

SUPPLEMENTARY MATERIAL

Guest–Host Interaction of Coinage Metals in π -Rich Cavities

Zhi Xiang Wong^A and Matthias Lein^{A,B}

^ASchool of Chemical and Physical Sciences, Victoria University of Wellington,
Wellington, New Zealand.

^BCorresponding author. Email: matthias.lein@vuw.ac.nz

File: Ag-1-c.xyz

49

scf done: -1075.113386

C	-2.892266	0.041844	0.176185
C	-2.622726	0.543467	-1.099222
C	-1.927200	1.736789	-1.269709
C	-1.482371	2.483854	-0.176185
C	-1.782020	1.999614	1.099222
C	-2.467704	0.800609	1.269709
H	-2.948424	-0.006516	-1.975252
H	-1.722659	2.093333	-2.273473
H	-1.468570	2.556668	1.975252
H	-2.674209	0.445200	2.273473
C	-0.671313	3.731501	-0.375309
H	-0.498219	3.869773	-1.444847
H	-1.243830	4.604038	-0.046541
C	0.671313	3.731501	0.375309
H	1.243830	4.604038	0.046541
H	0.498219	3.869773	1.444847
C	1.482371	2.483854	0.176185
C	1.782020	1.999614	-1.099222
C	1.927200	1.736789	1.269709
C	2.467704	0.800609	-1.269709
H	1.468570	2.556668	-1.975252
C	2.622726	0.543467	1.099222
H	1.722659	2.093333	2.273473
C	2.892266	0.041844	-0.176185
H	2.674209	0.445200	-2.273473
H	2.948424	-0.006516	1.975252
C	3.567231	-1.284377	-0.375309
H	4.609129	-1.224830	-0.046541
H	3.600431	-1.503416	-1.444847
C	2.895918	-2.447124	0.375309
H	3.365299	-3.379208	0.046541
H	3.102212	-2.366356	1.444847
C	-3.567231	-1.284377	0.375309
H	-3.600431	-1.503416	1.444847
H	-4.609129	-1.224830	0.046541
C	-2.895918	-2.447124	-0.375309
H	-3.365299	-3.379208	-0.046541
H	-3.102212	-2.366356	-1.444847
C	-1.409895	-2.525698	-0.176185
C	-0.840706	-2.543081	1.099222
C	-0.540504	-2.537399	-1.269709
C	0.540504	-2.537399	1.269709
H	-1.479855	-2.550153	1.975252
C	0.840706	-2.543081	-1.099222
H	-0.951550	-2.538533	-2.273473
C	1.409895	-2.525698	0.176185
H	0.951550	-2.538533	2.273473
H	1.479855	-2.550153	-1.975252
Ag	0.000000	0.000000	0.000000

File: Ag-1-p.xyz

49

scf done: -1075.126581

C	0.341252	2.867157	-0.086826
C	0.855507	2.601102	-1.348392
C	1.960575	1.776348	-1.517403
C	2.608379	1.191482	-0.437169
C	2.117941	1.475862	0.842312
C	0.995430	2.296501	1.013545
H	0.384036	3.037013	-2.222379
H	2.327099	1.581412	-2.519470
H	2.640959	1.106905	1.718716
H	0.676030	2.560833	2.017555
C	3.774590	0.269110	-0.637823
H	3.893640	0.086254	-1.707913
H	4.698235	0.755699	-0.308623
C	3.644906	-1.069216	0.107184
H	4.445076	-1.730793	-0.236865
H	3.815421	-0.919616	1.175968
C	2.312405	-1.729111	-0.086826
C	1.824867	-2.041442	-1.348392
C	1.491113	-2.010318	1.013545
C	0.558075	-2.586082	-1.517403
H	2.438113	-1.851092	-2.222379
C	0.219163	-2.572122	0.842312
H	1.879732	-1.865876	2.017555
C	-0.272335	-2.854663	-0.437169
H	0.205993	-2.806033	-2.519470
H	-0.361871	-2.840591	1.718716
C	-1.654239	-3.403446	-0.637823
H	-1.694663	-4.446640	-0.308623
H	-1.872122	-3.415118	-1.707913
C	-2.748421	-2.621973	0.107184
H	-3.721449	-2.984153	-0.236865
H	-2.704121	-2.844444	1.175968
C	-0.896485	3.691189	0.107184
H	-1.111300	3.764060	1.175968
H	-0.723628	4.714946	-0.236865
C	-2.120351	3.134336	-0.637823
H	-3.003572	3.690942	-0.308623
H	-2.021518	3.328864	-1.707913
C	-2.336043	1.663181	-0.437169
C	-2.337105	1.096260	0.842312
C	-2.518650	0.809734	-1.517403
C	-2.486543	-0.286183	1.013545
H	-2.279088	1.733685	1.718716
C	-2.680374	-0.559660	-1.348392
H	-2.533092	1.224621	-2.519470
C	-2.653657	-1.138046	-0.086826
H	-2.555762	-0.694958	2.017555
H	-2.822149	-1.185921	-2.222379
Ag	0.000000	0.000000	0.924497

File: Ag-2-c.xyz

61

scf done: -1307.216889

C	1.271542	2.415294	0.623198
C	1.182169	2.378949	-0.779671
C	-0.087680	2.414581	-1.366082
C	-1.271542	2.415294	-0.623198
C	-1.182169	2.378949	0.779671
C	0.087680	2.414581	1.366082
C	2.651315	-0.165686	0.779671
C	2.727477	-0.106459	-0.623198
C	2.134928	-1.131358	-1.366082
C	1.469146	-2.213263	-0.779671
C	1.455935	-2.308835	0.623198
C	2.047248	-1.283223	1.366082
C	-1.469146	-2.213263	0.779671
C	-1.455935	-2.308835	-0.623198
C	-2.047248	-1.283223	-1.366082
C	-2.651315	-0.165686	-0.779671
C	-2.727477	-0.106459	0.623198
C	-2.134928	-1.131358	1.366082
C	0.755898	-3.445055	1.309717
C	-0.740728	-3.194530	1.654940
C	0.740728	-3.194530	-1.654940
C	-0.755898	-3.445055	-1.309717
C	-3.136908	0.955776	-1.654940
C	-2.605556	2.377154	-1.309717
C	-3.361454	1.067901	1.309717
C	-2.396180	2.238754	1.654940
C	3.361454	1.067901	-1.309717
C	2.396180	2.238754	-1.654940
C	3.136908	0.955776	1.654940
C	2.605556	2.377154	1.309717
H	-0.156548	2.414233	-2.450046
H	0.156548	2.414233	2.450046
H	2.169062	-1.071542	-2.450046
H	2.012513	-1.342692	2.450046
H	-2.012513	-1.342692	-2.450046
H	-2.169062	-1.071542	2.450046
H	0.845071	-4.338149	0.690492
H	1.276095	-3.673256	2.242088
H	-0.806952	-2.832178	2.682447
H	-1.255719	-4.160352	1.643452
H	1.255719	-4.160352	-1.643452
H	0.806952	-2.832178	-2.682447
H	-0.845071	-4.338149	-0.690492
H	-1.276095	-3.673256	-2.242088
H	-4.230830	0.992691	-1.643452
H	-2.856214	0.717248	-2.682447
H	-2.543085	2.941759	-2.242088
H	-3.334412	2.900928	-0.690492
H	-4.179483	1.437221	0.690492
H	-3.819181	0.731497	2.242088
H	-2.975111	3.167661	1.643452
H	-2.049262	2.114930	2.682447
H	4.179483	1.437221	-0.690492
H	3.819181	0.731497	-2.242088
H	2.975111	3.167661	-1.643452
H	2.049262	2.114930	-2.682447
H	4.230830	0.992691	1.643452
H	2.856214	0.717248	2.682447
H	3.334412	2.900928	0.690492
H	2.543085	2.941759	2.242088
Ag	0.000000	0.000000	0.000000

File: Ag-2-p.xyz

61

scf done: -1307.227782

C	-2.600446	0.744474	-0.849962
C	-2.527722	0.783872	0.548299
C	-1.664692	1.722044	1.143623
C	-0.835463	2.573483	0.393091
C	-0.869298	2.471511	-1.002228
C	-1.774028	1.586415	-1.582335
C	-1.705742	-1.988590	-1.002228
C	-1.810971	-2.010273	0.393091
C	-0.658987	-2.302688	1.143623
C	0.585008	-2.581007	0.548299
C	0.655489	-2.624289	-0.849962
C	-0.486862	-2.329561	-1.582335
C	2.575040	-0.482921	-1.002228
C	2.646433	-0.563210	0.393091
C	2.323680	0.580644	1.143623
C	1.942714	1.797135	0.548299
C	1.944956	1.879815	-0.849962
C	2.260890	0.743146	-1.582335
C	1.951143	-2.929457	-1.543163
C	2.798505	-1.678424	-1.886504
C	1.800812	-2.779262	1.410323
C	3.006376	-1.849110	1.080433
C	1.506505	2.949180	1.410323
C	0.098188	3.528153	1.080433
C	1.561413	3.154468	-1.543163
C	0.054305	3.262789	-1.886504
C	-3.104564	-1.679043	1.080433
C	-3.307318	-0.169918	1.410323
C	-2.852810	-1.584365	-1.886504
C	-3.512556	-0.225011	-1.543163
H	-1.691530	1.840435	2.224917
H	-1.818032	1.533972	-2.666420
H	-0.748098	-2.385125	2.224917
H	-0.419443	-2.341447	-2.666420
H	2.439628	0.544690	2.224917
H	2.237474	0.807476	-2.666420
H	2.532990	-3.616519	-0.927625
H	1.743529	-3.463945	-2.472210
H	2.577684	-1.374879	-2.911298
H	3.856319	-1.961326	-1.879194
H	2.140161	-3.817479	1.347284
H	1.507499	-2.621220	2.450403
H	3.723518	-2.387291	0.460129
H	3.523772	-1.625597	2.015514
H	2.235954	3.762174	1.347284
H	1.516293	2.616142	2.450403
H	-0.354078	3.864474	2.015514
H	0.205695	4.418306	0.460129
H	1.865502	4.001893	-0.927625
H	2.128100	3.241913	-2.472210
H	-0.229601	4.320333	-1.879194
H	-0.098162	2.919780	-2.911298
H	-3.929213	-2.031016	0.460129
H	-3.169694	-2.238878	2.015514
H	-4.376115	0.055306	1.347284
H	-3.023792	0.005078	2.450403
H	-3.626718	-2.359007	-1.879194
H	-2.479522	-1.544900	-2.911298
H	-4.398492	-0.385374	-0.927625
H	-3.871629	0.222033	-2.472210
Ag	0.000000	0.000000	1.026960

File: Au-1-c.xyz

49

scf done: -1063.807703

C	-2.899357	0.044365	0.174713
C	-2.630443	0.548339	-1.100611
C	-1.933692	1.742430	-1.269276
C	-1.488100	2.488734	-0.174713
C	-1.790097	2.003861	1.100611
C	-2.475835	0.803411	1.269276
H	-2.954662	-0.000195	-1.977870
H	-1.727185	2.099494	-2.272265
H	-1.477162	2.558910	1.977870
H	-2.681807	0.446039	2.272265
C	-0.671142	3.731295	-0.375591
H	-0.497085	3.865554	-1.445598
H	-1.240152	4.607458	-0.049731
C	0.671142	3.731295	0.375591
H	1.240152	4.607458	0.049731
H	0.497085	3.865554	1.445598
C	1.488100	2.488734	0.174713
C	1.790097	2.003861	-1.100611
C	1.933692	1.742430	1.269276
C	2.475835	0.803411	-1.269276
H	1.477162	2.558910	-1.977870
C	2.630443	0.548339	1.100611
H	1.727185	2.099494	2.272265
C	2.899357	0.044365	-0.174713
H	2.681807	0.446039	-2.272265
H	2.954662	-0.000195	1.977870
C	3.566968	-1.284421	-0.375591
H	4.610251	-1.229726	-0.049731
H	3.596211	-1.502289	-1.445598
C	2.895825	-2.446874	0.375591
H	3.370099	-3.377732	0.049731
H	3.099126	-2.363266	1.445598
C	-3.566968	-1.284421	0.375591
H	-3.596211	-1.502289	1.445598
H	-4.610251	-1.229726	0.049731
C	-2.895825	-2.446874	-0.375591
H	-3.370099	-3.377732	-0.049731
H	-3.099126	-2.363266	-1.445598
C	-1.411257	-2.533099	-0.174713
C	-0.840346	-2.552200	1.100611
C	-0.542143	-2.545842	-1.269276
C	0.542143	-2.545842	1.269276
H	-1.477500	-2.558715	1.977870
C	0.840346	-2.552200	-1.100611
H	-0.954622	-2.545533	-2.272265
C	1.411257	-2.533099	0.174713
H	0.954622	-2.545533	2.272265
H	1.477500	-2.558715	-1.977870
Au	0.000000	0.000000	0.000000

File: Au-1-p.xyz

49

scf done: -1063.852005

C	-2.741954	-0.949077	-0.222575
C	-2.806703	-0.350043	-1.465387
C	-2.529981	1.007063	-1.632919
C	-2.193096	1.822061	-0.568095
C	-2.139464	1.234704	0.708832
C	-2.403277	-0.137713	0.877967
H	-3.073730	-0.943696	-2.333019
H	-2.586309	1.437078	-2.627150
H	-2.019463	1.859320	1.587340
H	-2.499801	-0.540610	1.881667
C	-1.886313	3.276444	-0.764821
H	-1.786521	3.467003	-1.835633
H	-2.730871	3.885257	-0.425096
C	-0.623406	3.761430	-0.032347
H	-0.385683	4.765470	-0.393868
H	-0.827625	3.863941	1.036082
C	0.549261	2.849636	-0.222754
C	1.100505	2.606114	-1.465531
C	1.082519	2.150686	0.877815
C	2.137349	1.687742	-1.632990
H	0.720079	3.134280	-2.333180
C	2.138962	1.235738	0.708790
H	0.781656	2.435650	1.881467
C	2.674450	0.988305	-0.568136
H	2.538099	1.521555	-2.627156
H	2.619809	0.819494	1.587347
C	3.780409	-0.004810	-0.764900
H	4.730095	0.422031	-0.425417
H	3.895187	-0.186588	-1.835737
C	3.568841	-1.340893	-0.032396
H	4.319358	-2.048897	-0.393997
H	3.759808	-1.215553	1.036014
C	-2.945529	-2.420422	-0.032106
H	-2.932080	-2.648571	1.036301
H	-3.934092	-2.716224	-0.393408
C	-1.894534	-3.271737	-0.765006
H	-1.999843	-4.307652	-0.425700
H	-2.109558	-3.279986	-1.835803
C	-0.481401	-2.810668	-0.568301
C	0.000618	-2.470811	0.708606
C	0.392870	-2.694973	-1.633163
C	1.321066	-2.013057	0.877715
H	-0.600379	-2.679063	1.587098
C	1.706515	-2.256037	-1.465645
H	0.048621	-2.958771	-2.627384
C	2.192879	-1.900330	-0.222841
H	1.718354	-1.894969	1.881352
H	2.354201	-2.190465	-2.333234
Au	-0.000036	0.000049	0.824459

File: Au-2-c.xyz

61

scf done: -1295.912400

C	1.273173	2.424273	0.623647
C	1.183538	2.386644	-0.780132
C	-0.087805	2.422369	-1.366871
C	-1.273173	2.424273	-0.623647
C	-1.183538	2.386644	0.780132
C	0.087805	2.422369	1.366871
C	2.658664	-0.168348	0.780132
C	2.736069	-0.109536	-0.623647
C	2.141736	-1.135143	-1.366871
C	1.475126	-2.218296	-0.780132
C	1.462895	-2.314737	0.623647
C	2.053930	-1.287226	1.366871
C	-1.475126	-2.218296	0.780132
C	-1.462895	-2.314737	-0.623647
C	-2.053930	-1.287226	-1.366871
C	-2.658664	-0.168348	-0.780132
C	-2.736069	-0.109536	0.623647
C	-2.141736	-1.135143	1.366871
C	0.757170	-3.446424	1.309334
C	-0.740664	-3.193571	1.655537
C	0.740664	-3.193571	-1.655537
C	-0.757170	-3.446424	-1.309334
C	-3.136046	0.955352	-1.655537
C	-2.606106	2.378940	-1.309334
C	-3.363275	1.067484	1.309334
C	-2.395382	2.238219	1.655537
C	3.363275	1.067484	-1.309334
C	2.395382	2.238219	-1.655537
C	3.136046	0.955352	1.655537
C	2.606106	2.378940	1.309334
H	-0.156595	2.417676	-2.450614
H	0.156595	2.417676	2.450614
H	2.172066	-1.073222	-2.450614
H	2.015471	-1.344453	2.450614
H	-2.015471	-1.344453	-2.450614
H	-2.172066	-1.073222	2.450614
H	0.843350	-4.340246	0.690828
H	1.274640	-3.676030	2.242910
H	-0.804520	-2.827332	2.681744
H	-1.252398	-4.161141	1.649058
H	1.252398	-4.161141	-1.649058
H	0.804520	-2.827332	-2.681744
H	-0.843350	-4.340246	-0.690828
H	-1.274640	-3.676030	-2.242910
H	-4.229853	0.995962	-1.649058
H	-2.850801	0.716932	-2.681744
H	-2.546215	2.941885	-2.242910
H	-3.337088	2.900485	-0.690828
H	-4.180438	1.439760	0.690828
H	-3.820855	0.734144	2.242910
H	-2.977455	3.165179	1.649058
H	-2.046282	2.110401	2.681744
H	4.180438	1.439760	-0.690828
H	3.820855	0.734144	-2.242910
H	2.977455	3.165179	-1.649058
H	2.046282	2.110401	-2.681744
H	4.229853	0.995962	1.649058
H	2.850801	0.716932	2.681744
H	3.337088	2.900485	0.690828
H	2.546215	2.941885	2.242910
Au	0.000000	0.000000	0.000000

File: Cu-1-c.xyz

49

scf done: -2568.408562

C	0.218152	2.828310	0.178194
C	0.677966	2.501280	-1.097929
C	1.816425	1.723529	-1.271332
C	2.544570	1.254060	-0.178168
C	2.069920	1.559112	1.097980
C	0.924578	2.326737	1.271380
H	0.147553	2.863624	-1.971419
H	2.155747	1.490997	-2.274833
H	2.603375	1.201306	1.971502
H	0.582466	2.555119	2.274892
C	3.763652	0.404529	-0.370912
H	3.911600	0.232865	-1.439191
H	4.652412	0.938114	-0.021812
C	3.667940	-0.935567	0.371084
H	4.471798	-1.590073	0.021931
H	3.838856	-0.786838	1.439350
C	2.340444	-1.603180	0.178368
C	1.827291	-1.837550	-1.097805
C	1.552822	-1.964318	1.271479
C	0.584444	-2.434471	-1.271309
H	2.406191	-1.559049	-1.971254
C	0.315370	-2.572316	1.097960
H	1.921649	-1.782402	2.275034
C	-0.186166	-2.830586	-0.178215
H	0.213441	-2.611921	-2.274857
H	-0.261287	-2.855534	1.971392
C	-1.531441	-3.461578	-0.371014
H	-1.513730	-4.498110	-0.022061
H	-1.754017	-3.503731	-1.439294
C	-2.644108	-2.708676	0.371110
H	-3.612906	-3.077693	0.022218
H	-2.600418	-2.930999	1.439383
C	-1.023683	3.644285	0.370677
H	-1.238038	3.718263	1.438914
H	-0.858659	4.667587	0.021251
C	-2.232200	3.057094	-0.371190
H	-3.138630	3.560004	-0.021983
H	-2.157732	3.271024	-1.439481
C	-2.358416	1.576558	-0.178407
C	-2.385307	1.013120	1.097802
C	-2.400950	0.711101	-1.271491
C	-2.477485	-0.362547	1.271346
H	-2.342038	1.654113	1.971229
C	-2.505278	-0.663702	-1.097924
H	-2.369176	1.121107	-2.275052
C	-2.558633	-1.225245	0.178273
H	-2.504455	-0.772879	2.274896
H	-2.553625	-1.304342	-1.971354
Cu	0.000006	-0.000015	0.000029

File: Cu-1-p.xyz

49

scf done: -2568.426763

C	2.858175	0.387547	0.031880
C	2.853758	-0.226706	-1.210396
C	2.311974	-1.495176	-1.386260
C	1.768304	-2.207654	-0.328088
C	1.777680	-1.601490	0.935872
C	2.308138	-0.319263	1.110801
H	3.278148	0.290069	-2.064499
H	2.320779	-1.942998	-2.374174
H	1.451940	-2.160371	1.806281
H	2.389440	0.091611	2.112981
C	1.187307	-3.575443	-0.530139
H	1.038426	-3.734702	-1.600539
H	1.905494	-4.336201	-0.206703
C	-0.135432	-3.804738	0.216455
H	-0.577995	-4.736859	-0.143954
H	0.053037	-3.949822	1.282711
C	-1.093646	-2.668969	0.031710
C	-1.623371	-2.358257	-1.210639
C	-1.430700	-1.838943	1.110445
C	-2.450898	-1.254811	-1.386773
H	-1.388160	-2.984474	-2.064557
C	-2.275923	-0.738497	0.935224
H	-1.115678	-2.114637	2.112721
C	-2.796075	-0.427495	-0.328784
H	-2.843129	-1.038757	-2.374734
H	-2.597093	-0.176760	1.805489
C	-3.690154	0.759467	-0.531141
H	-4.708086	0.517924	-0.207682
H	-3.753605	0.967803	-1.601589
C	-3.227511	2.019896	0.215214
H	-3.813264	2.869133	-0.145730
H	-3.447830	1.929575	1.281420
C	3.362696	1.785282	0.216449
H	3.394104	2.021149	1.282695
H	4.391226	1.867975	-0.143960
C	2.502829	2.816140	-0.530282
H	2.802511	3.818469	-0.206735
H	2.715365	2.766885	-1.600648
C	1.027767	2.635371	-0.328473
C	0.497964	2.339766	0.935252
C	0.139065	2.750617	-1.386696
C	-0.877729	2.158085	1.109936
H	1.144745	2.336688	1.805726
C	-1.230387	2.585678	-1.211078
H	0.522625	2.982745	-2.374417
C	-1.764723	2.281684	0.030958
H	-1.274326	2.022644	2.112014
H	-1.890054	2.695494	-2.065151
Cu	0.000232	-0.000522	0.844978

File: Cu-2-c.xyz

61

scf done: -2800.524721

C	2.459525	1.069717	0.620433
C	2.364363	1.095388	-0.779943
C	1.376186	1.887632	-1.365115
C	0.469765	2.640621	-0.620433
C	0.516818	2.554013	0.779943
C	1.516749	1.776658	1.365115
C	1.953432	-1.724584	0.779943
C	2.051962	-1.727138	-0.620433
C	0.946645	-2.135628	-1.365115
C	-0.233547	-2.595292	-0.779943
C	-0.303360	-2.664869	0.620433
C	0.780256	-2.201872	1.365115
C	-2.470250	-0.829429	0.779943
C	-2.521727	-0.913482	-0.620433
C	-2.322830	0.247996	-1.365115
C	-2.130815	1.499904	-0.779943
C	-2.156164	1.595152	0.620433
C	-2.297006	0.425215	1.365115
C	-1.536609	-3.163571	1.309596
C	-2.555611	-2.045827	1.653677
C	-1.396931	-2.960598	-1.653677
C	-2.720631	-2.228793	-1.309596
C	-1.865487	2.690077	-1.653677
C	-0.569876	3.470532	-1.309596
C	-1.971429	2.912528	1.309596
C	-0.493933	3.236138	1.653677
C	3.290507	-1.241739	-1.309596
C	3.262419	0.270521	-1.653677
C	3.049544	-1.190311	1.653677
C	3.508037	0.251043	1.309596
H	1.319312	1.928563	-2.448776
H	1.569761	1.730835	2.448776
H	1.010528	-2.106839	-2.448776
H	0.714067	-2.224870	2.448776
H	-2.329840	0.178276	-2.448776
H	-2.283827	0.494035	2.448776
H	-2.011053	-3.923018	0.687613
H	-1.253130	-3.665339	2.236596
H	-2.400369	-1.728032	2.686154
H	-3.564685	-2.467517	1.615248
H	-1.572947	-4.039982	-1.615248
H	-1.123837	-2.735847	-2.686154
H	-3.349248	-2.866521	-0.687613
H	-3.274484	-2.069492	-2.236596
H	-2.712254	3.382203	-1.615248
H	-1.807394	2.341195	-2.686154
H	-0.154990	3.870532	-2.236596
H	-0.807856	4.333794	-0.687613
H	-2.391907	3.703132	0.687613
H	-2.547711	2.917912	2.236596
H	-0.354590	4.320866	1.615248
H	-0.296335	2.942797	2.686154
H	4.157104	-1.467273	-0.687613
H	3.429474	-1.801041	-2.236596
H	4.285201	0.657779	-1.615248
H	2.931231	0.394652	-2.686154
H	3.919275	-1.853349	1.615248
H	2.696704	-1.214764	2.686154
H	4.402960	0.219886	0.687613
H	3.800841	0.747427	2.236596
Cu	0.000000	0.000000	0.000000

File: Cu-2-p.xyz

61

scf done: -2800.533209

C	2.236959	-1.610407	0.366329
C	1.942142	-1.514494	-1.001779
C	2.017875	-0.256025	-1.615746
C	2.394256	0.899300	-0.916695
C	2.609885	0.807187	0.461142
C	2.547641	-0.448593	1.059529
C	-0.382231	-2.559063	0.984205
C	-0.556925	-2.626594	-0.400917
C	-1.550048	-1.832803	-0.991468
C	-2.433382	-1.048798	-0.235561
C	-2.300081	-1.047982	1.160791
C	-1.272725	-1.789328	1.728109
C	-1.759590	1.752298	1.224962
C	-2.090252	1.728666	-0.132900
C	-1.110571	2.090028	-1.068142
C	0.153521	2.563071	-0.687680
C	0.448896	2.657231	0.680401
C	-0.507649	2.237120	1.594394
C	-3.208266	-0.218726	2.020642
C	-2.692051	1.222238	2.276897
C	-3.483516	-0.238459	-0.935779
C	-3.438419	1.273393	-0.599322
C	1.144623	2.949875	-1.745035
C	2.500640	2.207945	-1.636777
C	1.788598	3.146086	1.147446
C	2.849124	2.024408	1.308454
C	0.326825	-3.479351	-1.257731
C	1.549823	-2.710681	-1.817738
C	0.762845	-3.246013	1.672506
C	2.161760	-2.928065	1.080438
H	1.889031	-0.195321	-2.694012
H	2.741329	-0.520944	2.125899
H	-1.714564	-1.914176	-2.063511
H	-1.150301	-1.758890	2.806997
H	-1.377510	2.111181	-2.122300
H	-0.262994	2.278372	2.651904
H	-4.199260	-0.183578	1.566272
H	-3.338616	-0.711130	2.985987
H	-2.162650	1.243474	3.230996
H	-3.553509	1.887114	2.395778
H	-4.477122	-0.628876	-0.696776
H	-3.356281	-0.371651	-2.011901
H	-4.179164	1.510714	0.163994
H	-3.725418	1.837067	-1.488997
H	1.323221	4.028698	-1.711848
H	0.699787	2.746134	-2.721030
H	2.887115	2.039457	-2.643691
H	3.233259	2.835833	-1.130070
H	2.153801	3.906701	0.456106
H	1.673056	3.646869	2.110339
H	3.838416	2.445843	1.103665
H	2.869337	1.704281	2.351581
H	0.657328	-4.343267	-0.681483
H	-0.250126	-3.874369	-2.096042
H	2.396569	-3.398142	-1.902871
H	1.329316	-2.374216	-2.832696
H	0.618234	-4.331069	1.666433
H	0.747068	-2.947082	2.721990
H	2.467016	-3.723454	0.399266
H	2.887271	-2.937174	1.895861
Cu	-0.157306	-0.001006	-0.902541

File: delta.xyz

60

scf done: -1160.394569

C	1.171026	2.335438	0.777600
C	-0.090345	2.360157	1.358485
C	-1.262623	2.373099	0.616022
C	-1.171026	2.335438	-0.777600
C	0.090345	2.360157	-1.358485
C	1.262623	2.373099	-0.616022
H	-0.163040	2.349015	2.443121
H	0.163040	2.349015	-2.443121
C	2.595239	2.367048	-1.306963
C	3.121745	0.952487	-1.656495
H	3.323610	2.890009	-0.684352
H	2.836066	0.714973	-2.683754
C	2.385751	2.227267	1.656495
C	3.347543	1.064019	1.306963
H	2.953164	3.165141	1.645381
H	3.810518	0.713123	2.232775
C	2.608061	-0.153581	-0.777600
C	1.998783	-1.258320	-1.358485
C	2.686476	-0.093086	0.616022
C	1.423853	-2.280014	-0.616022
H	1.952787	-1.315705	-2.443121
C	2.089128	-1.101837	1.358485
C	1.437036	-2.181857	0.777600
H	2.115827	-1.033311	2.443121
C	0.752304	-3.431066	-1.306963
C	-0.735994	-3.179754	-1.656495
H	0.841016	-4.323336	-0.684352
H	1.287676	-3.656567	-2.232775
H	-1.264510	-4.140085	-1.645381
H	-0.798849	-2.813591	-2.683754
C	0.735994	-3.179754	1.656495
C	-0.752304	-3.431066	1.306963
H	0.798849	-2.813591	2.683754
H	1.264510	-4.140085	1.645381
H	-0.841016	-4.323336	0.684352
H	-1.287676	-3.656567	2.232775
C	-1.437036	-2.181857	-0.777600
C	-1.423853	-2.280014	0.616022
C	-2.089128	-1.101837	-1.358485
C	-1.998783	-1.258320	1.358485
C	-2.686476	-0.093086	-0.616022
H	-2.115827	-1.033311	-2.443121
C	-2.608061	-0.153581	0.777600
H	-1.952787	-1.315705	2.443121
C	-3.347543	1.064019	-1.306963
C	-2.385751	2.227267	-1.656495
H	-4.164626	1.433327	-0.684352
H	-3.810518	0.713123	-2.232775
H	-2.953164	3.165141	-1.645381
H	-2.037217	2.098619	-2.683754
C	-3.121745	0.952487	1.656495
C	-2.595239	2.367048	1.306963
H	-2.836066	0.714973	2.683754
H	-4.217674	0.974944	1.645381
H	-3.323610	2.890009	0.684352
H	-2.522842	2.943444	2.232775
H	2.522842	2.943444	-2.232775
H	2.037217	2.098619	2.683754
H	4.217674	0.974944	-1.645381
H	4.164626	1.433327	0.684352

File: para.xyz

48

scf done: -928.293820

C	-1.400511	2.512959	0.177376
C	-0.838580	2.528447	-1.094118
C	0.535621	2.522412	-1.265832
C	1.400511	2.512959	-0.177376
C	0.838580	2.528447	1.094118
C	-0.535621	2.522412	1.265832
H	-1.481831	2.519250	-1.967975
H	0.948282	2.505907	-2.269637
H	1.481831	2.519250	1.967975
H	-0.948282	2.505907	2.269637
C	2.887922	2.438154	-0.378230
H	3.089942	2.341253	-1.448255
H	3.361741	3.375015	-0.064633
C	3.555464	1.281937	0.378230
H	4.603719	1.223846	0.064633
H	3.572556	1.505341	1.448255
C	2.876542	-0.043601	0.177376
C	2.608989	-0.537992	-1.094118
C	2.452284	-0.797345	1.265832
C	1.916663	-1.725068	-1.265832
H	2.922650	0.023678	-1.967975
C	1.770409	-1.990455	1.094118
H	2.644320	-0.431717	2.269637
C	1.476031	-2.469358	-0.177376
H	1.696037	-2.074190	-2.269637
H	1.440819	-2.542928	1.967975
C	0.667542	-3.720091	-0.378230
H	1.241978	-4.598860	-0.064633
H	0.482614	-3.846595	-1.448255
C	-0.667542	-3.720091	0.378230
H	-1.241978	-4.598860	0.064633
H	-0.482614	-3.846595	1.448255
C	-2.887922	2.438154	0.378230
H	-3.089942	2.341253	1.448255
H	-3.361741	3.375015	0.064633
C	-3.555464	1.281937	-0.378230
H	-4.603719	1.223846	-0.064633
H	-3.572556	1.505341	-1.448255
C	-2.876542	-0.043601	-0.177376
C	-2.608989	-0.537992	1.094118
C	-2.452284	-0.797345	-1.265832
C	-1.916663	-1.725068	1.265832
H	-2.922650	0.023678	1.967975
C	-1.770409	-1.990455	-1.094118
H	-2.644320	-0.431717	-2.269637
C	-1.476031	-2.469358	0.177376
H	-1.696037	-2.074190	2.269637
H	-1.440819	-2.542928	-1.967975