

## Supporting Information for

### How easy is CO<sub>2</sub> fixation by M-C bonds containing complexes (M = Cu, Ni, Co, Rh, Ir)?

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**XYZ Coordinates** (Coordinate data sets, absolute energies, 3D view for DFT optimized complexes (main distances in Å))

**CO<sub>2</sub>**

E : -188.572427564 A.U.  
C 0.000000 0.000000 -0.000006  
O 0.000000 0.000000 1.172763  
O 0.000000 0.000000 -1.172759

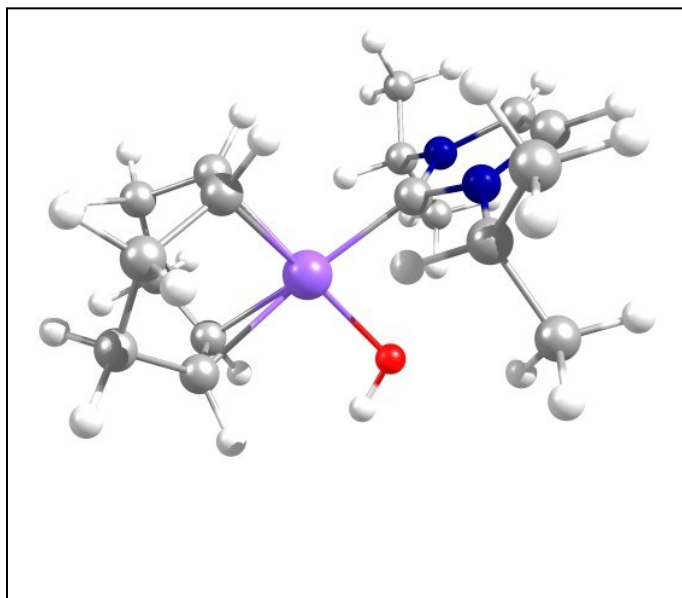
**Phenylacetylide CCPH**

E : -308.245246694 A.U.  
C -0.597955 -0.000036 -0.000043  
C 0.119713 1.216671 -0.000016  
C 0.119797 -1.216704 -0.000017  
C 1.515167 1.211192 0.000025  
H -0.431235 2.158745 -0.000032  
C 1.515242 -1.211132 0.000026  
H -0.431103 -2.158806 -0.000035  
C 2.217763 0.000056 0.000046  
H 2.058280 2.158781 0.000040  
H 2.058429 -2.158679 0.000043  
H 3.309803 0.000085 0.000080  
C -2.024654 -0.000110 -0.000118  
C -3.240587 -0.000056 -0.000146  
H -4.311086 0.000596 0.001373

1

E : -954.037291796 A.U.

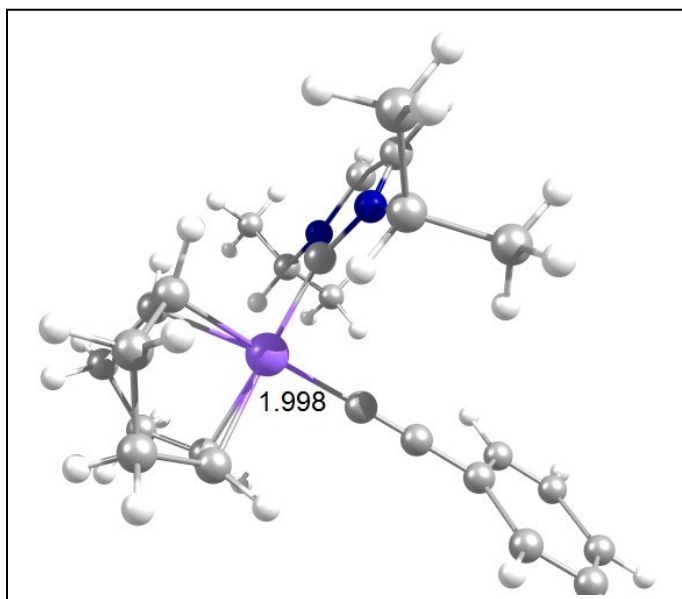
Ir	0.595880	-0.008621	0.337292
N	-2.184624	1.113445	-0.374401
N	-2.222127	-1.054804	-0.334080
C	-1.378885	0.018263	-0.198522
C	-3.504458	0.728769	-0.594171
C	-3.527899	-0.633528	-0.569522
C	-1.713701	2.501699	-0.162669
C	-2.050015	2.959149	1.261920
C	-2.250850	3.441356	-1.244822
C	-1.803328	-2.448352	-0.054049
C	-2.167818	-2.827289	1.386480
C	-2.362706	-3.417739	-1.097950
C	2.543357	0.742661	0.991951
C	2.623750	-0.665125	0.914490
C	3.339028	-1.414734	-0.205998
C	2.381642	-1.806557	-1.357886
C	1.233925	-0.823087	-1.531740
C	1.374025	0.606479	-1.574601
C	2.729231	1.318152	-1.490131
C	3.089528	1.714858	-0.038621
H	-4.303027	1.440826	-0.765728
H	-4.350635	-1.323539	-0.714986
H	-0.617009	2.413060	-0.250368
H	-1.611058	2.261544	1.990749
H	-3.139802	3.005430	1.418000
H	-1.637989	3.964410	1.439446
H	-3.341057	3.580138	-1.165264
H	-2.020018	3.067433	-2.253039
H	-1.788089	4.432453	-1.131311
H	-0.703688	-2.405340	-0.132113
H	-3.259679	-2.830272	1.534384
H	-1.709714	-2.111175	2.084755
H	-1.790674	-3.836100	1.614040
H	-2.104594	-3.102362	-2.119445
H	-3.458344	-3.510344	-1.027794
H	-1.940804	-4.419323	-0.930121
H	3.805133	-2.323122	0.207298
H	4.167553	-0.799252	-0.588800
H	2.946552	-1.934529	-2.302611
H	1.939955	-2.791969	-1.132355
H	3.516874	0.679629	-1.922052
H	2.707095	2.224497	-2.116458
H	4.185598	1.828880	0.074978
H	2.654816	2.703184	0.182210
H	2.397688	1.179964	1.987621
H	2.511001	-1.219770	1.853163
H	0.395974	-1.240913	-2.105469
H	0.622605	1.144865	-2.164327
O	-0.130757	0.025044	2.242343
H	0.606897	0.004819	2.879814



### 8-Ir

E : -1185.87913985 A.U.

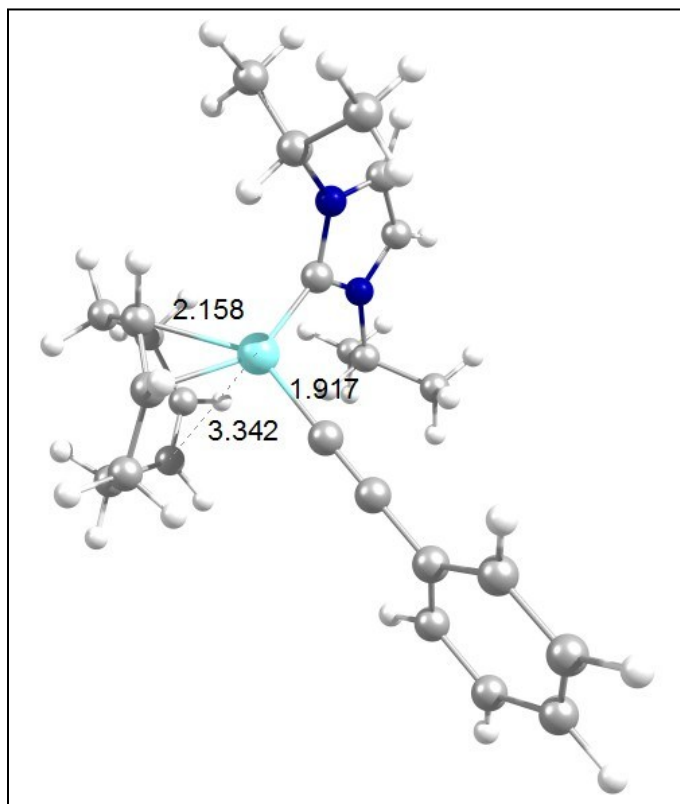
Ir	-0.790872	-0.550243	-0.043332
N	-0.782049	2.427084	-0.846207
N	-0.567973	2.218338	1.301337
C	-0.736250	1.487766	0.152751
C	-0.629401	3.711117	-0.329560
C	-0.496805	3.579834	1.019774
C	-0.854924	2.080829	-2.283332
C	0.509125	2.278977	-2.953635
C	-1.982600	2.848296	-2.979561
C	-0.356763	1.605309	2.632774
C	1.108027	1.747402	3.060868
C	-1.341342	2.169192	3.661786
C	-0.830510	-2.524933	-1.033804
C	-0.856039	-2.742374	0.357781
C	-2.097624	-3.158235	1.138563
C	-2.869530	-1.949622	1.722863
C	-2.789773	-0.707578	0.854640
C	-2.955350	-0.673421	-0.553062
C	-3.289797	-1.896794	-1.403340
C	-2.028068	-2.603289	-1.960205
H	-0.639134	4.598618	-0.951379
H	-0.369198	4.331855	1.789542
H	-1.087230	1.000981	-2.267186
H	1.274912	1.679797	-2.441223
H	0.814903	3.337305	-2.938717
H	0.459571	1.955732	-4.004269
H	-1.777804	3.930190	-3.019960
H	-2.944351	2.697684	-2.468107
H	-2.084382	2.495107	-4.016100
H	-0.570419	0.536650	2.454539
H	1.386535	2.804505	3.198151
H	1.770450	1.299067	2.307119
H	1.268821	1.228974	4.017987
H	-2.381854	2.060329	3.322817
H	-1.153825	3.235568	3.865824
H	-1.230799	1.628761	4.613242
H	-1.796007	-3.823741	1.962643
H	-2.758683	-3.759393	0.494991
H	-3.925357	-2.226294	1.914350
H	-2.439465	-1.693935	2.705413
H	-3.896589	-2.604018	-0.816219
H	-3.926972	-1.586492	-2.246819
H	-2.257255	-3.658922	-2.206211
H	-1.740027	-2.127100	-2.911390
H	0.139333	-2.628768	-1.530644
H	0.102392	-2.970745	0.832339
H	-3.009124	0.221961	1.393909
H	-3.267804	0.285163	-0.980657
C	1.206242	-0.541316	-0.113939
C	2.444079	-0.565255	-0.144490
C	3.866001	-0.613546	-0.159296
C	4.575628	-1.498725	0.690923
C	4.622106	0.220584	-1.020377
C	5.970195	-1.540049	0.680573
H	4.009049	-2.151217	1.358212
C	6.016310	0.165422	-1.032105
H	4.093540	0.909708	-1.681968
C	6.700981	-0.711711	-0.181253
H	6.492927	-2.230122	1.347789
H	6.575196	0.816448	-1.709241
H	7.792404	-0.750187	-0.190170



## 8-Cu

E : -1278.85108844 A.U.

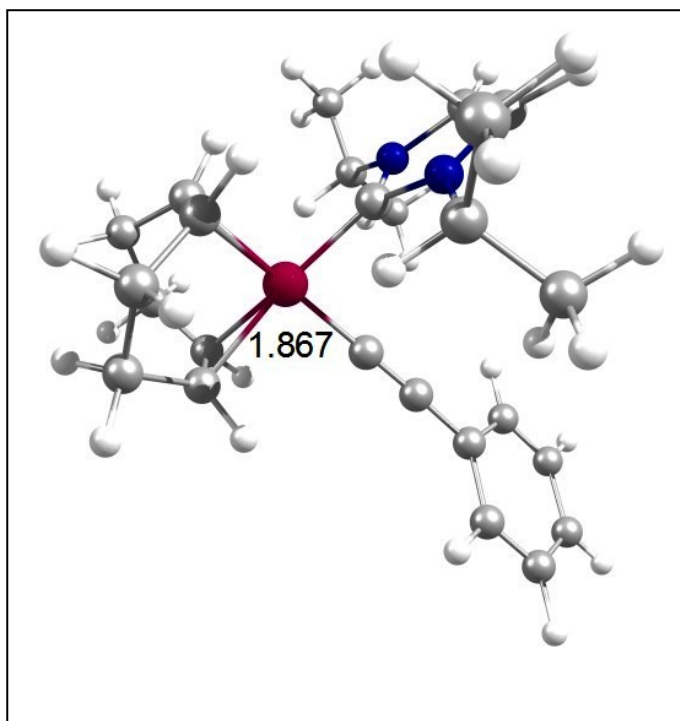
Cu	-0.587105	0.481951	-0.529835
N	-1.332934	-1.659242	1.437589
N	-2.399183	-1.959138	-0.414081
C	-1.555495	-1.076901	0.215931
C	-2.011629	-2.866244	1.560284
C	-2.684831	-3.058057	0.390798
C	-0.392032	-1.118009	2.446525
C	0.857720	-1.999594	2.540862
C	-1.091591	-0.923235	3.795737
C	-2.859621	-1.797998	-1.808551
C	-2.221849	-2.856218	-2.717182
C	-4.390080	-1.788199	-1.890055
C	-1.363949	2.555639	1.735708
C	-0.289655	3.249386	1.320804
C	-0.170064	4.125966	0.100183
C	0.261390	3.374732	-1.180660
C	-0.622818	2.246006	-1.664311
C	-1.947416	1.944911	-1.346037
C	-2.881311	2.695188	-0.399869
C	-2.732918	2.425025	1.113549
H	-1.965924	-3.480586	2.452097
H	-3.330416	-3.870170	0.076761
H	-0.095641	-0.141510	2.034533
H	1.356982	-2.055076	1.563825
H	0.610480	-3.016742	2.884697
H	1.565940	-1.562085	3.259796
H	-1.376467	-1.885605	4.250147
H	-1.998122	-0.308962	3.693217
H	-0.409962	-0.418695	4.495936
H	-2.475908	-0.807590	-2.094708
H	-2.565492	-3.869518	-2.456082
H	-1.126186	-2.828492	-2.637017
H	-2.498586	-2.667312	-3.765030
H	-4.817219	-1.023181	-1.226046
H	-4.817534	-2.764612	-1.613403
H	-4.707171	-1.568657	-2.920161
H	0.591104	4.898303	0.298827
H	-1.107194	4.669529	-0.083323
H	0.331196	4.116075	-2.000771
H	1.279034	2.972502	-1.047492
H	-2.811526	3.776414	-0.594687
H	-3.914654	2.421912	-0.669884
H	-3.443306	3.078784	1.657344
H	-3.079443	1.395352	1.306551
H	-1.250657	1.997040	2.672329
H	0.620063	3.157423	1.924135
H	-0.244864	1.794313	-2.589966
H	-2.471159	1.330683	-2.086474
C	1.305618	0.179149	-0.496050
C	2.525163	-0.037539	-0.476609
C	3.925537	-0.297987	-0.458521
C	4.533828	-1.094685	-1.460803
C	4.759108	0.225108	0.561401
C	5.904901	-1.353552	-1.439459
H	3.906717	-1.504335	-2.255202
C	6.129458	-0.039351	0.576393
H	4.308912	0.844045	1.340265
C	6.713234	-0.829935	-0.421988
H	6.348383	-1.970640	-2.225276
H	6.749315	0.376673	1.374975
H	7.785977	-1.034833	-0.407746



## 8-Co

E : -1227.31156941 A.U.

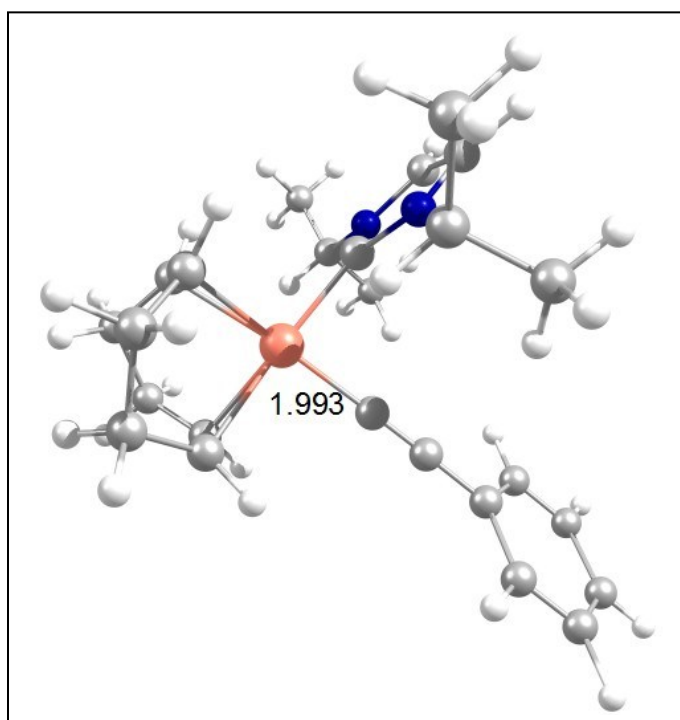
Co	-1.028954	-0.649999	-0.078367
N	-0.816474	2.215621	-0.734352
N	-0.558563	1.890630	1.390418
C	-0.822681	1.230018	0.218811
C	-0.537361	3.458600	-0.169514
C	-0.376100	3.253857	1.167446
C	-0.955434	1.939995	-2.180451
C	0.390637	2.109402	-2.893106
C	-2.072162	2.785478	-2.800848
C	-0.367805	1.203795	2.687056
C	1.104726	1.244878	3.110215
C	-1.310500	1.770439	3.754411
C	-1.127962	-2.397259	-1.226753
C	-1.092187	-2.766545	0.119627
C	-2.292708	-3.228033	0.924247
C	-2.954354	-2.044979	1.674384
C	-2.843786	-0.742987	0.909347
C	-3.100654	-0.571239	-0.461532
C	-3.562641	-1.675474	-1.398703
C	-2.362995	-2.361111	-2.099727
H	-0.489404	4.371763	-0.751372
H	-0.160037	3.955794	1.964404
H	-1.237642	0.873281	-2.207198
H	1.148143	1.465680	-2.424522
H	0.737085	3.154421	-2.855060
H	0.293581	1.823548	-3.951193
H	-1.825478	3.859022	-2.784978
H	-3.024317	2.643111	-2.269457
H	-2.216942	2.496238	-3.852069
H	-0.641371	0.159369	2.464072
H	1.439287	2.276812	3.301764
H	1.738247	0.804030	2.328293
H	1.241381	0.669215	4.037931
H	-2.359083	1.733462	3.424937
H	-1.063136	2.815463	3.999995
H	-1.218735	1.183950	4.680274
H	-1.974830	-3.990126	1.653436
H	-3.024690	-3.723139	0.267674
H	-4.012316	-2.278969	1.910524
H	-2.451796	-1.912088	2.647060
H	-4.157705	-2.417797	-0.843946
H	-4.238852	-1.254927	-2.160376
H	-2.639939	-3.380975	-2.434350
H	-2.113455	-1.802975	-3.016891
H	-0.175312	-2.400215	-1.764486
H	-0.109745	-2.987106	0.545062
H	-2.912748	0.154121	1.535301
H	-3.312918	0.449947	-0.795125
C	0.835365	-0.651230	-0.180150
C	2.075684	-0.656139	-0.221413
C	3.497881	-0.708480	-0.243984
C	4.209201	-1.601152	0.597617
C	4.254032	0.128691	-1.102344
C	5.603556	-1.646377	0.581571
H	3.644066	-2.257446	1.262447
C	5.647974	0.069566	-1.119845
H	3.726648	0.824688	-1.757622
C	6.333887	-0.814797	-0.277548
H	6.126533	-2.342635	1.242178
H	6.205705	0.723537	-1.795127
H	7.425114	-0.856349	-0.291035



### 8-Rh

E : -1192.05773182 A.U.

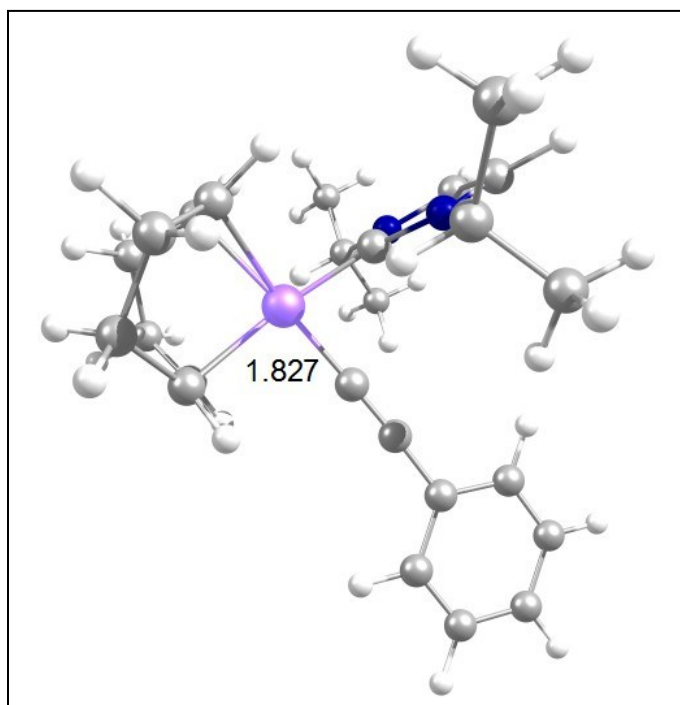
Rh	-0.935466	-0.620671	-0.053571
N	-0.802846	2.353635	-0.824043
N	-0.575135	2.117233	1.315733
C	-0.795869	1.405766	0.165844
C	-0.575754	3.624628	-0.301923
C	-0.433774	3.475612	1.044953
C	-0.913686	2.022607	-2.261695
C	0.446855	2.163533	-2.952856
C	-2.017167	2.844771	-2.934226
C	-0.387203	1.484138	2.640558
C	1.082734	1.558315	3.067489
C	-1.345183	2.079952	3.677102
C	-1.006969	-2.575965	-1.076576
C	-1.023382	-2.821109	0.300260
C	-2.260233	-3.213813	1.095817
C	-2.985550	-1.995547	1.720223
C	-2.927015	-0.746599	0.862470
C	-3.112299	-0.690882	-0.529670
C	-3.459877	-1.889960	-1.404394
C	-2.210042	-2.589309	-1.997173
H	-0.544227	4.516108	-0.917522
H	-0.254620	4.213355	1.818335
H	-1.194788	0.954929	-2.250565
H	1.192643	1.529565	-2.452932
H	0.798748	3.207467	-2.939906
H	0.367340	1.846426	-4.003532
H	-1.765911	3.916992	-2.966826
H	-2.976796	2.731522	-2.409191
H	-2.149820	2.506987	-3.972432
H	-0.646168	0.427713	2.453870
H	1.406699	2.600529	3.218065
H	1.723037	1.091786	2.305880
H	1.222364	1.021326	4.017676
H	-2.390245	2.017668	3.340170
H	-1.112782	3.136054	3.887948
H	-1.254843	1.528470	4.624364
H	-1.963665	-3.903217	1.902105
H	-2.952180	-3.782222	0.455395
H	-4.036662	-2.258198	1.955191
H	-2.511584	-1.757430	2.686713
H	-4.061166	-2.609203	-0.826757
H	-4.107152	-1.556739	-2.231403
H	-2.459960	-3.628214	-2.291414
H	-1.920161	-2.076154	-2.928461
H	-0.038263	-2.646951	-1.580495
H	-0.060379	-3.036369	0.771122
H	-3.084787	0.185611	1.416821
H	-3.373150	0.286154	-0.948748
C	1.055544	-0.622484	-0.137721
C	2.293514	-0.646576	-0.168485
C	3.716297	-0.700261	-0.184034
C	4.423178	-1.593340	0.660002
C	4.475743	0.136936	-1.038980
C	5.817680	-1.640251	0.648941
H	3.854294	-2.248299	1.322951
C	5.869889	0.077932	-1.050402
H	3.949824	0.832542	-1.695886
C	6.551640	-0.807951	-0.206330
H	6.337841	-2.337110	1.311156
H	6.430982	0.732212	-1.722615
H	7.642949	-0.850051	-0.215369



## 8-Ni

E : -1252.28124421 A.U.

Ni	-1.049522	-0.606962	0.029643
N	-0.609539	2.057070	-1.093485
N	-0.463580	2.076196	1.076197
C	-0.704230	1.263206	0.009813
C	-0.312460	3.363262	-0.718289
C	-0.221677	3.375061	0.641573
C	-0.711237	1.574772	-2.497343
C	0.658471	1.621583	-3.181638
C	-1.790205	2.346925	-3.262737
C	-0.376322	1.621193	2.489958
C	1.062006	1.741731	3.002571
C	-1.389316	2.365022	3.365652
C	-1.145338	-2.634762	-0.749366
C	-1.251884	-2.715603	0.625929
C	-2.533321	-2.913006	1.409106
C	-3.154943	-1.570353	1.867909
C	-3.028608	-0.463002	0.849517
C	-3.155549	-0.575933	-0.524550
C	-3.522489	-1.834011	-1.287578
C	-2.276831	-2.633972	-1.748082
H	-0.204068	4.167477	-1.436360
H	-0.021552	4.191950	1.324905
H	-1.018097	0.521408	-2.390045
H	1.398972	1.037486	-2.618473
H	1.020753	2.656234	-3.278691
H	0.579360	1.199924	-4.193937
H	-1.506909	3.399916	-3.410443
H	-2.758574	2.322379	-2.741946
H	-1.923131	1.902238	-4.259084
H	-0.641668	0.553046	2.438755
H	1.382152	2.793290	3.057470
H	1.755019	1.191636	2.351865
H	1.128018	1.320395	4.015835
H	-2.413524	2.274355	2.975216
H	-1.146625	3.435473	3.443334
H	-1.370807	1.950350	4.383414
H	-2.312379	-3.521137	2.298622
H	-3.253179	-3.490623	0.813807
H	-4.219762	-1.712551	2.131892
H	-2.662805	-1.241095	2.796253
H	-4.181507	-2.462421	-0.672992
H	-4.108698	-1.551566	-2.174497
H	-2.561053	-3.675755	-1.987416
H	-1.897327	-2.210237	-2.690875
H	-0.141488	-2.734031	-1.171078
H	-0.315488	-2.829114	1.180188
H	-3.043507	0.551726	1.259946
H	-3.217717	0.362284	-1.085282
C	0.776584	-0.641278	-0.011400
C	2.009879	-0.688872	-0.032040
C	3.430114	-0.804396	-0.047661
C	4.050774	-2.071226	0.067130
C	4.247557	0.343758	-0.177047
C	5.440692	-2.180317	0.053950
H	3.427895	-2.961763	0.167740
C	5.636989	0.223962	-0.191783
H	3.778033	1.325152	-0.266731
C	6.237781	-1.035817	-0.076011
H	5.907086	-3.163368	0.144684
H	6.256708	1.117184	-0.293618
H	7.325701	-1.125737	-0.086917

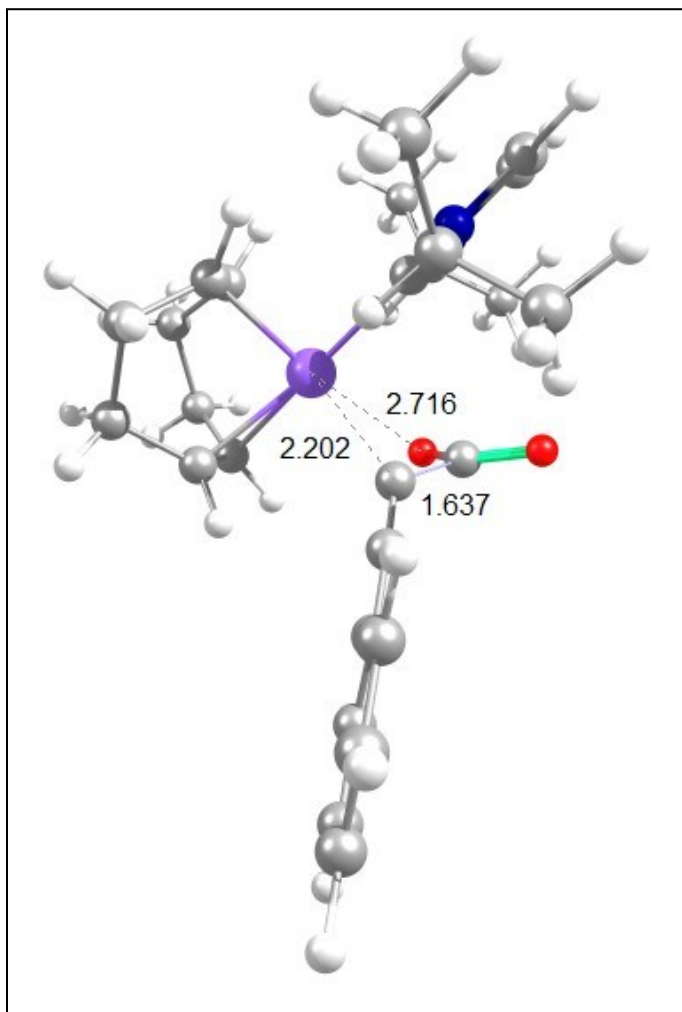




**TS<sub>8</sub>-Ir**

E : -1375.48103770 A.U.

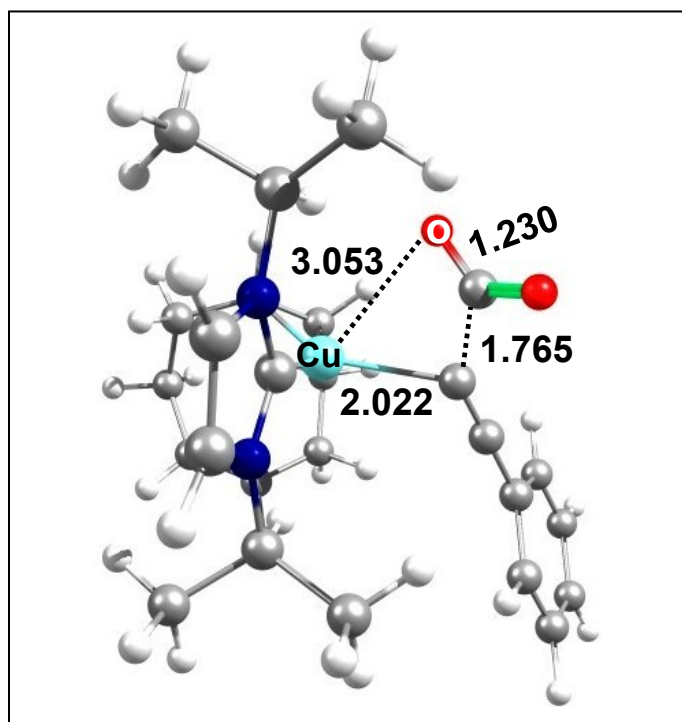
Ir	0.469415	0.663126	0.028832
O	0.513780	0.028545	-2.611147
O	-0.210872	-2.132577	-2.348702
N	2.750775	-1.400098	-0.302436
N	1.256252	-2.142050	1.085642
C	1.551221	-1.070707	0.279150
C	3.177736	-2.651954	0.122936
C	2.241944	-3.117813	0.994231
C	3.457316	-0.590517	-1.328123
C	3.509618	-1.343489	-2.661897
C	4.848301	-0.181614	-0.829353
C	-0.012952	-2.308551	1.830720
C	-0.864952	-3.405867	1.181013
C	0.254221	-2.566459	3.317895
C	-0.040059	2.664547	-0.758433
C	-0.953953	2.404315	0.276970
C	-0.872374	3.009497	1.671526
C	-0.113774	2.089319	2.655102
C	0.979201	1.287826	1.971345
C	1.963584	1.825237	1.054831
C	2.011598	3.298038	0.639802
C	1.184364	3.559365	-0.644342
C	-0.170839	-0.920654	-2.152039
H	4.096419	-3.105879	-0.229170
H	2.194799	-4.051350	1.542318
H	2.819236	0.297839	-1.448230
H	2.499227	-1.627201	-2.984554
H	4.140126	-2.244818	-2.592121
H	3.943014	-0.688485	-3.432013
H	5.508065	-1.055756	-0.709313
H	4.795553	0.345048	0.134593
H	5.319188	0.489361	-1.562726
H	-0.517521	-1.336668	1.706257
H	-0.388348	-4.394052	1.282449
H	-1.016703	-3.198804	0.112353
H	-1.845879	-3.458378	1.677227
H	0.872357	-1.771468	3.759574
H	0.763998	-3.529686	3.478023
H	-0.699674	-2.604056	3.864176
H	-1.893319	3.181588	2.046196
H	-0.395587	4.000121	1.625142
H	0.300248	2.673787	3.500235
H	-0.825327	1.372073	3.096673
H	1.660843	3.937053	1.466023
H	3.057944	3.591219	0.460363
H	0.886419	4.623760	-0.711674
H	1.818908	3.362144	-1.522373
H	-0.371830	2.460944	-1.782056
H	-1.933864	2.020834	-0.013454
H	1.337598	0.451758	2.586428
H	2.940006	1.328294	1.056632
C	-1.181072	-0.393894	-0.975897
C	-2.422843	-0.427778	-0.827874
C	-3.822523	-0.428615	-0.650702
C	-4.663272	0.272739	-1.554918
C	-4.424389	-1.127344	0.428096
C	-6.046455	0.260242	-1.387610
H	-4.207758	0.812284	-2.386936
C	-5.806711	-1.108903	0.600080
H	-3.785538	-1.673756	1.123449
C	-6.624058	-0.422204	-0.308163
H	-6.680965	0.794795	-2.098036
H	-6.254299	-1.644329	1.440534
H	-7.708031	-0.420155	-0.175787



### TS<sub>8</sub>-Cu

E : -1468.39317516 A.U.

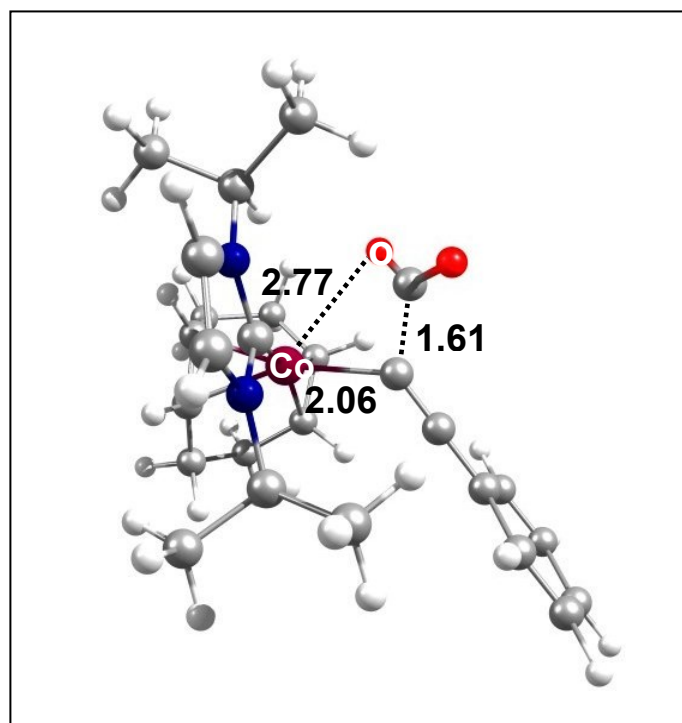
Cu	0.563041	0.528983	-0.372882
O	0.087794	-0.635160	-3.154452
O	0.074967	-2.548346	-1.873357
N	2.992699	-1.213222	-0.087856
N	1.884015	-1.147743	1.763310
C	1.898281	-0.630640	0.494986
C	3.639693	-2.069086	0.794577
C	2.939368	-2.030962	1.963288
C	3.407551	-0.992416	-1.495282
C	3.471064	-2.316790	-2.262002
C	4.720925	-0.202683	-1.551612
C	0.797054	-0.897839	2.733739
C	-0.094126	-2.138433	2.867197
C	1.355820	-0.416227	4.076716
C	1.408501	2.396176	-0.994014
C	0.114583	2.305956	-1.487620
C	-1.079452	3.165678	-1.093125
C	-1.854669	2.774828	0.190493
C	-1.059397	2.453043	1.430796
C	0.136641	2.933344	1.816580
C	0.984797	3.939208	1.081176
C	1.974689	3.312839	0.069537
C	-0.140652	-1.391786	-2.212250
H	4.525306	-2.632762	0.525418
H	3.102865	-2.555280	2.897593
H	2.594772	-0.388138	-1.925563
H	2.506321	-2.840196	-2.205294
H	4.269748	-2.971353	-1.877393
H	3.687837	-2.111471	-3.320289
H	5.556484	-0.783591	-1.130121
H	4.644391	0.742430	-0.994195
H	4.969943	0.031117	-2.597071
H	0.212459	-0.088304	2.270366
H	0.458385	-2.981713	3.310455
H	-0.471508	-2.445836	1.882107
H	-0.951179	-1.915783	3.520340
H	2.002118	0.463952	3.947539
H	1.940213	-1.202802	4.579488
H	0.528242	-0.142319	4.747280
H	-1.800979	3.124885	-1.923844
H	-0.760174	4.217427	-1.035110
H	-2.575459	3.582733	0.422040
H	-2.468079	1.891110	-0.039363
H	0.350622	4.677142	0.571282
H	1.578050	4.509233	1.815163
H	2.508887	4.137164	-0.442802
H	2.754466	2.760901	0.622661
H	2.186649	1.938287	-1.617533
H	0.002332	1.749123	-2.425773
H	-1.552551	1.745839	2.107986
H	0.548552	2.561492	2.761857
C	-1.042517	-0.559529	-0.943986
C	-2.255011	-0.693552	-0.680083
C	-3.633069	-0.856068	-0.391469
C	-4.617488	-0.184281	-1.160442
C	-4.064288	-1.696730	0.665606
C	-5.973145	-0.348862	-0.879294
H	-4.294200	0.454460	-1.984323
C	-5.421859	-1.848007	0.944723
H	-3.313852	-2.229135	1.252181
C	-6.381295	-1.176225	0.175347
H	-6.718651	0.170645	-1.485663
H	-5.737225	-2.500055	1.762594
H	-7.444036	-1.300627	0.394342



**TS<sub>8</sub>-Co**

E: -1416.87907678 A.U.

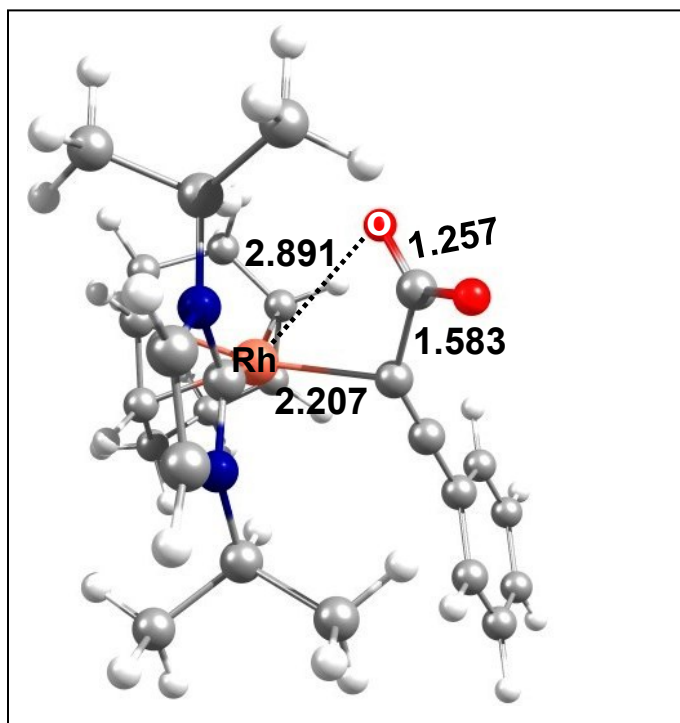
Co	0.505801	0.762009	0.146450
O	0.774600	0.669406	-2.616257
O	0.171254	-1.537536	-2.727245
N	2.662122	-1.297224	-0.293144
N	1.133777	-1.967930	1.088126
C	1.483302	-0.904096	0.293321
C	3.021885	-2.574306	0.123389
C	2.063662	-2.996605	0.991794
C	3.443886	-0.528940	-1.299993
C	3.511412	-1.291432	-2.628175
C	4.839154	-0.193939	-0.756581
C	-0.108885	-2.041875	1.885758
C	-0.997776	-3.181969	1.376203
C	0.198405	-2.165559	3.382962
C	-0.184115	2.656402	-0.568576
C	-0.896428	2.383734	0.587957
C	-0.628221	3.014268	1.938478
C	0.253920	2.083389	2.797313
C	1.244014	1.311771	1.950353
C	2.045689	1.853380	0.903135
C	2.048522	3.310696	0.459981
C	1.021849	3.560746	-0.672923
C	0.149151	-0.373204	-2.316670
H	3.911381	-3.075116	-0.239472
H	1.965314	-3.929953	1.533494
H	2.860971	0.388483	-1.459060
H	2.503304	-1.547015	-2.983385
H	4.110860	-2.211713	-2.533180
H	3.992635	-0.654033	-3.384259
H	5.449253	-1.102036	-0.626331
H	4.792937	0.326973	0.211186
H	5.363521	0.456550	-1.471848
H	-0.604288	-1.077155	1.688958
H	-0.537189	-4.164889	1.563279
H	-1.174424	-3.079673	0.296693
H	-1.964018	-3.162902	1.901808
H	0.839043	-1.342990	3.731147
H	0.702850	-3.116990	3.614057
H	-0.739417	-2.138737	3.957302
H	-1.584098	3.203560	2.452224
H	-0.145733	3.994259	1.811277
H	0.775489	2.655331	3.591249
H	-0.389257	1.356503	3.321514
H	1.851019	3.969597	1.321151
H	3.054089	3.579352	0.100137
H	0.713742	4.624177	-0.692570
H	1.496072	3.354944	-1.643804
H	-0.610982	2.342480	-1.523992
H	-1.853265	1.867700	0.480680
H	1.664568	0.437931	2.461912
H	2.976656	1.316954	0.701119
C	-0.877281	-0.149010	-1.085971
C	-2.110986	-0.265077	-0.910808
C	-3.511781	-0.319673	-0.735387
C	-4.322033	0.785681	-1.110280
C	-4.149137	-1.473007	-0.208212
C	-5.706266	0.733403	-0.959861
H	-3.841154	1.671997	-1.527745
C	-5.533146	-1.510720	-0.054003
H	-3.537440	-2.333768	0.063961
C	-6.317199	-0.410458	-0.428179
H	-6.315693	1.589140	-1.258734
H	-6.008691	-2.406708	0.351310
H	-7.402396	-0.446979	-0.311228



**TS<sub>8</sub>-Rh**

E : -1380.60267387 A.U.

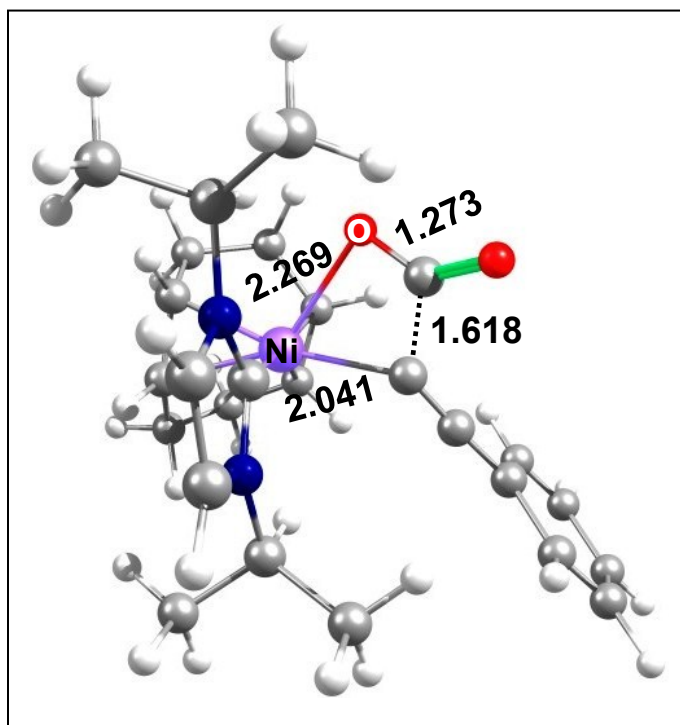
Rh	0.398847	0.714006	0.125967
O	0.795506	0.611535	-2.735536
O	0.344596	-1.627213	-2.894753
N	2.766753	-1.242577	-0.240596
N	1.250307	-2.098168	1.051104
C	1.542782	-0.975230	0.318438
C	3.214273	-2.505010	0.129994
C	2.264490	-3.043299	0.942226
C	3.504487	-0.355444	-1.179912
C	3.697942	-1.046881	-2.533682
C	4.833539	0.094408	-0.560349
C	-0.016724	-2.316152	1.782107
C	-0.797338	-3.477936	1.156470
C	0.239459	-2.518297	3.280235
C	-0.275132	2.700405	-0.611268
C	-1.139633	2.363068	0.425305
C	-1.066820	2.933314	1.832362
C	-0.258124	2.021424	2.783411
C	0.899066	1.325987	2.093905
C	1.812078	1.935317	1.175627
C	1.777029	3.403281	0.753134
C	0.913949	3.633122	-0.512081
C	0.210992	-0.470387	-2.474225
H	4.152778	-2.917146	-0.221009
H	2.223814	-4.008298	1.433600
H	2.834923	0.505564	-1.321968
H	2.734673	-1.381922	-2.943240
H	4.381910	-1.907699	-2.450846
H	4.141452	-0.332246	-3.242085
H	5.524702	-0.753735	-0.431550
H	4.689049	0.570413	0.420668
H	5.321342	0.820709	-1.226745
H	-0.573548	-1.377625	1.624871
H	-0.259754	-4.432310	1.271358
H	-0.966185	-3.300330	0.085339
H	-1.770013	-3.585475	1.659729
H	0.809088	-1.679678	3.705620
H	0.798793	-3.447324	3.473018
H	-0.718743	-2.590145	3.815527
H	-2.088312	3.053460	2.226050
H	-0.630936	3.943053	1.804745
H	0.101583	2.595192	3.660807
H	-0.925461	1.240883	3.184004
H	1.417286	4.024024	1.589449
H	2.804373	3.742874	0.548835
H	0.580842	4.687786	-0.566174
H	1.532661	3.459118	-1.405177
H	-0.573416	2.444599	-1.632600
H	-2.078794	1.874092	0.155582
H	1.297000	0.476466	2.662183
H	2.803635	1.474842	1.124629
C	-0.886348	-0.315716	-1.343326
C	-2.103117	-0.447973	-1.093334
C	-3.491795	-0.491108	-0.828810
C	-4.342503	0.526739	-1.335614
C	-4.074099	-1.541767	-0.074955
C	-5.714776	0.488758	-1.094767
H	-3.903889	1.332661	-1.926600
C	-5.445229	-1.561270	0.172565
H	-3.431096	-2.337140	0.303989
C	-6.271367	-0.549486	-0.336050
H	-6.356042	1.275596	-1.498110
H	-5.878180	-2.376205	0.757112
H	-7.346362	-0.572901	-0.145216



**TS<sub>8</sub>-Ni**

E : -1440.80251645 A.U.

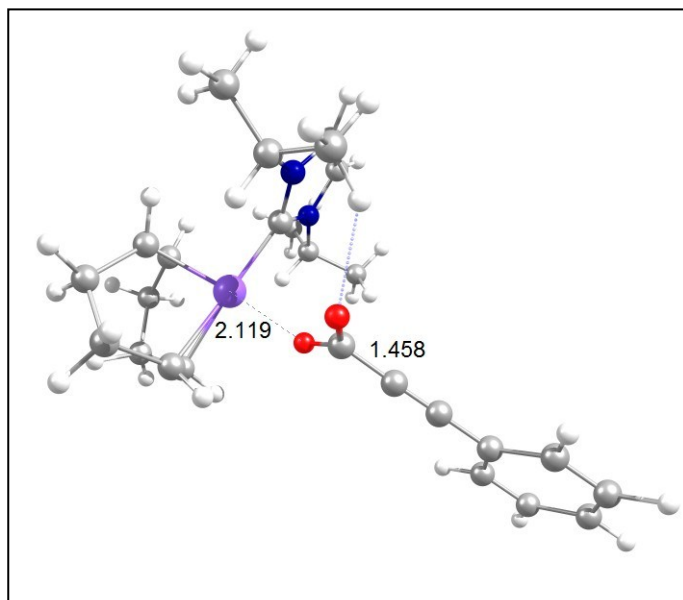
Ni	0.598070	0.763012	0.037770
O	0.926558	0.707750	-2.207090
O	-0.157956	-1.090722	-3.119497
N	2.505747	-1.518720	-0.319403
N	0.976146	-1.942727	1.168031
C	1.408897	-0.982019	0.296276
C	2.743584	-2.800760	0.161678
C	1.788202	-3.067129	1.092580
C	3.371174	-0.890118	-1.366985
C	3.345904	-1.721571	-2.653789
C	4.790959	-0.688133	-0.825473
C	-0.204907	-1.842332	2.063434
C	-1.208818	-2.954000	1.740637
C	0.222822	-1.855197	3.535500
C	-0.229454	2.718878	-0.542930
C	-0.760447	2.437554	0.698798
C	-0.290164	3.033014	2.008281
C	0.700042	2.095592	2.727163
C	1.624307	1.374320	1.777757
C	2.241183	1.912043	0.635745
C	2.139500	3.351514	0.163642
C	0.974437	3.577719	-0.832161
C	0.052032	-0.211792	-2.304230
H	3.559619	-3.413053	-0.202710
H	1.617993	-3.953032	1.692680
H	2.892192	0.073386	-1.579689
H	2.320718	-1.856168	-3.023818
H	3.814115	-2.708104	-2.513462
H	3.916844	-1.191978	-3.429574
H	5.297228	-1.647987	-0.641534
H	4.801184	-0.115457	0.114391
H	5.387469	-0.138796	-1.567550
H	-0.650052	-0.867628	1.812646
H	-0.816935	-3.943815	2.019140
H	-1.448836	-2.964826	0.669057
H	-2.135081	-2.793162	2.310313
H	0.953801	-1.064717	3.757215
H	0.669726	-2.820853	3.815684
H	-0.656361	-1.699837	4.177236
H	-1.163144	3.206787	2.654888
H	0.163375	4.017585	1.829564
H	1.304114	2.648970	3.471972
H	0.140303	1.342976	3.304012
H	2.043843	4.014346	1.036762
H	3.083143	3.626469	-0.328972
H	0.683050	4.643931	-0.845448
H	1.313385	3.333440	-1.847925
H	-0.810365	2.419282	-1.417802
H	-1.714144	1.904243	0.724291
H	2.090184	0.477004	2.195649
H	3.084351	1.343106	0.235810
C	-0.899533	-0.159788	-0.996841
C	-2.138737	-0.235722	-0.811042
C	-3.532944	-0.296298	-0.661177
C	-4.317886	0.880777	-0.821054
C	-4.186271	-1.529960	-0.389294
C	-5.701625	0.819805	-0.700081
H	-3.822206	1.824763	-1.053536
C	-5.571273	-1.575330	-0.274612
H	-3.590363	-2.437822	-0.292576
C	-6.329469	-0.404396	-0.425354
H	-6.299649	1.723714	-0.828145
H	-6.069757	-2.525522	-0.075287
H	-7.416856	-0.447704	-0.337355



### II<sub>8</sub>-Ir

E : -1375.51228579 A.U.

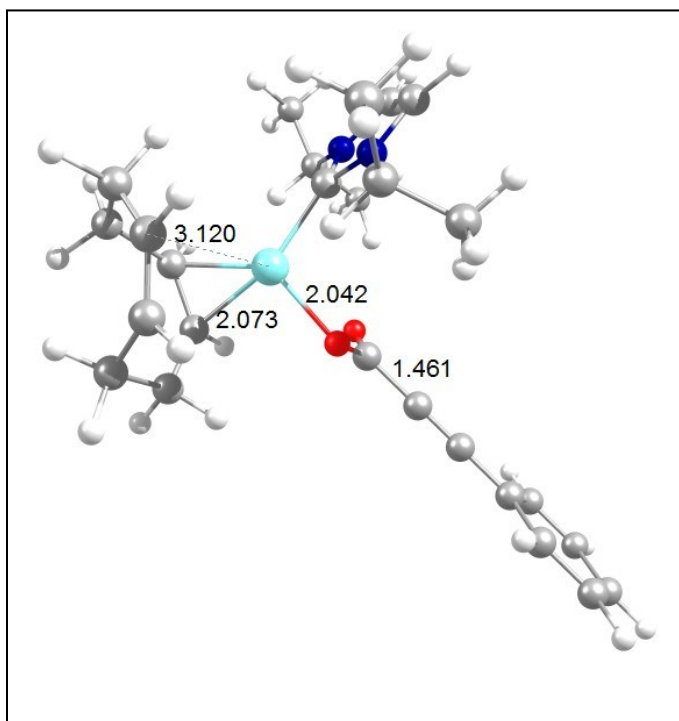
Ir	1.301068	-0.601832	-0.005396
O	-0.812698	-0.672247	0.125157
O	-1.117382	0.304712	-1.911373
N	0.931382	2.049727	1.487994
N	1.466560	2.455373	-0.575045
C	1.252216	1.426766	0.306622
C	0.940939	3.432576	1.339829
C	1.276510	3.686368	0.044305
C	0.553612	1.327316	2.725424
C	1.472876	1.717405	3.887698
C	-0.930827	1.534534	3.043645
C	1.780894	2.277747	-2.013894
C	3.150920	2.882676	-2.343745
C	0.657771	2.843736	-2.887987
C	-1.536862	-0.184459	-0.848436
C	3.227771	-0.793566	0.872448
C	3.368593	-0.705082	-0.552202
C	3.715505	-1.902167	-1.443167
C	2.452836	-2.608065	-1.997233
C	1.267742	-2.532529	-1.052936
C	1.308727	-2.792212	0.330499
C	2.556462	-3.255145	1.072988
C	3.345685	-2.071651	1.685925
H	0.712988	4.112013	2.152880
H	1.387896	4.628030	-0.480226
H	0.719371	0.267797	2.462295
H	1.337778	2.771709	4.177365
H	2.530551	1.562686	3.629975
H	1.238852	1.100661	4.767771
H	-1.555996	1.206006	2.202630
H	-1.152909	2.590795	3.264736
H	-1.206018	0.941155	3.928327
H	1.809117	1.183198	-2.137442
H	3.939034	2.479000	-1.691079
H	3.144431	3.979179	-2.236519
H	3.415650	2.653808	-3.386507
H	0.553683	3.932930	-2.755696
H	-0.292806	2.346805	-2.652740
H	0.890692	2.657105	-3.947011
H	4.335796	-1.559455	-2.286184
H	4.340919	-2.613831	-0.880826
H	2.152300	-2.123223	-2.939364
H	2.680755	-3.660893	-2.252962
H	2.261983	-3.949213	1.875587
H	3.200668	-3.835177	0.394280
H	2.951418	-1.859561	2.693533
H	4.409406	-2.347004	1.826397
H	3.492079	0.106200	1.443053
H	3.722971	0.257421	-0.937931
H	0.286976	-2.573254	-1.539599
H	0.350994	-2.991329	0.821967
C	-2.970376	-0.262488	-0.595905
C	-4.182425	-0.296689	-0.445563
C	-5.594441	-0.340593	-0.273234
C	-6.167566	-1.029787	0.820691
C	-6.452365	0.303074	-1.195223
C	-7.552649	-1.071651	0.982650
H	-5.509206	-1.529506	1.533478
C	-7.836128	0.257814	-1.023080
H	-6.014101	0.833482	-2.042410
C	-8.391900	-0.428726	0.063933
H	-7.981313	-1.609405	1.831409
H	-8.486556	0.759642	-1.743082
H	-9.475730	-0.463322	0.194168



## II<sub>8</sub>-Cu

E : -1467.43429141 A.U.

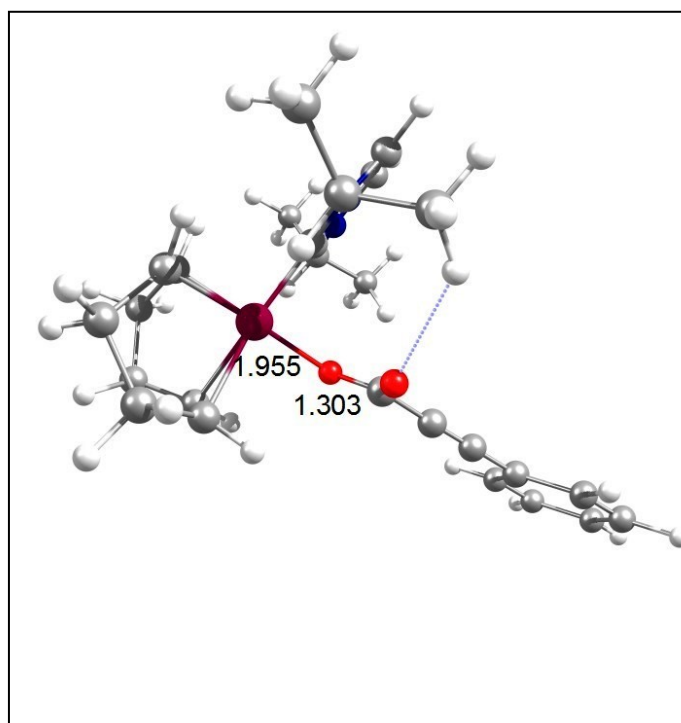
Cu	1.341997	0.470060	-0.474614
O	-0.839122	-0.550126	-1.791238
O	-0.609724	0.732653	0.063625
N	2.211506	-2.391217	-0.238981
N	1.592330	-1.609799	1.675861
C	1.815484	-1.232135	0.376962
C	2.222759	-3.460327	0.649155
C	1.834989	-2.966078	1.859398
C	2.474273	-2.496953	-1.692607
C	3.829774	-3.160959	-1.957517
C	1.309316	-3.193619	-2.404792
C	1.085314	-0.694483	2.723798
C	2.067254	-0.617174	3.898488
C	-0.329609	-1.092570	3.156191
C	-1.303983	0.068637	-0.804304
C	2.899006	2.440591	1.376250
C	1.916910	3.317388	1.102569
C	1.715118	4.117326	-0.159836
C	0.896184	3.380878	-1.244360
C	1.446359	2.077175	-1.779516
C	2.724584	1.528206	-1.676428
C	3.955626	2.132145	-1.006241
C	4.064822	1.993428	0.529069
H	2.498331	-4.467557	0.358830
H	1.717812	-3.463657	2.815194
H	2.512241	-1.448641	-2.024548
H	3.827859	-4.223051	-1.666455
H	4.638762	-2.652915	-1.412471
H	4.056737	-3.117674	-3.032675
H	0.372999	-2.643153	-2.234741
H	1.194300	-4.232081	-2.055010
H	1.501777	-3.222412	-3.487998
H	1.033276	0.281339	2.219174
H	3.077385	-0.346902	3.557816
H	2.131483	-1.575211	4.438514
H	1.728835	0.144168	4.616519
H	-0.345214	-2.088741	3.626389
H	-1.009517	-1.089732	2.294173
H	-0.708343	-0.367149	3.891192
H	1.167729	5.039269	0.095921
H	2.677845	4.445979	-0.574556
H	-0.120128	3.184484	-0.863001
H	0.766554	4.066368	-2.104377
H	4.843015	1.637357	-1.433356
H	4.048494	3.190216	-1.294285
H	4.246124	0.929938	0.761726
H	4.978489	2.523586	0.862786
H	2.875901	1.978307	2.369962
H	1.151568	3.458342	1.873921
H	0.802433	1.628814	-2.547461
H	2.954873	0.752096	-2.415128
C	-2.746497	0.066275	-0.575520
C	-3.957611	0.050342	-0.412698
C	-5.367981	0.037213	-0.220434
C	-6.213744	-0.650293	-1.121791
C	-5.952929	0.713514	0.875558
C	-7.595662	-0.658679	-0.928988
H	-5.767078	-1.172358	-1.969802
C	-7.335744	0.699073	1.060514
H	-5.304422	1.247182	1.572647
C	-8.162464	0.014423	0.160765
H	-8.236082	-1.193514	-1.634133
H	-7.772657	1.226458	1.911680
H	-9.244680	0.005928	0.307992



## II<sub>8</sub>-Co

E: -1415.88630477 A.U.

Co	1.568561	-0.719530	-0.082882
O	-0.382244	-0.790765	0.028356
O	-0.663368	0.254177	-1.973172
N	1.043122	1.580412	1.671906
N	1.627567	2.286276	-0.289404
C	1.443709	1.138930	0.436941
C	0.973992	2.969316	1.711198
C	1.342118	3.412867	0.477044
C	0.672805	0.678228	2.786401
C	1.558132	0.932646	4.011784
C	-0.822740	0.786290	3.100547
C	2.015052	2.329332	-1.720942
C	3.372619	3.023606	-1.890293
C	0.914640	2.979046	-2.565472
C	-1.096023	-0.264391	-0.925973
C	3.336955	-0.957259	0.857916
C	3.564625	-0.659661	-0.509808
C	3.994975	-1.678140	-1.558419
C	2.768356	-2.292612	-2.278534
C	1.558180	-2.362623	-1.373697
C	1.547380	-2.848586	-0.068763
C	2.753427	-3.421641	0.647097
C	3.449113	-2.328278	1.494725
H	0.672647	3.519254	2.595156
H	1.414606	4.420825	0.085904
H	0.878540	-0.327057	2.384125
H	1.386387	1.935199	4.434633
H	2.625078	0.843619	3.760893
H	1.325809	0.198049	4.796700
H	-1.418980	0.562159	2.206158
H	-1.086413	1.790865	3.468142
H	-1.089157	0.061813	3.884544
H	2.093969	1.268700	-2.002224
H	4.148858	2.556117	-1.266772
H	3.314593	4.090389	-1.621787
H	3.691413	2.963007	-2.941235
H	0.771098	4.038002	-2.296784
H	-0.028811	2.430842	-2.444240
H	1.200688	2.940935	-3.627246
H	4.647296	-1.190665	-2.300357
H	4.606770	-2.467520	-1.092727
H	2.502726	-1.664626	-3.143141
H	3.016149	-3.290784	-2.689608
H	2.437866	-4.251240	1.299442
H	3.458956	-3.852777	-0.079017
H	2.972099	-2.284029	2.488253
H	4.509710	-2.592798	1.680618
H	3.478196	-0.129208	1.563358
H	3.840899	0.375317	-0.734968
H	0.593083	-2.227609	-1.871350
H	0.569963	-3.029093	0.388184
C	-2.534274	-0.322023	-0.685112
C	-3.746831	-0.333436	-0.533182
C	-5.159293	-0.346829	-0.358419
C	-5.745632	-1.024928	0.735512
C	-6.004701	0.318688	-1.276484
C	-7.130765	-1.033901	0.902073
H	-5.097414	-1.542095	1.445144
C	-7.388667	0.305522	-1.100358
H	-5.556538	0.840761	-2.123667
C	-7.957358	-0.369464	-0.012769
H	-7.569442	-1.562903	1.751231
H	-8.029181	0.823975	-1.817457
H	-9.041287	-0.378421	0.120867

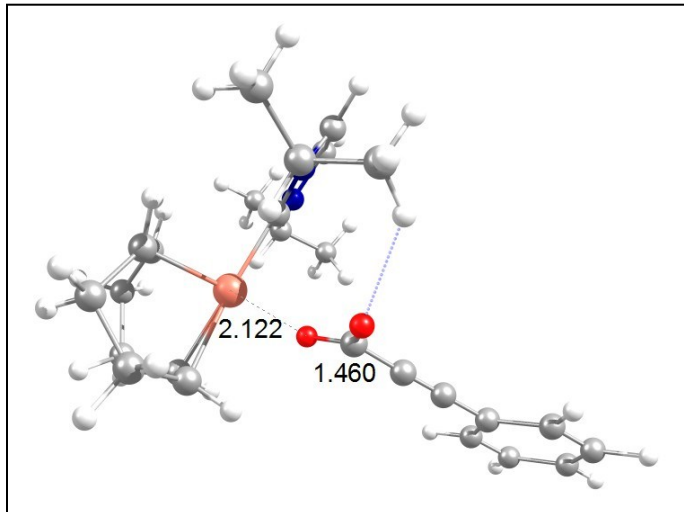




**II<sub>8</sub>-Rh**

E : -1380.62603526 A.U.

Rh	1.479900	-0.678086	-0.018193
O	-0.629448	-0.771842	0.197504
O	-0.897046	0.117003	-1.880030
N	1.058590	1.936760	1.505339
N	1.507419	2.381180	-0.567282
C	1.378810	1.339578	0.313029
C	0.984558	3.318947	1.367397
C	1.268245	3.597774	0.064234
C	0.753781	1.185017	2.744923
C	1.683261	1.613379	3.885555
C	-0.730265	1.309002	3.105970
C	1.797175	2.227318	-2.013885
C	3.147514	2.865630	-2.362217
C	0.646316	2.778489	-2.860769
C	-1.335843	-0.324064	-0.799880
C	3.418560	-0.825324	0.831035
C	3.542966	-0.726598	-0.583478
C	3.887283	-1.901535	-1.499808
C	2.626586	-2.618760	-2.045506
C	1.462902	-2.605211	-1.074305
C	1.537754	-2.877178	0.294077
C	2.806746	-3.304004	1.015654
C	3.550950	-2.100345	1.644303
H	0.740204	3.980412	2.190480
H	1.311542	4.546784	-0.457279
H	0.964968	0.138437	2.466017
H	1.500019	2.656445	4.188879
H	2.740384	1.518410	3.597930
H	1.507068	0.977871	4.765774
H	-1.357755	0.949745	2.279409
H	-1.003432	2.350079	3.341560
H	-0.946717	0.696172	3.993766
H	1.843831	1.135883	-2.153208
H	3.955848	2.472602	-1.728152
H	3.118717	3.960315	-2.241389
H	3.398255	2.654480	-3.412167
H	0.519350	3.863398	-2.714532
H	-0.287816	2.255961	-2.615583
H	0.865003	2.609213	-3.925659
H	4.485831	-1.534849	-2.348548
H	4.534344	-2.613597	-0.963140
H	2.293316	-2.110991	-2.963962
H	2.874338	-3.656285	-2.343594
H	2.548424	-4.024375	1.807730
H	3.469170	-3.842330	0.320938
H	3.132333	-1.902409	2.644860
H	4.618924	-2.348521	1.806375
H	3.638810	0.083844	1.404124
H	3.837616	0.253835	-0.972165
H	0.470191	-2.618160	-1.536230
H	0.593005	-3.058962	0.815759
C	-2.776366	-0.372935	-0.569994
C	-3.989970	-0.383944	-0.427701
C	-5.403547	-0.399747	-0.261900
C	-5.993570	-1.053051	0.845074
C	-6.246586	0.237667	-1.201798
C	-7.379786	-1.066086	1.002416
H	-5.347033	-1.547791	1.572032
C	-7.631622	0.221779	-1.034193
H	-5.795658	0.740331	-2.059211
C	-8.203960	-0.429231	0.066000
H	-7.821197	-1.576157	1.861704
H	-8.270105	0.718730	-1.768172
H	-9.288706	-0.440919	0.192746



### II<sub>8</sub>-Ni

E : -1440.83813142 A.U.

Ni	-1.471156	-0.682015	-0.099954
O	0.360681	-0.566990	-0.740270
O	0.487909	-0.662110	1.495657
N	-1.314175	2.072145	-1.055596
N	-1.404283	2.037724	1.118102
C	-1.423391	1.236586	0.015363
C	-1.226054	3.390940	-0.626993
C	-1.283100	3.369300	0.733539
C	-1.236780	1.641516	-2.478765
C	-2.386944	2.248312	-3.289351
C	0.141243	1.966226	-3.062664
C	-1.448965	1.592985	2.542558
C	-2.735383	2.084124	3.216343
C	-0.188093	2.044901	3.285347
C	1.053773	-0.577575	0.377049
C	-3.508013	-0.631393	-0.578781
C	-3.354776	-0.957132	0.773881
C	-3.509052	-2.338854	1.385581
C	-2.168211	-3.109730	1.465436
C	-1.251246	-2.836248	0.299560
C	-1.611192	-2.705799	-1.024411
C	-2.998222	-2.921276	-1.586669
C	-3.764452	-1.585533	-1.719164
H	-1.127467	4.223544	-1.313412
H	-1.240296	4.179697	1.451489
H	-1.351231	0.547676	-2.432923
H	-2.291606	3.341462	-3.371120
H	-3.366643	2.023241	-2.843104
H	-2.372055	1.841228	-4.310313
H	0.935387	1.499224	-2.466023
H	0.312646	3.052520	-3.106466
H	0.204448	1.578074	-4.089355
H	-1.433737	0.496674	2.483682
H	-3.637350	1.773749	2.667561
H	-2.752947	3.181119	3.301281
H	-2.795742	1.673620	4.234245
H	-0.133016	3.141147	3.366313
H	0.714712	1.668680	2.788210
H	-0.207587	1.637803	4.306210
H	-3.914241	-2.229363	2.401992
H	-4.257521	-2.910508	0.818372
H	-1.633034	-2.819901	2.381330
H	-2.353954	-4.195937	1.552465
H	-2.910406	-3.384602	-2.580453
H	-3.556200	-3.630670	-0.961257
H	-3.475371	-1.087257	-2.657832
H	-4.853474	-1.764428	-1.803832
H	-3.724554	0.417933	-0.802569
H	-3.429137	-0.119694	1.473518
H	-0.183923	-2.875033	0.527740
H	-0.795811	-2.597361	-1.746439
C	2.475437	-0.502058	0.230643
C	3.693970	-0.454192	0.136454
C	5.107618	-0.399749	0.027678
C	5.721106	-0.244289	-1.237832
C	5.917817	-0.504032	1.182952
C	7.110248	-0.194397	-1.338622
H	5.095706	-0.166375	-2.128647
C	7.305990	-0.453547	1.068033
H	5.443952	-0.625816	2.158276
C	7.904371	-0.298867	-0.189175
H	7.578436	-0.074913	-2.317547
H	7.926456	-0.536049	1.962373
H	8.992221	-0.260648	-0.273616

