C	1.446192	-3.738092	-2.046045
C	0.094482	-2.431750	3.045945
C	-3.004072	1.909042	-0.663468
H	2.045812	-3.178792	-2.769001
H	2.097588	-3.998137	-1.207539
H	1.157549	-4.682573	-2.530224
H	0.570782	-1.536344	-4.146710

H	-0.214985	-3.087592	-4.410970
H	-1.162609	-1.608847	-4.480072
H	-3.102877	-1.357627	-3.439382
H	-3.851583	-2.499018	-2.329731
H	-3.681585	-0.814852	-1.863150
H	-3.497692	-1.768226	0.511525
H	-3.562860	-3.492473	0.170652
H	-2.564095	-2.898611	1.492806
H	2.119549	1.362675	-3.586445
H	0.722469	0.679517	-4.418275
H	0.936620	2.426448	-4.346432
H	-1.681703	0.292229	-4.249756
H	-3.059107	0.874383	-3.308244
H	-2.049489	2.007819	-4.192251
H	-3.100905	1.780185	0.420592
H	-3.413787	2.902495	-0.896438
H	-3.661086	1.176542	-1.139754
H	0.249127	3.940159	0.882906
H	-1.381675	4.209582	0.280559
H	-1.100154	2.998761	1.520499
H	3.188106	-2.707621	0.299703
H	3.794627	-2.440199	1.928714
H	2.421312	-3.507974	1.674777
H	-0.972035	-2.566813	2.839136
H	0.584051	-3.395824	2.908030
H	0.174618	-2.180426	4.112246
H	3.817028	1.358592	0.477678
H	4.450224	0.308981	1.742205
H	4.198738	-0.325453	0.117119
H	2.191370	2.836145	1.504260
H	0.874907	2.750987	2.681058
H	2.482262	2.185898	3.108920
H	2.831961	2.329410	-1.315694
H	2.070980	3.721231	-2.073848
H	2.074799	3.578000	-0.322075
H	0.868108	-4.420960	0.831300
H	-0.794746	-4.357218	1.426852
H	-0.400996	-5.306643	0.002756
H	-1.044397	1.533051	3.048402
H	-1.648038	-0.120587	3.162348
H	-0.467926	0.467547	4.325922

Calculations with 11 electron ECP for uranium

CO complexes

$(C_5H_5)_3U(CO)$

E = -725.879717 au

33

C	-2.346136	-0.740958	-1.513480
C	-2.445061	-1.510508	-0.333216
C	-2.654044	-0.626312	0.745025
C	-2.710866	0.699847	0.227638
C	-2.530238	0.627688	-1.165010
U	-0.000134	-0.000546	-0.167220
C	0.533146	2.402939	-1.510813
C	1.809888	1.874437	-1.164500
C	1.964851	1.993164	0.228169
C	0.789686	2.608385	0.747763
C	-0.081802	2.871821	-0.329156
C	1.806276	-1.673015	-1.505273
C	2.529409	-1.360098	-0.332865
C	1.876966	-1.973637	0.755901
C	0.754808	-2.693659	0.253344
C	0.717285	-2.515525	-1.140827
H	-2.206191	-1.126066	-2.516711
H	-2.538076	1.461319	-1.855498
H	2.831422	1.692373	0.803549
H	-0.003546	-2.948413	-1.822604
H	-2.360450	-2.587287	-0.266126
H	0.620411	2.879087	1.783495
H	3.418302	-0.745335	-0.278139
H	2.534223	1.465317	-1.857205
H	2.203845	-1.949336	1.788998
H	0.127957	2.476401	-2.513211
H	2.062019	-1.368663	-2.513439
H	-2.804084	-0.910179	1.780206
H	-2.886755	1.599020	0.804708
H	-1.055490	3.339014	-0.260362
H	0.068602	-3.290306	0.841304
C	-0.005218	0.006104	2.503214
O	-0.008049	0.009378	3.640622

$(C_5H_4SiMe_3)_3U(CO)$
E = -1095.0165717 au
69

C	1.618643	0.208815	1.930774
C	0.580002	-0.606699	2.459886
C	0.857049	-1.944542	2.098746
C	2.025239	-1.942614	1.315387
C	2.533542	-0.598615	1.216865
U	-0.017155	-0.614640	-0.265654
C	1.459874	-2.166653	-1.713659

O	2.066361	-2.890180	-2.351519
C	-1.999746	-2.489537	0.589245
C	-2.778540	-1.447541	-0.003788
C	-2.502943	-1.495599	-1.402578
C	-1.575254	-2.519950	-1.656974
C	-1.259810	-3.142140	-0.409072
C	-0.957734	1.516793	-1.907905
C	-0.059425	2.205851	-1.024806
C	1.242553	1.745716	-1.358852
C	1.151200	0.813471	-2.415237
C	-0.222840	0.678241	-2.760584
Si	-0.481831	3.744973	-0.013764
H	-2.032091	1.652540	-1.935047
H	-0.601764	-3.991707	-0.268045
H	1.707023	1.276980	2.080174
H	2.164717	2.070418	-0.893660
H	-1.209327	-2.822299	-2.631450
H	0.275050	-2.815790	2.366839
H	-1.997284	-2.743603	1.642040
H	2.518433	-2.829248	0.930785
Si	-4.163163	-0.491343	0.851690
H	-0.243652	-0.267657	3.077490
H	1.983830	0.342305	-2.924240
H	-0.623508	0.048867	-3.545744
H	-2.942285	-0.848211	-2.151147
Si	4.288391	-0.114534	0.719483
C	-4.934933	0.744950	-0.357596
C	-5.490724	-1.738352	1.388722
C	-3.519929	0.394161	2.401310
H	-6.324814	-1.234053	1.888982
H	-5.889737	-2.280467	0.525605
H	-5.078048	-2.476887	2.083601
H	-5.769869	1.272043	0.116295
H	-4.214358	1.497104	-0.690924
H	-5.326640	0.232138	-1.242055
H	-4.330972	0.920127	2.916569
H	-3.091913	-0.325982	3.106844
H	-2.744191	1.126560	2.157452
C	4.587806	1.712765	1.129345
C	5.480083	-1.173371	1.752672
C	4.683343	-0.420500	-1.111333
H	6.523027	-0.924851	1.527074
H	5.315638	-1.015710	2.823163
H	5.338818	-2.239914	1.548668
H	5.734236	-0.184316	-1.312250
H	4.522889	-1.466749	-1.389563
H	4.069367	0.204781	-1.765372
H	5.627925	1.978563	0.912365
H	3.948328	2.382645	0.546472
H	4.406914	1.911438	2.190468

C	-2.363168	3.952385	0.086722
C	0.230999	3.711633	1.742988
C	0.253627	5.243534	-0.919551
H	-0.021820	4.640927	2.265476
H	-0.170047	2.878179	2.327432
H	1.322425	3.627715	1.731603
H	-2.610641	4.885764	0.603835
H	-2.814239	3.997711	-0.909767
H	-2.835593	3.133663	0.637514
H	0.026116	6.174980	-0.389416
H	1.342177	5.157640	-0.999152
H	-0.147838	5.322140	-1.934735

$(C_5HMe_4)_3U(CO)$
E = -1197.5106231 au

69

C	2.814265	-0.816509	0.290692
C	2.583124	-1.228560	-1.044843
C	2.525811	-0.047773	-1.845710
C	2.783025	1.076293	-1.036093
C	2.921408	0.612511	0.300355
C	2.705487	-2.613942	-1.599394
C	3.116232	2.450875	-1.527913
C	3.401803	1.438096	1.455969
C	3.149283	-1.695604	1.455895
U	0.092748	-0.066392	-0.385651
C	0.238291	0.854749	1.965866
O	0.259199	1.296297	3.018702
C	-0.222970	2.412848	-1.590406
C	-1.297175	1.679197	-2.145328
C	-2.368350	1.667822	-1.208504
C	-1.923248	2.329438	-0.045845
C	-0.585648	2.805483	-0.282859
C	-3.783605	1.289818	-1.519279
C	-2.767711	2.701142	1.134744
C	0.126394	3.801709	0.583046
C	-0.872654	-2.767339	-0.663300
C	-2.072138	-2.032011	-0.385701
C	-2.022585	-1.603384	0.959245
C	-0.794814	-2.082259	1.530346
C	-0.112802	-2.802460	0.522320
C	-3.249411	-2.013337	-1.310415
C	-0.630291	-3.533089	-1.928399
C	-0.459627	-2.105055	2.992305
C	-3.130647	-0.964509	1.738237
H	2.408885	-0.031710	-2.924965
H	0.695583	2.664838	-2.097746
H	0.822237	-3.330328	0.657188

H	0.294893	-4.109857	-1.877369
H	-1.448585	-4.242314	-2.111374
H	-0.575828	-2.889134	-2.815028
H	-4.060879	-1.389463	-0.934215
H	-2.993022	-1.659197	-2.314854
H	-3.653018	-3.028899	-1.429456
H	-2.757337	-0.261508	2.489688
H	-3.819061	-0.414687	1.092169
H	-3.723113	-1.718421	2.275498
H	0.619550	-2.168036	3.160961
H	-0.835151	-1.229603	3.529916
H	-0.909358	-2.985039	3.472806
H	3.159654	0.983424	2.420829
H	4.494991	1.550548	1.423854
H	2.980686	2.448282	1.449146
H	2.633869	3.249988	-0.957186
H	4.198647	2.625011	-1.459070
H	2.840578	2.576164	-2.579369
H	2.856183	-2.733600	1.283023
H	4.231281	-1.695903	1.647653
H	2.665682	-1.364832	2.381448
H	2.361781	-3.383954	-0.904432
H	2.143492	-2.725703	-2.530929
H	3.756228	-2.837902	-1.830099
H	-4.307933	0.849846	-0.665623
H	-4.356710	2.180456	-1.812298
H	-3.842568	0.584113	-2.351053
C	-1.356821	1.148844	-3.493537
H	-2.207691	2.676181	2.075813
H	-3.164493	3.721388	1.033291
H	-3.626866	2.034470	1.246250
H	1.210884	3.760662	0.454408
H	-0.187447	4.824086	0.330647
H	-0.086696	3.663392	1.647244
H	-2.303482	0.630329	-3.638091
H	-1.277623	1.966075	-4.208926
H	-0.534154	0.451814	-3.646145

$(C_5Me_5)_3UCO$
E = -1315.407501 au

78

C	1.740242	1.015391	2.074158
C	0.557642	0.403698	2.543870
C	0.629815	-0.998566	2.256532
C	1.859127	-1.239582	1.583275
C	2.528040	0.016573	1.445210
U	0.024519	-0.376660	-0.355199
C	2.172953	-0.640375	-1.696303

O	3.133518	-0.754006	-2.303136
C	-1.610186	-2.960035	-0.306894
C	-0.381944	-3.643238	-0.440782
C	0.228683	-3.210060	-1.646532
C	-0.658032	-2.297648	-2.299632
C	-1.795851	-2.133194	-1.462995
C	0.488856	2.209902	-1.386015
C	-0.735948	2.264066	-0.665176
C	-1.775775	1.804185	-1.537948
C	-1.201587	1.493358	-2.789700
C	0.198499	1.704493	-2.692111
C	-0.485833	1.025867	3.419048
C	1.156520	1.684609	-3.844412
C	0.062852	-4.830783	0.359842
C	2.525313	-2.564620	1.369706
C	1.779656	2.874933	-1.017430
C	-3.120191	-1.537565	-1.827237
C	-1.945541	1.283653	-4.075137
C	-0.531924	-1.899543	-3.738789
C	-2.673726	-3.219726	0.714486
C	3.941185	0.195060	0.980034
C	2.234059	2.383024	2.441569
C	-1.017181	3.011478	0.601622
C	1.449282	-3.819798	-2.266640
C	-0.269820	-2.005302	2.903373
C	-3.236401	1.895841	-1.221825
H	1.843280	-3.208761	-3.082987
H	2.258432	-3.968969	-1.543123
H	1.221880	-4.808613	-2.690092
H	0.408297	-1.385255	-3.966109
H	-0.572819	-2.786069	-4.386512
H	-1.345702	-1.242097	-4.042410
H	-3.042155	-0.858924	-2.676192
H	-3.837031	-2.325412	-2.101344
H	-3.570011	-0.978670	-0.999769
H	-3.125136	-2.295135	1.093343
H	-3.494320	-3.810918	0.283111
H	-2.292920	-3.777110	1.573509
H	2.198955	1.653161	-3.516351
H	0.991996	0.831102	-4.511108
H	1.045338	2.588663	-4.460272
H	-1.338012	0.773847	-4.827702
H	-2.871948	0.713606	-3.952602
H	-2.234272	2.251329	-4.509724
H	-3.480285	1.476572	-0.238465
H	-3.567742	2.944077	-1.202180
H	-3.850745	1.378485	-1.962532
H	-0.111682	3.188029	1.181487
H	-1.460635	3.993167	0.379403
H	-1.727198	2.486760	1.249119

H	2.930687	-2.687832	0.359323
H	3.368351	-2.684735	2.064321
H	1.839310	-3.390801	1.551168
H	-1.327565	-1.734339	2.820942
H	-0.150419	-2.997393	2.468861
H	-0.048828	-2.087822	3.977598
H	4.083884	1.126970	0.422259
H	4.633290	0.230969	1.833602
H	4.270267	-0.628278	0.340623
H	3.001429	2.745949	1.752332
H	1.440896	3.135875	2.484560
H	2.694868	2.363946	3.439478
H	2.655909	2.241362	-1.193265
H	1.925600	3.787776	-1.611840
H	1.792999	3.167733	0.031483
H	1.137953	-5.008836	0.271594
H	-0.175675	-4.752537	1.425237
H	-0.436054	-5.741501	-0.001056
H	-0.440600	2.117247	3.401733
H	-1.502579	0.731976	3.133010
H	-0.355801	0.713106	4.465094