

Do QTAIM metrics correlate with the strength of heavy
element–ligand bonds?

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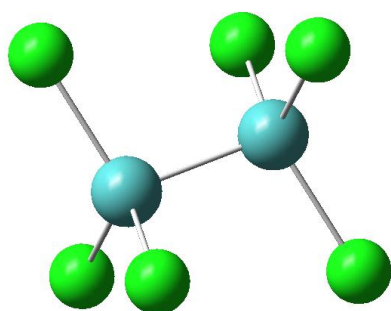
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Supplementary Information

Cartesian atomic coordinates (Å) and ball-and-stick representations of all molecules studied

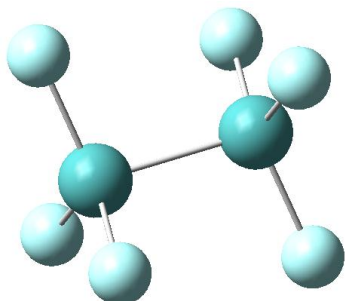
Mo_2Cl_6

```
Mo 0.000000 0.000000 1.115000
Cl 0.000000 2.182589 1.618890
Cl -1.890177 -1.091294 1.618890
Cl 1.890177 -1.091294 1.618890
Mo 0.000000 0.000000 -1.115000
Cl 1.890177 1.091294 -1.618890
Cl 0.000000 -2.182589 -1.618890 Cl -1.890177 1.091294 -1.618890
```



Mo_2F_6

```
Mo 0.000000 0.000000 1.125000
F 0.000000 1.825827 1.479905
F -1.581212 -0.912913 1.479905
F 1.581212 -0.912913 1.479905
Mo 0.000000 0.000000 -1.125000
F 1.581212 0.912913 -1.479905
F 0.000000 -1.825827 -1.479905
F -1.581212 0.912913 -1.479905
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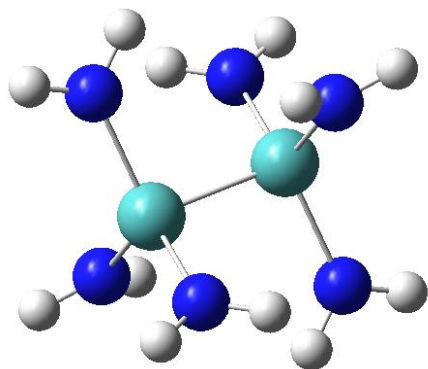


$\text{Mo}_2(\text{OH})_6$

Mo	0.000000	0.000000	1.100000
O	0.000000	1.890831	1.433405
O	-1.637508	-0.945415	1.433405
O	1.637508	-0.945416	1.433405
Mo	0.000000	0.000000	-1.100000
O	0.000000	-1.890831	-1.433405
O	-1.637508	0.945416	-1.433405
O	1.637508	0.945415	-1.433405
H	0.000000	2.125802	2.377654
H	-1.840999	-1.062901	2.377654
H	1.840999	-1.062901	2.377654
H	0.000000	-2.125802	-2.377654
H	-1.840999	1.062901	-2.377654
H	1.840999	1.062901	-2.377654

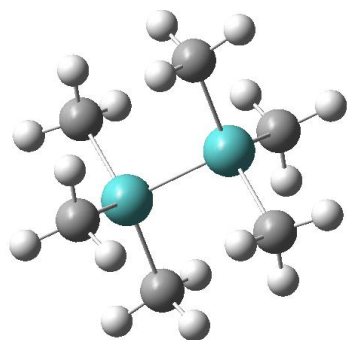
$\text{Mo}_2(\text{NH}_2)_6$

Mo	0.000000	0.000000	1.100000
N	0.000000	1.995131	1.415998
N	-1.727834	-0.997565	1.415998
N	1.727834	-0.997565	1.415998
Mo	0.000000	0.000000	-1.100000
N	0.000000	-1.995131	-1.415998
N	-1.727834	0.997565	-1.415998
N	1.727834	0.997565	-1.415998
H	0.000000	2.435512	2.330542
H	-2.109215	-1.217756	2.330542
H	2.109215	-1.217756	2.330542
H	0.000000	-2.435512	-2.330542
H	-2.109215	1.217756	-2.330542
H	2.109215	1.217756	-2.330542
H	0.000000	2.696568	0.682299
H	-2.335296	-1.348284	0.682299
H	2.335296	-1.348284	0.682299
H	0.000000	-2.696568	-0.682299
H	-2.335296	1.348284	-0.682299
H	2.335296	1.348284	-0.682299



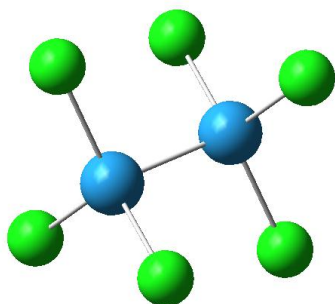
$\text{Mo}_2(\text{CH}_3)_6$

Mo	0.000000	0.000000	1.105000
C	0.000000	2.054110	1.541615
C	-1.778911	-1.027055	1.541615
C	1.778911	-1.027055	1.541615
Mo	0.000000	0.000000	-1.105000
C	0.000000	-2.054110	-1.541615
C	-1.778911	1.027055	-1.541615
C	1.778911	1.027055	-1.541615
H	0.000000	2.222432	2.627932
H	-1.924683	-1.111216	2.627932
H	1.924683	-1.111216	2.627932
H	0.000000	-2.222432	-2.627932
H	-1.924683	1.111216	-2.627932
H	1.924683	1.111216	-2.627932
H	0.889913	2.542902	1.120240
H	-0.889913	2.542902	1.120240
H	-2.647174	-0.500764	1.120240
H	-1.757261	-2.042138	1.120240
H	1.757261	-2.042138	1.120240
H	2.647174	-0.500764	1.120240
H	0.889913	-2.542902	-1.120240
H	-0.889913	-2.542902	-1.120240
H	-2.647174	0.500764	-1.120240
H	-1.757261	2.042138	-1.120240
H	1.757261	2.042138	-1.120240
H	2.647174	0.500764	-1.120240



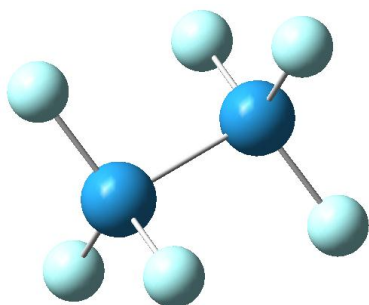
W_2Cl_6

W	0.000000	0.000000	1.150000
Cl	0.000000	2.192333	1.656140
Cl	-1.898616	-1.096166	1.656140
Cl	1.898616	-1.096166	1.656140
W	0.000000	0.000000	-1.150000
Cl	1.898616	1.096166	-1.656140
Cl	0.000000	-2.192333	-1.656140
Cl	-1.898616	1.096166	-1.656140



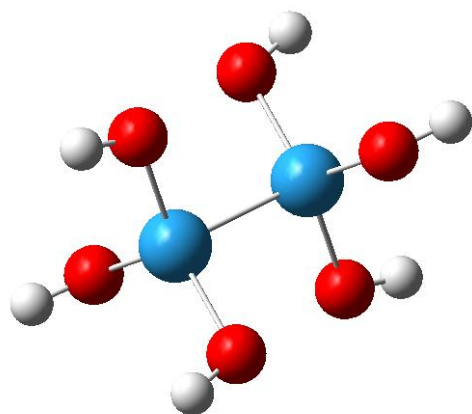
W_2F_6

W	0.000000	0.000000	1.155000
F	0.000000	1.838917	1.545874
F	-1.592549	-0.919459	1.545874
F	1.592549	-0.919459	1.545874
W	0.000000	0.000000	-1.155000
F	1.592549	0.919459	-1.545874
F	0.000000	-1.838917	-1.545874
F	-1.592549	0.919459	-1.545874



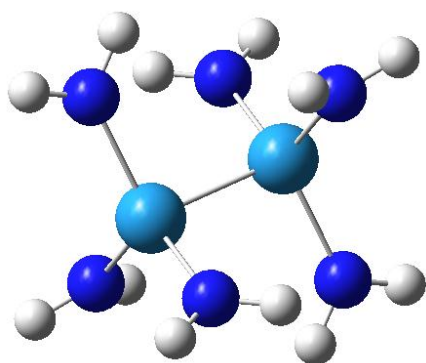
$W_2(OH)_6$

W	0.000000	0.000000	1.150000
O	0.000000	1.900679	1.485141
O	-1.646036	-0.950339	1.485141
O	1.646036	-0.950340	1.485141
W	0.000000	0.000000	-1.150000
O	0.000000	-1.900679	-1.485141
O	-1.646036	0.950340	-1.485141
O	1.646036	0.950339	-1.485141
H	0.000000	2.143361	2.427966
H	-1.856205	-1.071681	2.427966
H	1.856205	-1.071681	2.427966
H	0.000000	-2.143361	-2.427966
H	-1.856205	1.071681	-2.427966
H	1.856205	1.071680	-2.427966



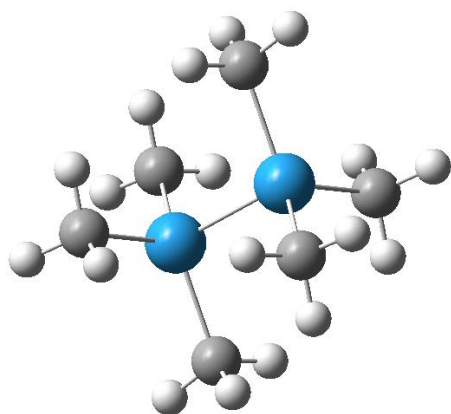


W	0.000000	0.000000	1.145000
N	0.000000	1.995130	1.460998
N	-1.727833	-0.997565	1.460998
N	1.727833	-0.997565	1.460998
W	0.000000	0.000000	-1.145000
N	0.000000	-1.995130	-1.460998
N	-1.727833	0.997565	-1.460998
N	1.727833	0.997565	-1.460998
H	0.000000	2.436927	2.374807
H	-2.110441	-1.218463	2.374807
H	2.110441	-1.218463	2.374807
H	0.000000	-2.436927	-2.374807
H	-2.110441	1.218463	-2.374807
H	2.110441	1.218463	-2.374807
H	0.000000	2.697686	0.728436
H	-2.336265	-1.348843	0.728436
H	2.336265	-1.348843	0.728436
H	0.000000	-2.697686	-0.728436
H	-2.336265	1.348843	-0.728436
H	2.336265	1.348843	-0.728436



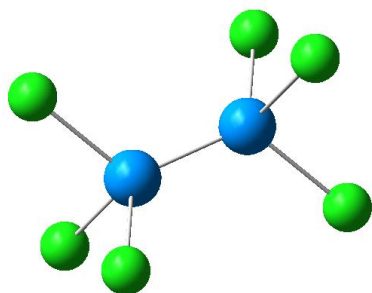
$W_2(CH_3)_6$

W	0.000000	0.000000	1.145000
C	0.000000	2.046177	1.617397
C	-1.772041	-1.023088	1.617397
C	1.772041	-1.023089	1.617397
W	0.000000	0.000000	-1.145000
C	0.000000	-2.046177	-1.617397
C	-1.772041	1.023089	-1.617397
C	1.772041	1.023088	-1.617397
H	0.000000	2.206899	2.706262
H	-1.911231	-1.103449	2.706262
H	1.911231	-1.103450	2.706262
H	0.000000	-2.206899	-2.706262
H	-1.911231	1.103450	-2.706262
H	1.911231	1.103449	-2.706262
H	0.887506	2.552695	1.208456
H	-0.887506	2.552695	1.208456
H	-2.654452	-0.507745	1.208456
H	-1.766946	-2.044950	1.208456
H	1.766946	-2.044950	1.208456
H	2.654452	-0.507745	1.208456
H	0.887506	-2.552695	-1.208456
H	-0.887506	-2.552695	-1.208456
H	-2.654452	0.507745	-1.208456
H	-1.766946	2.044950	-1.208456
H	1.766946	2.044950	-1.208456
H	2.654452	0.507745	-1.208456



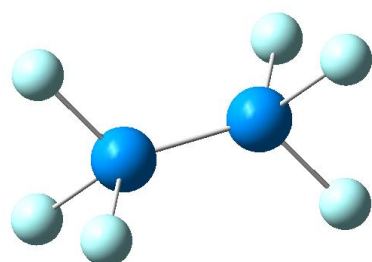
U_2Cl_6

```
U 0.000000 0.000000 1.175000
Cl 0.000000 2.151564 2.367632
Cl -1.863309 -1.075782 2.367632
Cl 1.863309 -1.075782 2.367632
U 0.000000 0.000000 -1.175000
Cl 1.863309 1.075782 -2.367632
Cl 0.000000 -2.151564 -2.367632
Cl -1.863309 1.075782 -2.367632
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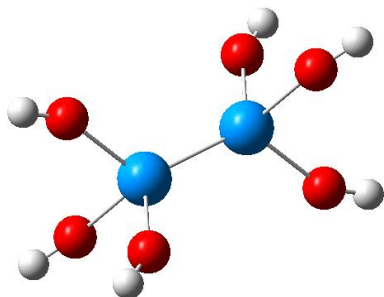
U_2F_6

```
U 0.000000 0.000000 1.190000
F 0.000000 1.710888 2.301064
F -1.481672 -0.855444 2.301064
F 1.481672 -0.855444 2.301064
U 0.000000 0.000000 -1.190000
F 1.481672 0.855444 -2.301064
F 0.000000 -1.710888 -2.301064
F -1.481672 0.855444 -2.301064
```



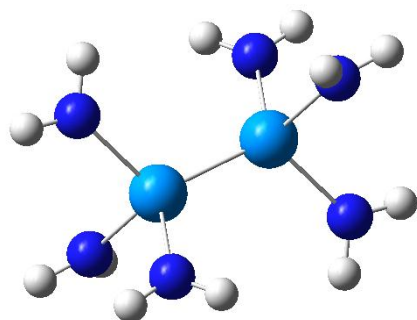


U	0.000000	0.000000	1.185000
O	0.000000	1.763940	2.287232
O	-1.527617	-0.881970	2.287232
O	1.527617	-0.881970	2.287232
U	0.000000	0.000000	-1.185000
O	0.000000	-1.763940	-2.287232
O	-1.527617	0.881970	-2.287232
O	1.527617	0.881970	-2.287232
H	0.000000	2.267335	3.110671
H	-1.963570	-1.133668	3.110671
H	1.963570	-1.133668	3.110671
H	0.000000	-2.267335	-3.110671
H	-1.963570	1.133668	-3.110671
H	1.963570	1.133667	-3.110671



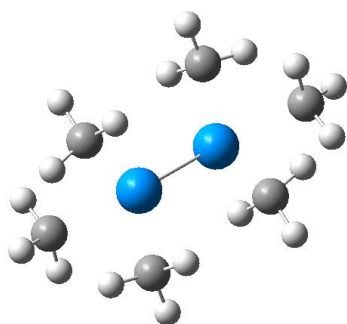


U	0.000000	0.000000	1.175000
N	0.000000	1.959371	2.130649
N	-1.696865	-0.979685	2.130649
N	1.696865	-0.979686	2.130649
U	0.000000	0.000000	-1.175000
N	0.000000	-1.959371	-2.130649
N	-1.696865	0.979686	-2.130649
N	1.696865	0.979685	-2.130649
H	0.000000	2.149183	3.133612
H	-1.861247	-1.074591	3.133612
H	1.861247	-1.074592	3.133612
H	0.000000	-2.149183	-3.133612
H	-1.861247	1.074592	-3.133612
H	1.861247	1.074591	-3.133612
H	0.000000	2.866577	1.662737
H	-2.482529	-1.433289	1.662737
H	2.482529	-1.433289	1.662737
H	0.000000	-2.866577	-1.662737
H	-2.482529	1.433289	-1.662737
H	2.482529	1.433288	-1.662737



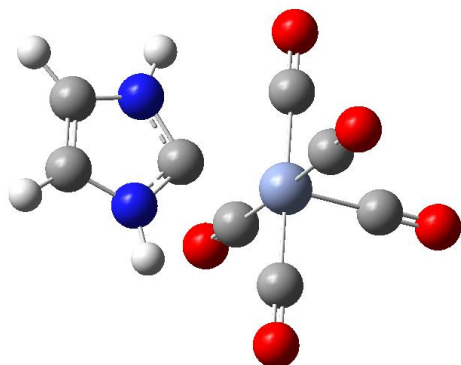


U	-0.301633	1.140797	0.000000
C	-2.511613	1.909944	0.000000
C	0.301633	2.653781	1.680044
C	0.301633	2.653781	-1.680044
U	0.301633	-1.140797	0.000000
C	2.511613	-1.909944	0.000000
C	-0.301633	-2.653781	1.680044
C	-0.301633	-2.653781	-1.680044
H	-2.551669	3.010346	0.000000
H	-0.090177	3.661178	1.469980
H	-0.090177	3.661178	-1.469980
H	2.551669	-3.010346	0.000000
H	0.090177	-3.661178	1.469980
H	0.090177	-3.661178	-1.469980
H	-3.057577	1.556727	-0.888623
H	-3.057577	1.556727	0.888623
H	-0.091965	2.340851	2.659658
H	1.396040	2.734287	1.771036
H	1.396040	2.734287	-1.771036
H	-0.091965	2.340851	-2.659658
H	3.057577	-1.556727	-0.888623
H	3.057577	-1.556727	0.888623
H	0.091965	-2.340851	2.659658
H	-1.396040	-2.734287	1.771036
H	-1.396040	-2.734287	-1.771036
H	0.091965	-2.340851	-2.659658



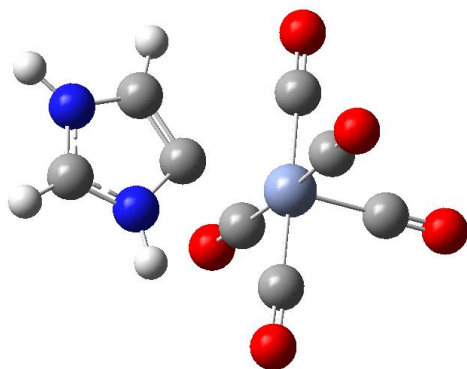
(CO)₅Cr-nNHC

C	0.000000	0.000000	-1.421798
N	0.000000	1.060438	-2.280638
N	0.000000	-1.060438	-2.280638
C	0.000000	0.679233	-3.614995
C	0.000000	-0.679233	-3.614995
H	0.000000	2.017876	-1.952182
H	0.000000	-2.017876	-1.952182
H	0.000000	1.389186	-4.430296
H	0.000000	-1.389186	-4.430296
Cr	0.000000	0.000000	0.667699
C	-1.895480	0.000000	0.623420
C	0.000000	0.000000	2.540765
C	1.895480	0.000000	0.623420
C	0.000000	-1.884431	0.671854
C	0.000000	1.884431	0.671854
O	0.000000	-3.046607	0.664142
O	3.052704	0.000000	0.597229
O	-3.052704	0.000000	0.597229
O	0.000000	3.046607	0.664142
O	0.000000	0.000000	3.701258



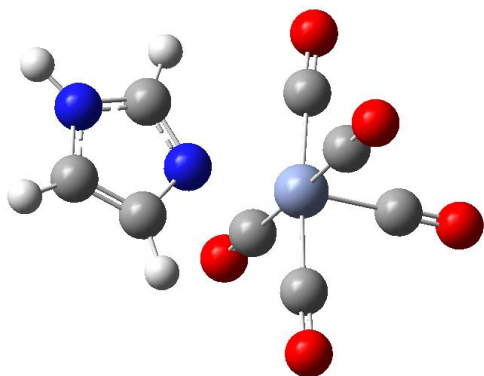
(CO)₅Cr-aNHC

C	-0.091901	1.407064	0.000000
C	-1.141227	2.312155	0.000000
N	1.026106	2.256056	0.000000
N	-0.635182	3.605624	0.000000
C	0.702377	3.559089	0.000000
H	-2.208567	2.139751	0.000000
H	1.980493	1.910824	0.000000
H	-1.176719	4.462160	0.000000
H	1.375187	4.404959	0.000000
Cr	-0.002481	-0.699148	0.000000
C	1.872592	-0.626554	0.000000
C	0.049412	-2.566950	0.000000
C	-1.891551	-0.740068	0.000000
C	-0.006502	-0.634089	1.892013
C	-0.006502	-0.634089	-1.892013
O	-0.006502	-0.584533	3.049903
O	-3.051786	-0.762600	0.000000
O	3.035333	-0.543329	0.000000
O	-0.006502	-0.584533	-3.049903
O	0.083517	-3.728662	0.000000



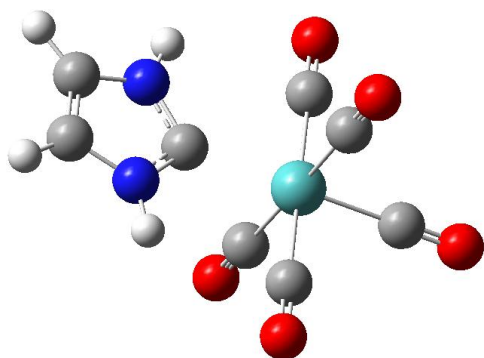
(CO)₅Cr-IMID

N	0.829524	1.272296	0.000000
C	0.373869	2.578862	0.000000
C	2.155324	1.341743	0.000000
C	1.439651	3.439848	0.000000
N	2.561134	2.637691	0.000000
H	-0.682073	2.811993	0.000000
H	2.835759	0.501152	0.000000
H	1.497686	4.519662	0.000000
H	3.523022	2.952608	0.000000
Cr	-0.356749	-0.534637	0.000000
C	1.174911	-1.641887	0.000000
C	-1.376834	-2.077135	0.000000
C	-1.980368	0.439892	0.000000
C	-0.339703	-0.508698	1.899675
C	-0.339703	-0.508698	-1.899675
O	-0.339703	-0.513234	3.056509
O	-3.006082	0.979930	0.000000
O	2.079502	-2.369093	0.000000
O	-0.339703	-0.513234	-3.056509
O	-2.017756	-3.047818	0.000000



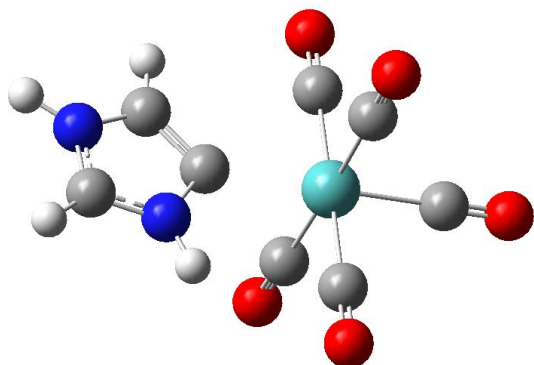
(CO)₅Mo-nNHC

C	0.000000	0.000000	-1.637867
N	0.000000	1.059909	-2.498005
N	0.000000	-1.059909	-2.498005
C	0.000000	0.679453	-3.832044
C	0.000000	-0.679453	-3.832044
H	0.000000	2.017069	-2.168942
H	0.000000	-2.017069	-2.168942
H	0.000000	1.388812	-4.648030
H	0.000000	-1.388812	-4.648030
Mo	0.000000	0.000000	0.600100
C	0.000000	-2.043289	0.610204
C	0.000000	0.000000	2.625233
C	0.000000	2.043289	0.610204
C	2.053762	0.000000	0.578699
C	-2.053762	0.000000	0.578699
O	3.210515	0.000000	0.569237
O	0.000000	3.204215	0.612870
O	0.000000	-3.204215	0.612870
O	-3.210515	0.000000	0.569237
O	0.000000	0.000000	3.785195



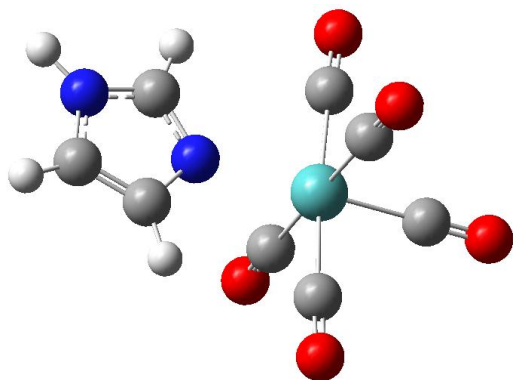
(CO)₅Mo-aNHC

C	-0.063146	1.625338	0.000000
C	-1.090695	2.555072	0.000000
N	1.073560	2.450802	0.000000
N	-0.556507	3.837619	0.000000
C	0.779956	3.760727	0.000000
H	-2.161970	2.407403	0.000000
H	2.019289	2.083852	0.000000
H	-1.078223	4.706491	0.000000
H	1.471024	4.591913	0.000000
Mo	-0.015967	-0.625906	0.000000
C	2.020377	-0.602820	0.000000
C	0.001548	-2.647179	0.000000
C	-2.064383	-0.631094	0.000000
C	-0.017561	-0.584231	2.050963
C	-0.017561	-0.584231	-2.050963
O	-0.017561	-0.552069	3.208561
O	-3.223831	-0.627563	0.000000
O	3.183830	-0.568292	0.000000
O	-0.017561	-0.552069	-3.208561
O	0.013864	-3.808766	0.000000



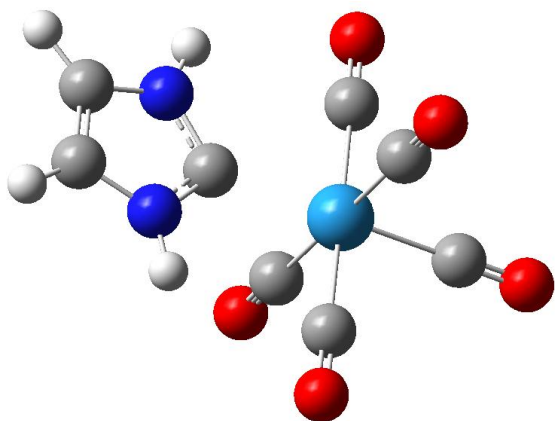
(CO)₅Mo-IMID

N	0.066385	1.724722	0.000000
C	-0.996803	2.611692	0.000000
C	1.167524	2.467662	0.000000
C	-0.526094	3.898477	0.000000
N	0.848850	3.787364	0.000000
H	-2.021854	2.266592	0.000000
H	2.183241	2.095573	0.000000
H	-1.031151	4.854880	0.000000
H	1.511286	4.552837	0.000000
Mo	-0.027531	-0.572343	0.000000
C	2.010054	-0.740574	0.000000
C	-0.114515	-2.557656	0.000000
C	-2.076190	-0.564773	0.000000
C	-0.027466	-0.585452	2.053444
C	-0.027466	-0.585452	-2.053444
O	-0.027466	-0.630842	3.209316
O	-3.233287	-0.622148	0.000000
O	3.159780	-0.894050	0.000000
O	-0.027466	-0.630842	-3.209316
O	-0.164828	-3.719568	0.000000



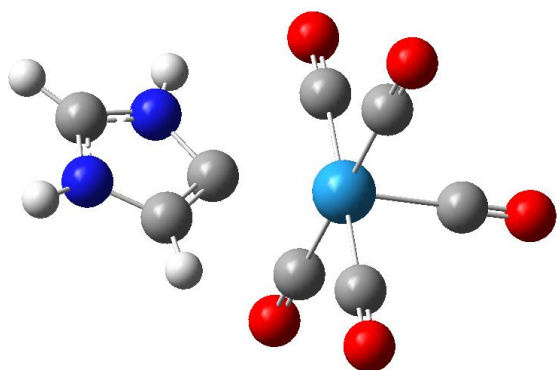
(CO)₅W-nNHC

C	0.000000	0.000000	-1.736446
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N	0.000000	-1.060310	-2.596219
C	0.000000	0.679649	-3.929281
C	0.000000	-0.679649	-3.929281
H	0.000000	2.017234	-2.266162
H	0.000000	-2.017234	-2.266162
H	0.000000	1.389060	-4.745046
H	0.000000	-1.389060	-4.745046
W	0.000000	0.000000	0.491259
C	-2.052260	0.000000	0.484766
C	0.000000	0.000000	2.519742
C	2.052260	0.000000	0.484766
C	0.000000	-2.041675	0.485420
C	0.000000	2.041675	0.485420
O	0.000000	-3.203897	0.468557
O	3.210171	0.000000	0.492872
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O	0.000000	3.203897	0.468557
O	0.000000	0.000000	3.680362



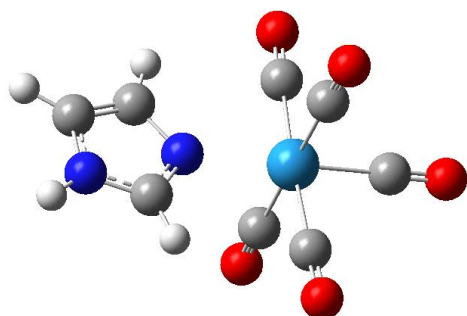
(CO)₅W-aNHC

C	1.144464	1.307398	0.000000
C	2.528496	1.378121	0.000000
N	0.784453	2.664849	0.000000
N	2.923804	2.708876	0.000000
C	1.839558	3.494025	0.000000
H	3.264556	0.586078	0.000000
H	-0.181056	2.976721	0.000000
H	3.877296	3.051927	0.000000
H	1.828636	4.574674	0.000000
W	-0.310469	-0.402577	0.000000
C	-0.300274	-0.393354	2.050529
C	-1.607231	-1.954568	0.000000
C	-0.300274	-0.393354	-2.050529
C	-1.861877	0.915325	0.000000
C	1.274686	-1.697882	0.000000
O	-2.731577	1.691170	0.000000
O	-0.300274	-0.394122	-3.209713
O	-0.300274	-0.394122	3.209713
O	2.177709	-2.427117	0.000000
O	-2.355311	-2.844444	0.000000



(CO)₅W-IMID

N	0.829524	1.272296	0.000000
C	0.373869	2.578862	0.000000
C	2.155324	1.341743	0.000000
C	1.439651	3.439848	0.000000
N	2.561134	2.637691	0.000000
H	-0.682073	2.811993	0.000000
H	2.835759	0.501152	0.000000
H	1.497686	4.519662	0.000000
H	3.523022	2.952608	0.000000
Cr	-0.356749	-0.534637	0.000000
C	1.174911	-1.641887	0.000000
C	-1.376834	-2.077135	0.000000
C	-1.980368	0.439892	0.000000
C	-0.339703	-0.508698	1.899675
C	-0.339703	-0.508698	-1.899675
O	-0.339703	-0.513234	3.056509
O	-3.006082	0.979930	0.000000
O	2.079502	-2.369093	0.000000
O	-0.339703	-0.513234	-3.056509
O	-2.017756	-3.047818	0.000000

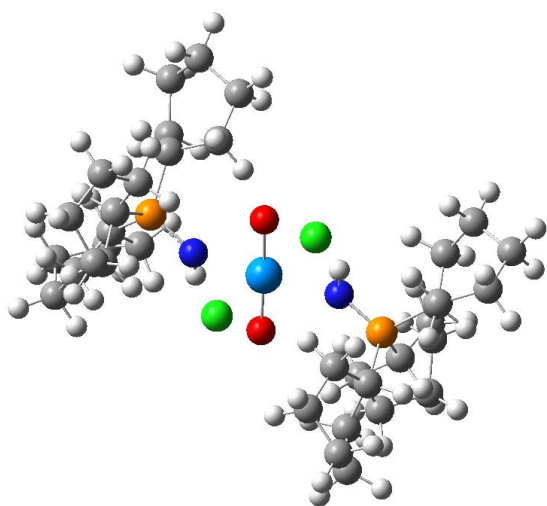


Uranyl 1

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Cl 0.144289 2.722482 -0.267795
O 0.214824 0.246872 1.787870
Cl -0.024278 -2.590777 0.299564
N -2.399373 0.022370 0.523002
P -3.895280 0.077422 -0.092945
H -2.404210 -0.260110 1.509554
C -4.160588 1.656520 -1.039978
C -3.547163 1.641687 -2.451581
C -3.639516 2.895026 -0.261218
C -4.046656 2.854459 -3.260507
C -3.248923 4.046704 -1.201919
C -4.203761 4.114246 -2.388415
H -5.263492 1.713525 -1.150256
H -2.450128 1.666745 -2.358079
H -3.798625 0.724015 -3.000669
H -4.421578 3.244858 0.428512
H -2.759861 2.612589 0.337948
H -3.325200 3.045291 -4.072091
H -5.008905 2.608724 -3.741799
H -3.251770 4.989297 -0.632169
H -2.215481 3.898915 -1.554850
H -5.239953 4.186440 -2.010149
H -4.029234 5.019815 -2.991652
C -4.342607 -1.283413 -1.305333
C -5.099419 -2.488931 -0.732805
C -3.096946 -1.801692 -2.059584
C -5.746559 -3.312969 -1.912424
C -3.381738 -3.127337 -2.793242
C -4.882054 -3.251412 -3.187466
H -5.026154 -0.769736 -2.011448
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H -6.759271 -2.921027 -2.118533
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H -3.121467 -3.980727 -2.145379
H -5.164274 -2.376151 -3.802130
H -5.052337 -4.145080 -3.813325
C -5.159579 -0.013476 1.269421
C -5.371762 1.311747 2.028672
C -4.795778 -1.108960 2.283529
C -6.076251 1.073094 3.421894
C -6.041868 -1.448893 3.186162
C -6.941793 -0.217093 3.389601

H -6.103794 -0.291205 0.764702
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H -3.984118 -0.727645 2.925541
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C 5.138091 -2.308167 -3.264713
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H 5.930566 -1.244912 -0.477713
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C 4.373331 2.042759 1.959145

C	4.058442	2.608004	-0.477152
C	5.269835	3.273466	2.224140
C	4.195812	4.038931	0.084142
C	5.431893	4.159491	0.972677
H	5.690356	1.414872	0.384891
H	3.309884	2.312121	2.080967
H	4.602925	1.268185	2.707599
H	4.600674	2.532608	-1.434717
H	2.991536	2.411047	-0.681600
H	4.821409	3.860239	3.046435
H	6.262688	2.939394	2.577773
H	4.234257	4.756858	-0.753521
H	3.294389	4.293210	0.670424
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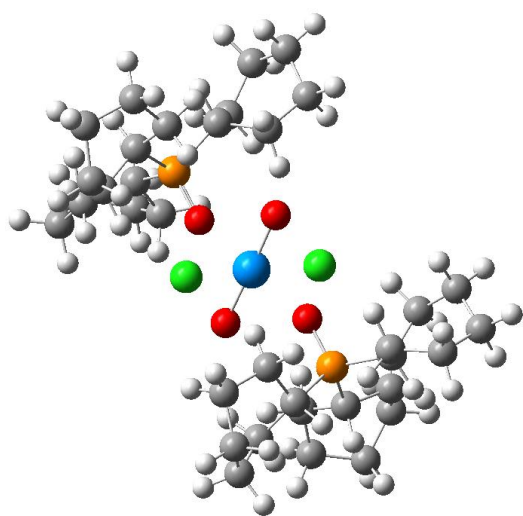


Uranyl 2

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Cl 0.038274 -2.596717 0.152694
O -2.382040 0.012096 0.349893
P -3.845621 0.105956 -0.106819
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C -3.603347 1.855094 -2.301594
C -3.655189 2.913762 -0.005577
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C -3.268450 4.139525 -0.842755
C -4.266184 4.314061 -2.019784
H -5.297015 1.803619 -0.957801
H -2.505157 1.876074 -2.221443
H -3.860713 0.984065 -2.920923
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H -3.403937 3.393801 -3.800189
H -5.085385 2.923724 -3.487145
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H -2.247151 4.018822 -1.236101
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C -5.731908 -3.220194 -2.010031
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H 2.628138 -2.032380 4.550137
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C 5.524955 0.316151 -2.195310
C 4.196246 -1.827487 -2.111852
C 6.645577 -0.307634 -3.055350
C 4.825659 -1.975895 -3.511850
C 6.336930 -1.767549 -3.442749
H 5.775322 -1.222572 -0.716424
H 4.720928 0.711693 -2.841075
H 5.941208 1.171293 -1.640696
H 4.247162 -2.797331 -1.593380
H 3.128589 -1.565456 -2.203074
H 6.771650 0.306942 -3.965322
H 7.603515 -0.259603 -2.505531
H 4.577948 -2.972998 -3.915812
H 4.389165 -1.237997 -4.209726
H 6.757672 -2.458687 -2.687715
H 6.823787 -2.020510 -4.401089
C 4.502238 1.526584 0.602944
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C 3.901818 2.636118 -0.306322
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C	4.033665	4.030489	0.339509
C	5.307802	4.121126	1.176375
H	5.593329	1.435783	0.416666
H	3.270512	2.165843	2.264635
H	4.611949	1.116019	2.768357
H	4.414724	2.631019	-1.282357
H	2.836454	2.427228	-0.496134
H	4.788186	3.694128	3.252148
H	6.227413	2.832373	2.676124
H	4.018437	4.799744	-0.452101
H	3.156122	4.226917	0.981397
H	6.173563	3.850545	0.541871
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Uranyl 3

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O 0.226368 0.201412 1.824134
Cl -0.084506 -2.602180 0.242197
O -2.420458 0.037399 0.375305
P -3.868803 0.112272 -0.127357
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C -3.576627 1.822105 -2.351049
C -3.692142 2.922758 -0.074286
C -4.068815 3.089153 -3.078649
C -3.302919 4.140830 -0.929606
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H -3.820226 0.943658 -2.962806
H -4.483394 3.216147 0.628686
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H -3.335386 3.342459 -3.859937
H -5.019236 2.876778 -3.594071
H -3.319465 5.040204 -0.296680
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H -5.287480 4.316710 -1.747900
H -4.079471 5.228979 -2.652973
C -4.299807 -1.208562 -1.370904
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C -3.047821 -1.675372 -2.152543
C -5.665391 -3.202322 -2.063977
C -3.318691 -2.979039 -2.935773
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H -2.222068 -1.853160 -1.450510
H -5.802535 -4.259286 -1.785947
H -6.669244 -2.797855 -2.270789
H -2.667793 -3.010930 -3.820933
H -3.039331 -3.847820 -2.317806
H -5.078282 -2.213081 -3.918511
H -4.958287 -3.969656 -3.978574
C -5.040155 -0.110196 1.281587
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C -4.562281 -1.244169 2.208959
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C -5.734836 -1.721712 3.089339
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H -5.986565 -0.419445 0.800906

H	-4.402248	1.698840	2.328636
H	-6.011316	1.809299	1.593306
H	-4.126499	-2.089133	1.662012
H	-3.747490	-0.841197	2.828825
H	-5.176350	0.661247	4.265137
H	-6.631259	1.559082	3.836987
H	-6.273792	-2.540722	2.586924
H	-5.328388	-2.141389	4.022950
H	-7.487015	-0.502869	2.625848
H	-7.252560	-0.785193	4.347340
N	2.323678	-0.078984	-0.489605
P	3.845344	-0.127941	0.065083
H	2.305978	0.126353	-1.496660
C	3.994393	-1.254793	1.514427
C	3.974061	-2.755926	1.124609
C	2.947972	-1.036983	2.620152
C	3.680750	-3.650489	2.350922
C	3.444251	-1.697506	3.918831
C	4.201224	-3.013450	3.636937
H	4.995331	-1.004837	1.919345
H	3.194590	-2.930338	0.369271
H	4.945591	-3.036656	0.689782
H	2.705919	0.015695	2.796535
H	2.009295	-1.503915	2.293374
H	2.593898	-3.807465	2.436755
H	4.127825	-4.643057	2.190178
H	4.096678	-1.003137	4.473113
H	2.572561	-1.892795	4.562035
H	5.282233	-2.816593	3.530135
H	4.099583	-3.703327	4.488027
C	5.039183	-0.786558	-1.219256
C	5.621695	0.269862	-2.174254
C	4.419108	-1.952134	-2.043763
C	6.791268	-0.324858	-2.984512
C	5.051942	-2.080816	-3.439937
C	6.549616	-1.798203	-3.372427
H	5.879951	-1.175105	-0.612293
H	4.829955	0.617607	-2.857239
H	5.983673	1.155316	-1.636323
H	4.568404	-2.894096	-1.500417
H	3.330626	-1.820463	-2.136048
H	6.932441	0.286112	-3.889777
H	7.721789	-0.239728	-2.401191
H	4.854499	-3.089962	-3.830759
H	4.579142	-1.378136	-4.145839
H	7.001058	-2.467512	-2.620166
H	7.045024	-2.027808	-4.327178
C	4.544203	1.530257	0.574277
C	4.360853	1.926954	2.049347
C	3.969481	2.648872	-0.332528

C	5.243189	3.153278	2.369908
C	4.100559	4.041390	0.314574
C	5.358238	4.123285	1.179512
H	5.633139	1.425036	0.403189
H	3.300983	2.167609	2.222867
H	4.624699	1.111273	2.734110
H	4.489071	2.644008	-1.302418
H	2.904061	2.450742	-0.530352
H	4.809734	3.673848	3.238817
H	6.247269	2.815789	2.675342
H	4.107910	4.808876	-0.471762
H	3.214501	4.244592	0.936799
H	6.234420	3.863781	0.560556
H	5.528448	5.148868	1.538530

