Supporting Information

A relativistic DFT probe for small-molecule activation mediated by low-valence uranium metallocenes

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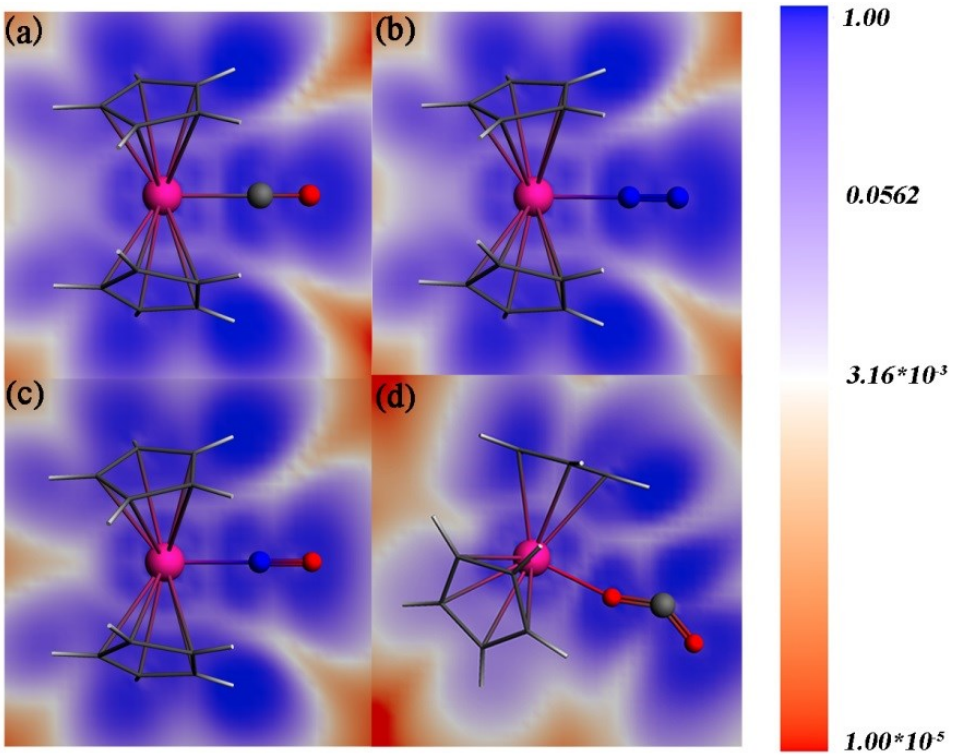

Figure S1. Plots of electron localization function (ELF) of [$Cp_3U(X)$], where X = CO (a), N_2 (b), NO (c) and CO_2 (d), on the selected plane. The color scale for the ELF values is given on the right side.

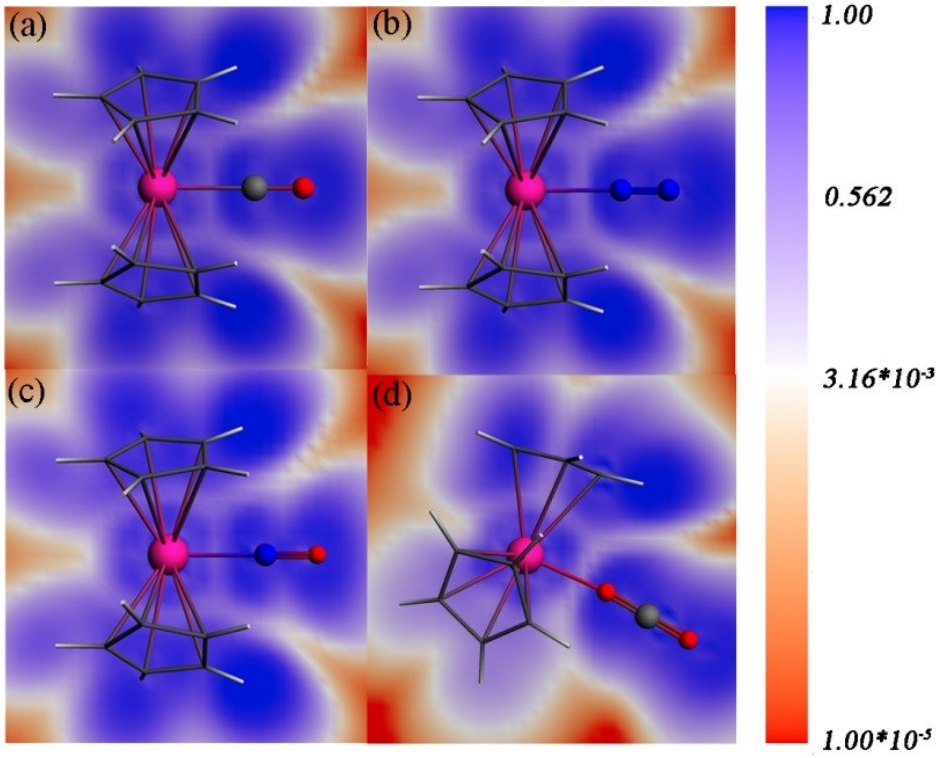

Figure S2. Plots of electron localization function (ELF) of $[Cp_3U(X)]^+$, where X = CO (a), N_2 (b), NO (c) and CO_2 (d), on the selected plane. The color scale for the ELF values is given on the right side.

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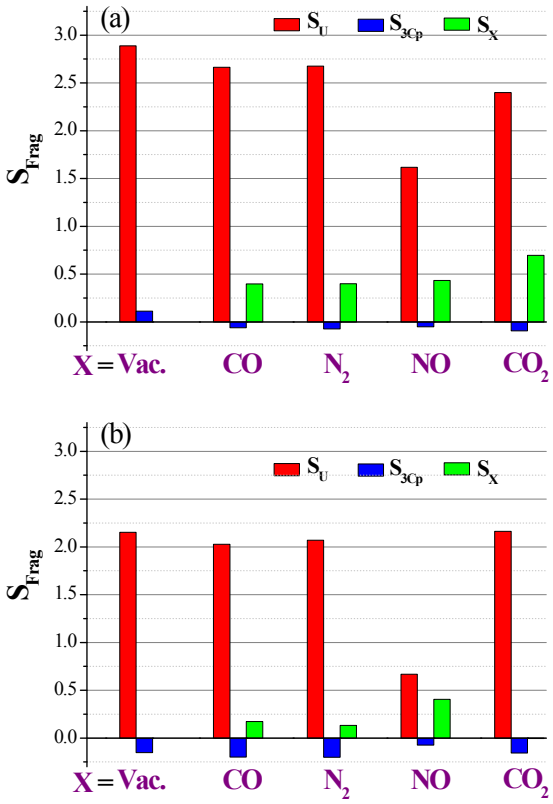

Figure S3. Electron-spin density of each fragment (S_{Frag}) for $[Cp_3U(X)]$ (a) and $[Cp_3U(X)]^+$ (b). $[Cp_3U(NO)]$ and $[Cp_3U(NO)]^+$ have the ^1A and ^2A ground states, respectively. Considering the one electron reduction from the ^2A state of $[Cp_3U(NO)]^+$, the S_{Frag} values of the ^3A state of $[Cp_3U(NO)]$ were presented.

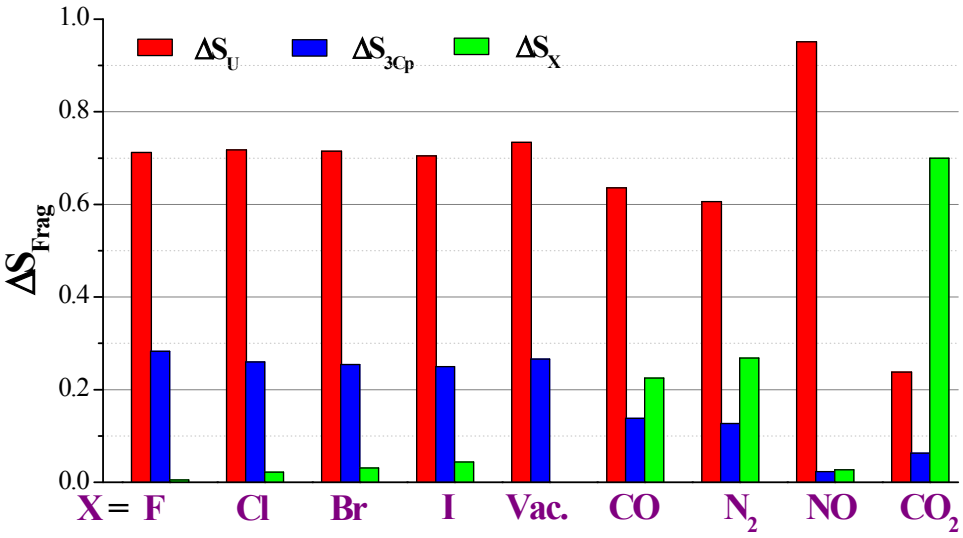

Figure S4. Difference of electron-spin density of each fragment (ΔS_{Frag}) between $[Cp_3U(X)]$ and $[Cp_3U(X)]^+$. S_{Frag} values of $[Cp_3U(NO)]$ in the ^3A state was used, because the complex has the ^1A ground state and $[Cp_3U(NO)]^+$ shows the ^2A ground state.

Table S1. Calculated relative energies (eV) of complexes [$Cp_3U(X)$] (X = Vac., CO, N_2, NO and CO_2) in various electronic states (ESSs).[a]

Complex	ESS	ESS	ΔE	ΔE_0	ΔH	ΔG	ΔG(sol)	ΔG(so)	ΔG(sol-so)
[Cp_3U]	Quartet	^4A	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	Doublet	^2A	0.555	0.582	0.562	0.649	0.688	0.644	0.655
[$Cp_3U(CO)$]	Quartet	^4A	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	Doublet	^2A	0.474	0.475	0.470	0.476	0.451	0.473	0.470
[$Cp_3U(N_2)$]	Quartet	^4A	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	Doublet	^2A	0.480	0.455	0.415	0.513	0.494	0.509	0.507
[$Cp_3U(NO)$]	Quintet	^5A	0.771	0.721	0.697	0.799	0.933	0.669	0.778
	Triplet	^3A	0.384	0.411	0.399	0.449	0.569	0.416	0.432
	Singlet	^1A	0.000	0.000	0.000	0.000	0.000	0.000	0.000
[$Cp_3U(NO)]^+$	Quartet	^4A	0.343	0.290	0.316	0.316	0.255	0.085	0.184
	Doublet	^2A	0.000	0.000	0.000	0.000	0.000	0.000	0.000
[$Cp_3U(CO_2)$]	Quartet	^4A	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	Doublet	^2A	0.329	0.317	0.318	0.296	0.326	0.332	0.352

[a] E is the total bonding energy in the gas phase. Frequency calculations afford E_0 (including zero-point vibrational energy), enthalpy H and free energy G. $\Delta G(sol) = \Delta G + \Delta G_{sol}$, $\Delta G(so) = \Delta G + \Delta G_{so}$ and $\Delta G(sol\text{-}so) = \Delta G + \Delta G_{sol} + \Delta G_{so}$, where G_{sol} and G_{so} correspond to the solvation and spin-orbit coupling energies, respectively.

Table S2. Calculated electron-spin density of each fragment ($S_{Frag.}$) of $[Cp_3U(X)]^z$.

	ESSs	S_U	S_{3Cp}	S_X
$[Cp_3U]$	^4A	2.887	0.113	—
$[Cp_3U(CO)]$	^4A	2.664	-0.061	0.397
$[Cp_3U(N_2)]$	^4A	2.675	-0.074	0.400
$[Cp_3U(NO)]$	^1A	0.000	0.000	—
	^3A	1.618	-0.051	0.433
$[Cp_3U(CO_2)]$	^4A	2.400	-0.094	0.695
$[Cp_3U(CO_2)]^{\#}$	^4A	2.825	-0.015	0.190
$[Cp_3U]^+$	^3A	2.153	-0.153	—
$[Cp_3U(CO)]^+$	^3A	2.028	-0.199	0.172
$[Cp_3U(N_2)]^+$	^3A	2.069	-0.201	0.132
$[Cp_3U(NO)]^+$	^2A	0.667	-0.074	0.406
$[Cp_3U(CO_2)]^+$	^3A	2.162	-0.157	-0.005

The full reference of Gaussian

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Gaussian 09, Revision D.01; Gaussian, Inc., Wallingford CT, 2009.

The full reference of ADF

Baerends, E. J.; Ziegler, T.; Autschbach, J.; Bashford, D.; Bérces, A.; Bickelhaupt, F. M.; Bo, C.; Boerrigter, P. M.; Cavallo, L.; Chong, D. P.; Deng, L.; Dickson, R. M.; Ellis, D. E.; van Faassen, M.; Fan, L.; Fischer, T. H.; Fonseca Guerra, C.; Franchini, M.; Ghysels, A.; Giammona, A.; van Gisbergen, S. J. A.; Götz, A. W.; Groeneveld, J. A.; Gritsenko, O. V.; Grüning, M.; Gusarov, S.; Harris, F. E.; van den Hoek, P.; Jacob, C. R.; Jacobsen, H.; Jensen, L.; Kaminski, J. W.; van Kesse, G.; Kootstra, F.; Kovalenko, A.; Krykunov, M. V.; van Lenthe, E.; McCormack, D. A.; Michalak, A.; Mitoraj, M.; Morton, S. M.; Neugebauer, J.; Nicu, V. P.; Noodleman, L.; Osinga, V. P.; Patchkovskii, S.; Pavanello, M.; Philipsen, P. H. T.; Post, D.; Pye, C. C.; Ravenek, W.; Rodríguez, J. I.; Ros, P.; Schipper, P. R. T.; van Schoot, H.; Schreckenbach, G.; Seldenthuis, J. S.; Seth, M.; Snijders, J. G.; Solà, M.; Swart, M.; Swerhone, D.; te Velde, G.; Vernooijs, P.; Versluis, L.; Visscher, L.; Visser, O.; Wang, F.; Wesolowski, T. A.; van Wezenbeek, E. M.; Wiesenekker, G.; Wolff, S. K.; Woo, T. K.; Yakovlev, A. L. ADF, ADF2014.06; SCM, Theoretical Chemistry, Vrije Universiteit: Amsterdam, The Netherlands, 2014.

Cartesian coordinates of optimized complexes

[Cp_3U]

C	2.56056241	-0.00105099	1.24683984
C	2.46745606	-1.14791544	0.41672405
C	2.30392392	-0.70858460	-0.92856872
C	2.30406222	0.71028141	-0.92733072
C	2.46749566	1.14728057	0.41873614
H	2.72391213	-0.00202945	2.32692877
H	-2.29935842	1.28468243	-1.81061797
H	2.57394757	-2.18012397	0.74563682
H	2.26234087	-1.34671670	-1.81123948
H	2.26245594	1.34997746	-1.80885305
H	2.57423321	2.17887976	0.74948972
C	-0.53767782	-2.35007552	-0.92814407
C	-1.28002493	-2.21797075	1.24679017
C	-2.22752997	-1.56350853	0.41795670
H	0.60071854	-3.31922987	0.74696703
C	-1.76651345	-1.64071689	-0.92782376
C	-0.23970470	-2.71089075	0.41742161
H	-1.36148711	-2.35971958	2.32686155
H	0.60066003	3.31936880	0.74554982
H	-3.17434111	-1.13975425	0.74808949
H	-2.29930266	-1.28524045	-1.80975593
H	0.03637138	-2.63316474	-1.81039613
C	-1.76659190	1.64035165	-0.92875168
C	-1.28014943	2.21831515	1.24568863
C	-0.23979493	2.71097111	0.41617837
H	-3.17449797	1.13998198	0.74721466
C	-0.53780605	2.34977893	-0.92927712
C	-2.22768007	1.56365543	0.41700527
H	-1.36176557	2.36050539	2.32570121
H	0.03632176	2.63255420	-1.81157395
U	-0.00023259	0.00010823	0.30429869

[$Cp_3U(CO)$]

C	-1.187090	-2.056100	1.146198
C	-2.226463	-1.556703	0.310019
C	-1.899730	-1.865436	-1.031539
C	-0.665650	-2.577933	-1.031539
C	-0.234913	-2.706526	0.310019
H	-1.165440	-2.018601	2.234494
H	2.665203	1.347972	-1.908815

H	-3.136385	-1.073396	0.649888
H	-2.499979	-1.634147	-1.908815
H	-0.165223	-2.982119	-1.908815
H	0.638604	-3.252887	0.649888
C	-1.899730	1.865436	-1.031539
C	-1.187090	2.056100	1.146198
C	-0.234913	2.706526	0.310019
H	-3.136385	1.073396	0.649888
C	-0.665650	2.577933	-1.031539
C	-2.226463	1.556703	0.310019
H	-1.165440	2.018601	2.234494
H	2.497781	-2.179491	0.649888
H	0.638604	3.252887	0.649888
H	-0.165223	2.982119	-1.908815
H	-2.499979	1.634147	-1.908815
C	2.565380	0.712497	-1.031539
C	2.374180	0.000000	1.146198
C	2.461376	-1.149822	0.310019
H	2.497781	2.179491	0.649888
C	2.565380	-0.712497	-1.031539
C	2.461376	1.149822	0.310019
H	2.330880	0.000000	2.234494
H	2.665203	-1.347972	-1.908815
U	0.000000	0.000000	-0.214918
C	0.000000	0.000000	-2.548070
O	0.000000	0.000000	-3.722241

$[Cp_3U(N_2)]$

C	-1.181172	2.045850	-1.053503
C	-2.224944	1.555064	-0.218253
C	-1.904124	1.874808	1.122751
C	-0.671569	2.586424	1.122751
C	-0.234253	2.704390	-0.218253
H	-1.153919	1.998647	-2.141276
H	2.673656	-1.348052	1.999923
H	-3.133493	1.069161	-0.558073
H	-2.504275	1.641429	1.999923
H	-0.169381	2.989480	1.999923
H	0.640825	3.248265	-0.558073
C	-1.904124	-1.874808	1.122751
C	-1.181172	-2.045850	-1.053503
C	-0.234253	-2.704390	-0.218253
H	-3.133493	-1.069161	-0.558073
C	-0.671569	-2.586424	1.122751

C	-2.224944	-1.555064	-0.218253
H	-1.153919	-1.998647	-2.141276
H	2.492667	2.179104	-0.558073
H	0.640825	-3.248265	-0.558073
H	-0.169381	-2.989480	1.999923
H	-2.504275	-1.641429	1.999923
C	2.575693	-0.711616	1.122751
C	2.362344	0.000000	-1.053503
C	2.459197	1.149326	-0.218253
H	2.492667	-2.179104	-0.558073
C	2.575693	0.711616	1.122751
C	2.459197	-1.149326	-0.218253
H	2.307838	0.000000	-2.141276
H	2.673656	1.348052	1.999923
U	0.000000	0.000000	0.341764
N	0.000000	0.000000	2.693565
N	0.000000	0.000000	3.832773

$[Cp_3U(NO)]$

C	-1.188836	-2.059124	1.044582
C	-2.222457	-1.557756	0.206664
C	-1.895603	-1.862658	-1.138245
C	-0.665308	-2.572969	-1.138245
C	-0.237827	-2.703582	0.206664
H	-1.163857	-2.015859	2.132472
H	2.636620	1.341727	-2.020363
H	-3.128830	-1.067413	0.546346
H	-2.480279	-1.612516	-2.020363
H	-0.156340	-2.954243	-2.020363
H	0.640008	-3.243353	0.546346
C	-1.895603	1.862658	-1.138245
C	-1.188836	2.059124	1.044582
C	-0.237827	2.703582	0.206664
H	-3.128830	1.067413	0.546346
C	-0.665308	2.572969	-1.138245
C	-2.222457	1.557756	0.206664
H	-1.163857	2.015859	2.132472
H	2.488821	-2.175940	0.546346
H	0.640008	3.243353	0.546346
H	-0.156340	2.954243	-2.020363
H	-2.480279	1.612516	-2.020363
C	2.560910	0.710311	-1.138245
C	2.377671	0.000000	1.044582
C	2.460285	-1.145827	0.206664

H	2.488821	2.175940	0.546346
C	2.560910	-0.710311	-1.138245
C	2.460285	1.145827	0.206664
H	2.327713	0.000000	2.132472
H	2.636620	-1.341727	-2.020363
U	0.000000	0.000000	-0.400708
N	0.000000	0.000000	-2.379650
O	0.000000	0.000000	-3.615561

$[Cp_3U(NO)]$

C	-1.159641	-2.008558	1.080228
C	-2.214514	-1.539348	0.247183
C	-1.914179	-1.892308	-1.089510
C	-0.681697	-2.603882	-1.089510
C	-0.225858	-2.687500	0.247183
H	-1.114273	-1.929978	2.165149
H	2.711196	1.345745	-1.965893
H	-3.119739	-1.048943	0.587915
H	-2.521047	-1.675092	-1.965893
H	-0.190149	-3.020837	-1.965893
H	0.651458	-3.226245	0.587915
C	-1.914179	1.892308	-1.089510
C	-1.159641	2.008558	1.080228
C	-0.225858	2.687500	0.247183
H	-3.119739	1.048943	0.587915
C	-0.681697	2.603882	-1.089510
C	-2.214514	1.539348	0.247183
H	-1.114273	1.929978	2.165149
H	2.468281	-2.177302	0.587915
H	0.651458	3.226245	0.587915
H	-0.190149	3.020837	-1.965893
H	-2.521047	1.675092	-1.965893
C	2.595876	0.711573	-1.089510
C	2.319283	0.000000	1.080228
C	2.440372	-1.148151	0.247183
H	2.468281	2.177302	0.587915
C	2.595876	-0.711573	-1.089510
C	2.440372	1.148151	0.247183
H	2.228547	0.000000	2.165149
H	2.711196	-1.345745	-1.965893
U	0.000000	0.000000	-0.420992
N	0.000000	0.000000	-2.506476
O	0.000000	0.000000	-3.727127

$[Cp_3U(CO_2)]$

C	-3.734717	0.926456	-2.299455
C	-4.204391	2.066912	-1.607671
C	-3.181038	3.057475	-1.636052
C	-2.073283	2.517040	-2.340269
C	-2.416625	1.192018	-2.743004
H	-4.284327	-0.000803	-2.445083
H	0.766111	2.202016	1.349028
H	-5.189032	2.174003	-1.161325
H	-3.258204	4.067021	-1.239836
H	-1.153784	3.041941	-2.585560
H	-1.798819	0.519203	-3.331012
C	-3.181038	3.057475	1.636052
C	-3.734717	0.926456	2.299455
C	-2.416625	1.192018	2.743004
H	-5.189032	2.174003	1.161325
C	-2.073283	2.517040	2.340269
C	-4.204391	2.066912	1.607671
H	-4.284327	-0.000803	2.445083
H	0.060712	-0.276182	-2.176902
H	-1.798819	0.519203	3.331012
H	-1.153784	3.041941	2.585560
H	-3.258204	4.067021	1.239836
C	0.484109	1.369434	0.709695
C	-0.086907	-0.742478	0.000000
C	0.125709	0.060783	-1.146165
H	0.060712	-0.276182	2.176902
C	0.484109	1.369434	-0.709695
C	0.125709	0.060783	1.146165
H	-0.393442	-1.787166	0.000000
H	0.766111	2.202016	-1.349028
U	-2.146762	1.112860	0.000000
O	-3.131408	-0.944050	0.000000
C	-3.304138	-2.201763	0.000000
O	-4.232058	-2.972482	0.000000

$[Cp_3U(CO_2)]^{\#}$ (Transition state)

C	-7.18806	1.71872	-4.26480
C	-7.99969	3.95428	-3.04927
C	-6.01254	5.75571	-3.19049
C	-3.96043	4.61866	-4.51443
C	-4.69436	2.10843	-5.16851
H	-8.30387	0.00578	-4.49583
H	1.51037	4.18952	2.55568

H	-9.83998	4.24806	-2.18742
H	-6.09485	7.69599	-2.51439
H	-2.20908	5.54423	-5.05763
H	-3.58953	0.76592	-6.26149
C	-6.01275	5.75567	3.19138
C	-7.18837	1.71927	4.26686
C	-4.69513	2.10895	5.17096
H	-9.84050	4.24797	2.18882
C	-3.96086	4.61868	4.51592
C	-8.00009	3.95422	3.05034
H	-8.30365	0.00569	4.49679
H	0.16015	-0.47891	-4.12130
H	-3.59004	0.76659	6.26377
H	-2.21021	5.54503	5.06022
H	-6.09559	7.69647	2.51677
C	0.96278	2.62086	1.34629
C	-0.14380	-1.36122	0.00026
C	0.27372	0.15434	-2.17131
H	0.16083	-0.47959	4.12155
C	0.96217	2.62111	-1.34532
C	0.27450	0.15402	2.17170
H	-0.65774	-3.35445	0.00008
H	1.50970	4.18990	-2.55454
U	-3.98096	2.20743	-0.00056
O	-6.08125	-2.25252	-0.00203
C	-6.86254	-4.36125	0.00672
O	-8.07210	-6.23904	-0.00255

$[Cp_3U]^+$

C	2.563715	0.000000	1.256388
C	2.471322	-1.148036	0.429287
C	2.308787	-0.711070	-0.916079
C	2.308787	0.711070	-0.916079
C	2.471322	1.148036	0.429287
H	2.717010	0.000000	2.335707
H	-2.304736	1.291661	-1.795054
H	2.568626	-2.177229	0.761586
H	2.270979	-1.350130	-1.795054
H	2.270979	1.350130	-1.795054
H	2.568626	2.177229	0.761586
C	-0.538589	-2.355003	-0.916079
C	-1.281858	-2.220242	1.256388
C	-2.229890	-1.566209	0.429287
H	0.601222	-3.313110	0.761586

C	-1.770198	-1.643933	-0.916079
C	-0.241432	-2.714246	0.429287
H	-1.358505	-2.352999	2.335707
H	0.601222	3.313110	0.761586
H	-3.169848	-1.135881	0.761586
H	-2.304736	-1.291661	-1.795054
H	0.033757	-2.641790	-1.795054
C	-1.770198	1.643933	-0.916079
C	-1.281858	2.220242	1.256388
C	-0.241432	2.714246	0.429287
H	-3.169848	1.135881	0.761586
C	-0.538589	2.355003	-0.916079
C	-2.229890	1.566209	0.429287
H	-1.358505	2.352999	2.335707
H	0.033757	2.641790	-1.795054
U	0.000000	0.000000	0.274134

$[Cp_3U(CO)]^+$

C	-1.223717	-2.119539	1.135168
C	-2.224144	-1.555374	0.298910
C	-1.844901	-1.770363	-1.051323
C	-0.610729	-2.482913	-1.051323
C	-0.234921	-2.703852	0.298910
H	-1.243630	-2.154030	2.224120
H	2.522208	1.349008	-1.930753
H	-3.150286	-1.102427	0.637614
H	-2.429379	-1.509792	-1.930753
H	-0.092829	-2.858800	-1.930753
H	0.620414	-3.279441	0.637614
C	-1.844901	1.770363	-1.051323
C	-1.223717	2.119539	1.135168
C	-0.234921	2.703852	0.298910
H	-3.150286	1.102427	0.637614
C	-0.610729	2.482913	-1.051323
C	-2.224144	1.555374	0.298910
H	-1.243630	2.154030	2.224120
H	2.529873	-2.177015	0.637614
H	0.620414	3.279441	0.637614
H	-0.092829	2.858800	-1.930753
H	-2.429379	1.509792	-1.930753
C	2.455630	0.712549	-1.051323
C	2.447433	0.000000	1.135168
C	2.459065	-1.148478	0.298910
H	2.529873	2.177015	0.637614

C	2.455630	-0.712549	-1.051323
C	2.459065	1.148478	0.298910
H	2.487259	0.000000	2.224120
H	2.522208	-1.349008	-1.930753
U	0.000000	0.000000	-0.058394
C	0.000000	0.000000	-2.408118
O	0.000000	0.000000	-3.563880

$[Cp_3U(N_2)]^+$

C	-1.215460	2.105239	-1.049232
C	-2.222291	1.552845	-0.213579
C	-1.849835	1.780493	1.136862
C	-0.617034	2.492251	1.136862
C	-0.233658	2.700983	-0.213579
H	-1.225983	2.123464	-2.138771
H	2.532855	-1.350535	2.014778
H	-3.146863	1.097148	-0.552829
H	-2.436025	1.518249	2.014778
H	-0.096830	2.868784	2.014778
H	0.623274	3.273838	-0.552829
C	-1.849835	-1.780493	1.136862
C	-1.215460	-2.105239	-1.049232
C	-0.233658	-2.700983	-0.213579
H	-3.146863	-1.097148	-0.552829
C	-0.617034	-2.492251	1.136862
C	-2.222291	-1.552845	-0.213579
H	-1.225983	-2.123464	-2.138771
H	2.523590	2.176690	-0.552829
H	0.623274	-3.273838	-0.552829
H	-0.096830	-2.868784	2.014778
H	-2.436025	-1.518249	2.014778
C	2.466870	-0.711758	1.136862
C	2.430920	0.000000	-1.049232
C	2.455948	1.148138	-0.213579
H	2.523590	-2.176690	-0.552829
C	2.466870	0.711758	1.136862
C	2.455948	-1.148138	-0.213579
H	2.451966	0.000000	-2.138771
H	2.532855	1.350535	2.014778
U	0.000000	0.000000	0.198105
N	0.000000	0.000000	2.649053
N	0.000000	0.000000	3.767305

$[Cp_3U(NO)]^+$

C	-1.187875	-2.057461	1.072004
C	-2.213729	-1.538245	0.235935
C	-1.871328	-1.818151	-1.111400
C	-0.638901	-2.529693	-1.111400
C	-0.225295	-2.686269	0.235935
H	-1.176706	-2.038114	2.161149
H	2.599388	1.345362	-1.990861
H	-3.134641	-1.077521	0.577329
H	-2.464812	-1.578455	-1.990861
H	-0.134576	-2.923818	-1.990861
H	0.634160	-3.253439	0.577329
C	-1.871328	1.818151	-1.111400
C	-1.187875	2.057461	1.072004
C	-0.225295	2.686269	0.235935
H	-3.134641	1.077521	0.577329
C	-0.638901	2.529693	-1.111400
C	-2.213729	1.538245	0.235935
H	-1.176706	2.038114	2.161149
H	2.500481	-2.175918	0.577329
H	0.634160	3.253439	0.577329
H	-0.134576	2.923818	-1.990861
H	-2.464812	1.578455	-1.990861
C	2.510229	0.711542	-1.111400
C	2.375751	0.000000	1.072004
C	2.439024	-1.148023	0.235935
H	2.500481	2.175918	0.577329
C	2.510229	-0.711542	-1.111400
C	2.439024	1.148023	0.235935
H	2.353411	0.000000	2.161149
H	2.599388	-1.345362	-1.990861
U	0.000000	0.000000	-0.282278
N	0.000000	0.000000	-2.364144
O	0.000000	0.000000	-3.559356

$[Cp_3U(CO_2)]^+$

C	-3.665293	0.918521	-2.273630
C	-4.175926	2.042761	-1.578646
C	-3.184096	3.064920	-1.606265
C	-2.061009	2.564152	-2.316421
C	-2.360567	1.233547	-2.727305
H	-4.197618	-0.012751	-2.459967
H	0.774754	2.243644	1.348043
H	-5.173441	2.129404	-1.157553

H	-3.297522	4.075554	-1.222939
H	-1.165316	3.124838	-2.570710
H	-1.728900	0.593586	-3.336626
C	-3.184096	3.064920	1.606265
C	-3.665293	0.918521	2.273630
C	-2.360567	1.233547	2.727305
H	-5.173441	2.129404	1.157553
C	-2.061009	2.564152	2.316421
C	-4.175926	2.042761	1.578646
H	-4.197618	-0.012751	2.459967
H	0.090756	-0.237144	-2.177815
H	-1.728900	0.593586	3.336626
H	-1.165316	3.124838	2.570710
H	-3.297522	4.075554	1.222939
C	0.480481	1.414434	0.710023
C	-0.083250	-0.698091	0.000000
C	0.128376	0.105349	-1.147715
H	0.090756	-0.237144	2.177815
C	0.480481	1.414434	-0.710023
C	0.128376	0.105349	1.147715
H	-0.333677	-1.757568	0.000000
H	0.774754	2.243644	-1.348043
U	-2.114387	1.173304	0.000000
O	-3.217861	-1.292960	0.000000
C	-3.806191	-2.318331	0.000000
O	-4.383866	-3.328428	0.000000