Supplementary Material For Dalton Trans. Manuscript

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"C-C Bond Coupling Between the Organometallic Cations $CH_3Ag_2^+$, $CH_3Cu_2^+$ and CH_3AgCu^+ and Allyliodide."

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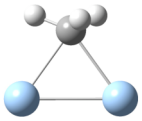
List of Supplementary Material:

(A) **Cartesian Coordinates**

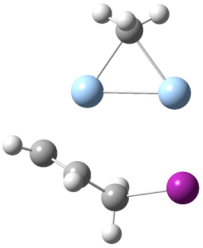
$CH_3Ag_2^+$



C	-0.003185	1.707147	0.008580
Ag	-1.346678	-0.176428	-0.000210
Ag	1.348053	-0.173862	-0.000250
H	0.192707	2.051935	1.023394
H	-0.971014	2.094606	-0.338832
H	0.732767	2.074214	-0.714431

E + ZPVE =-333.635265 Hartrees

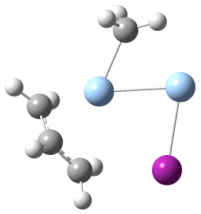
(B1) $CH_3Ag_2^+ + C_3H_5I$



C	-2.494996	-1.595752	0.021524
Ag	-1.813992	0.576979	-0.026066
Ag	-0.178060	-1.512970	0.029864
C	-1.161877	2.852583	0.121472
C	-0.028118	2.300704	-0.402531
C	1.187875	2.006611	0.412021
I	2.210532	0.053652	-0.039245
H	-1.256611	3.057944	1.186766
H	-1.912672	3.290672	-0.533889
H	0.083922	2.243375	-1.484755
H	1.988999	2.708028	0.167681
H	1.013181	1.989355	1.486833
H	-2.325929	-2.458160	0.681138
H	-2.752060	-1.944942	-0.979911
H	-3.387893	-1.123114	0.462716

E + ZPVE = -462.34075 Hartrees

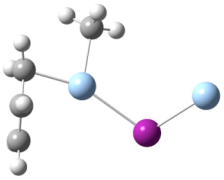
(TS(B1-C1)) $CH_3Ag_2^+ + C_3H_5I$ (TS)



Ag	1.446605	0.156440	-0.167249
Ag	-0.827020	1.544311	0.108441
I	-1.714076	-1.046604	-0.048939
C	3.073739	-1.374613	0.496095
C	2.104226	-2.094474	-0.214010
C	0.899319	-2.555559	0.365492
H	4.027593	-1.137915	0.033778
H	3.006241	-1.244745	1.574625
H	2.297282	-2.344416	-1.256220
H	0.280558	-3.262595	-0.173391
H	0.710856	-2.441960	1.428872
C	1.619269	2.333731	-0.017459
H	0.812015	3.091570	0.003394
H	2.199107	2.539519	-0.920087
H	2.212541	2.480750	0.886045

E + ZPVE = -462.30925 Hartrees
Imaginary Frequency = -124.4723 cm^{-1}

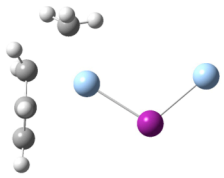
(C1) $CH_3Ag_2^+ + C_3H_5I$



Ag	-1.607337	0.371496	-0.125757
Ag	2.775049	0.561801	0.418742
I	0.796387	-1.062470	-0.412737
C	-3.664199	0.786239	0.306426
C	-3.580239	-0.361923	1.191863
C	-3.581862	-1.651214	0.748522
H	-3.795552	1.768830	0.749248
H	-4.152582	0.656890	-0.658818
H	-3.425901	-0.169852	2.252502
H	-3.457570	-2.483026	1.434766
H	-3.757081	-1.896743	-0.297208
C	-1.518188	2.345331	-0.944040
H	-0.687744	2.248278	-1.644501
H	-1.297425	3.006955	-0.106042
H	-2.450150	2.604014	-1.441823

E + ZPVE = -462.3331 Hartrees

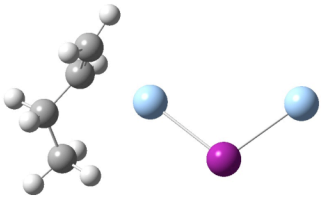
(TS(C1-D1)) $Ag_2I^+ + [C_4H_8]$ (TS)



Ag	-1.516428	0.350786	-0.032613
Ag	2.872773	0.627351	0.052843
I	0.821153	-1.113351	-0.044890
C	-3.732059	0.833021	-0.005436
C	-3.767254	-0.523621	0.578658
C	-3.833737	-1.659135	-0.154183
H	-4.178499	1.597415	0.619656
H	-4.027944	0.900594	-1.049836
H	-3.777516	-0.591106	1.665515
H	-3.914833	-2.630626	0.323503
H	-3.850976	-1.642373	-1.242065
C	-2.185914	2.505042	-0.147227
H	-2.958648	2.907512	-0.793921
H	-1.202056	2.679031	-0.596419
H	-2.245084	2.882883	0.871094

E + ZPVE = -462.3258 Hartrees
Imaginary Frequency = -260.1713 cm^{-1}

(D1) $Ag_2I^+ + [C_4H_8]$

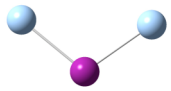


Ag	-1.337520	-0.365278	-0.253595
Ag	2.906955	-0.683090	0.343364
I	0.968703	1.086756	-0.276735
C	-4.562877	0.148219	0.296443
C	-3.639091	-1.034407	0.375309
C	-3.151649	-1.738483	-0.692846
H	-5.552601	-0.221749	0.605336
H	-4.664630	0.480447	-0.743294
H	-3.450632	-1.426244	1.377715
H	-2.671225	-2.705609	-0.552709
H	-3.433548	-1.474784	-1.711659
C	-4.166908	1.317934	1.211730
H	-4.923360	2.106409	1.167843
H	-4.075685	0.997585	2.255637

H -3.209859 1.759604 0.905128

E + ZPVE = -462.4149 Hartrees

Ag_2I^+



Ag 2.159177 -0.595151 0.000000
Ag -2.159177 -0.595179 0.000000
I 0.000000 1.055576 0.000000

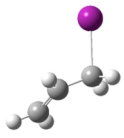
E + ZPVE = -305.2506 Hartrees

C_4H_8

C 1.861392 0.017370 -0.280254
C 0.723611 -0.295281 0.341619
C -0.540447 0.521255 0.308210
C -1.728941 -0.247249 -0.295032
H 1.958077 0.927275 -0.869913
H 2.740709 -0.618987 -0.223480
H 0.673336 -1.220878 0.919080
H -0.801871 0.827428 1.332401
H -0.366559 1.444456 -0.259112
H -1.526648 -0.527285 -1.334816
H -1.929874 -1.168946 0.264606
H -2.640865 0.360367 -0.276022

E + ZPVE = -157.1090 Hartrees

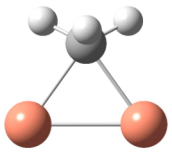
C_3H_5I



C 3.140275 -0.461360 -0.255861
C 2.148833 0.059367 0.474325
C 1.085144 0.918744 -0.090231
I -0.935951 -0.086515 -0.009799
H 3.202225 -0.305794 -1.330712
H 3.926011 -1.058704 0.197237
H 2.106641 -0.123708 1.546547
H 0.903029 1.826714 0.482880
H 1.221969 1.146253 -1.146020

E + ZPVE = -128.648932 Hartrees

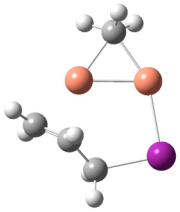
$CH_3Cu_2^+$



C	0.000212	1.414152	0.014300
Cu	-1.172268	-0.239685	-0.000240
Cu	1.172251	-0.239698	-0.000245
H	0.004321	1.808750	1.033165
H	-0.866518	1.804294	-0.548318
H	0.861423	1.804150	-0.556561

E + ZPVE = -434.3194 Hartrees

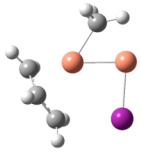
(B2) $CH_3Cu_2^+ + C_3H_5I$



C	-2.314855	-1.700473	0.042571
Cu	-1.888638	0.302938	-0.020722
Cu	-0.309602	-1.419531	0.016124
C	-1.772357	2.400334	0.117530
C	-0.584308	1.986290	-0.435443
C	0.689250	1.884847	0.338523
I	1.859573	-0.018880	-0.020930
H	-1.861021	2.621752	1.180452
H	-2.588301	2.730617	-0.523693
H	-0.493233	1.942387	-1.520952
H	1.410903	2.634150	0.006753
H	0.562766	1.920932	1.419394
H	-2.111869	-2.541073	0.727065
H	-2.614205	-2.098532	-0.931799
H	-3.219827	-1.254345	0.506363

E + ZPVE =-563.0484 Hartrees

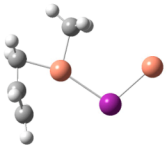
(TS(B2_C2)) $CH_3Cu_2^+ + C_3H_5I$ (TS)



Cu	1.487747	0.084901	-0.133747
Cu	-0.285805	1.562082	0.058015
I	-1.722353	-0.442752	-0.014069
C	2.867335	-1.390928	0.328108
C	1.787756	-1.988231	-0.345418
C	0.564785	-2.324144	0.283683
H	3.816458	-1.253195	-0.182431
H	2.884152	-1.320364	1.415279
H	1.893724	-2.215474	-1.405762
H	-0.152707	-2.943251	-0.240588
H	0.452703	-2.243907	1.361028
C	1.747007	2.080077	0.037408
H	1.033498	2.950010	0.080466
H	2.349597	2.285620	-0.852384
H	2.349679	2.183248	0.943602

E + ZPVE = -563.0275 Hartrees
Imaginary Frequency = -120.7537 cm^{-1}

(C2) Cu_2I^+ +[C_4H_8]



Cu	1.384200	0.444414	0.007056
Cu	-2.628210	0.785088	-0.005968
I	-0.861958	-0.924022	-0.012727
C	3.308300	0.871846	0.050298
C	3.306540	-0.492872	-0.437396
C	2.866853	-1.535755	0.332188
H	3.647366	1.659032	-0.614743
H	3.497368	1.051649	1.108534
H	3.485727	-0.657624	-1.498877
H	2.742588	-2.530499	-0.084893
H	2.722031	-1.432709	1.406772
C	1.012860	2.360688	0.070699
H	0.260838	2.412768	0.863714
H	0.591103	2.565211	-0.917557
H	1.845706	3.026349	0.285318

E + ZPVE = -563.0333 Hartrees

(TS(C2-D2)) Cu_2I^+ +[C_4H_8](TS)

Cu	-1.350620	0.299125	-0.006303
Cu	2.674409	0.861812	0.025931
I	0.948620	-0.884695	-0.005677
C	-3.283810	0.919730	-0.041942
C	-3.294663	-0.465401	0.482022
C	-3.054947	-1.562455	-0.283915
H	-3.743544	1.649192	0.615400
H	-3.578062	1.033303	-1.083997
H	-3.423484	-0.587999	1.556679
H	-3.030269	-2.556525	0.152153
H	-2.964417	-1.500623	-1.367318
C	-1.608396	2.318080	-0.112449
H	-2.368479	2.952362	-0.558819
H	-0.718930	2.340867	-0.754601
H	-1.388651	2.631345	0.909868

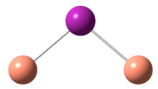
E + ZPVE = -563.0276 Hartrees
Imaginary Frequency = -266.8966 cm^{-1}

(D2) Cu_2I^+ + [C_4H_8]

Cu	1.034015	0.462013	-0.261097
Cu	-2.696127	0.863567	0.531423
I	-1.128969	-0.845780	-0.287699
C	4.013128	-0.224931	0.161949
C	3.111899	0.970596	0.308855
C	2.614093	1.728804	-0.721991
H	5.021738	0.125984	0.429901
H	4.062106	-0.535746	-0.888241
H	2.965710	1.333094	1.329754
H	2.164085	2.703017	-0.532144
H	2.865265	1.499595	-1.757827
C	3.643556	-1.407564	1.071550
H	4.385209	-2.205128	0.974237
H	3.609896	-1.107394	2.124777
H	2.666525	-1.830352	0.805989

E + ZPVE = -563.0989 Hartrees

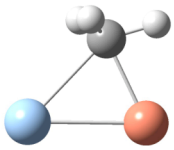
Cu_2I^+



Cu	1.887493	-0.765014	0.000000
Cu	-1.887493	-0.765043	0.000000
I	0.000000	0.837201	0.000000

E + ZPVE = -405.9202 Hartrees

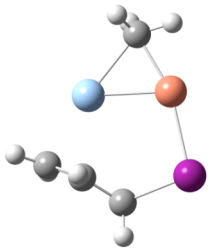
CH_3AgCu^+



C	0.799848	1.485386	0.000130
Ag	-1.051477	-0.077277	-0.000003
Cu	1.446206	-0.373071	-0.000002
H	0.397915	1.928951	0.913573
H	0.391213	1.930277	-0.909744
H	1.891203	1.679567	-0.004392

E + ZPVE = -383.9794 Hartrees

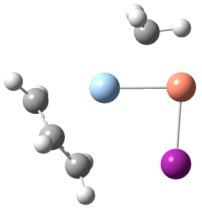
(B3) $CH_3AgCu^+ + C_3H_5I$



C	-1.976769	-2.059378	0.047994
Ag	-1.831390	0.247593	-0.015360
Cu	-0.046742	-1.483842	0.026338
C	-1.397294	2.594653	0.114238
C	-0.229342	2.136160	-0.424570
C	1.012399	1.922471	0.373641
I	2.089225	-0.025037	-0.029398
H	-1.496584	2.787798	1.181395
H	-2.188508	2.971012	-0.531560
H	-0.126270	2.088557	-1.508110
H	1.787737	2.636293	0.087113
H	0.860840	1.930173	1.451962
H	-1.396269	-3.011694	0.051925
H	-2.609487	-2.135753	-0.841475
H	-2.583500	-2.108305	0.957150

E + ZPVE = -512.6930 Hartrees

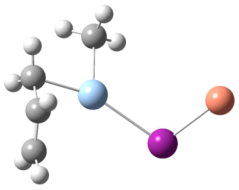
(TS(B3-C3)) CH_3AgCu^+ + C_3H_5I (TS)



Ag	1.381389	0.212152	-0.131891
Cu	-0.676195	1.546418	0.083300
I	-1.881201	-0.617930	-0.012729
C	2.964238	-1.416085	0.451974
C	1.947462	-2.023570	-0.296722
C	0.700132	-2.411252	0.250667
H	3.933759	-1.221295	0.003069
H	2.897614	-1.330043	1.535103
H	2.129684	-2.235617	-1.349429
H	0.013002	-3.004787	-0.340231
H	0.510367	-2.343174	1.317910
C	1.220151	2.438662	0.086162
H	0.348388	3.150090	0.141489
H	1.772434	2.761143	-0.798986
H	1.790872	2.630177	0.996443

E + ZPVE = -512.6637 Hartrees
Imaginary Frequency = -107.0309 Cm^{-1}

(C3) $AgCuI^+$ +[C_4H_8]

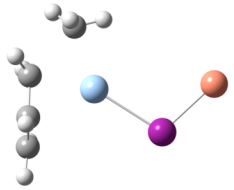


Ag	-1.285877	0.335746	-0.123788
Cu	2.744546	0.730424	0.766225
I	1.278434	-0.803942	-0.453545
C	-3.380702	0.498718	0.297848
C	-3.182780	-0.666259	1.143002
C	-3.044997	-1.931541	0.655087
H	-3.622765	1.444114	0.773797
H	-3.842430	0.353473	-0.678186
H	-3.063159	-0.497802	2.212140
H	-2.843470	-2.770378	1.313937
H	-3.179708	-2.155470	-0.401428

C	-1.415316	2.336397	-0.870317
H	-0.543528	2.372677	-1.524858
H	-1.327553	2.990220	-0.002509
H	-2.347259	2.485822	-1.411178

E + ZPVE = -512.6697 Hartrees

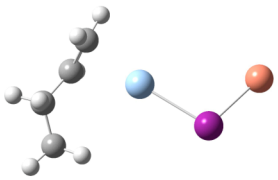
(TS(C3-D3)) $AgCuI^+$ + $[C_4H_8]$ (TS)



Ag	-1.184333	0.339604	-0.014034
Cu	2.915650	0.902443	0.008227
I	1.279682	-0.919447	0.003674
C	-3.440540	0.592745	-0.040571
C	-3.357659	-0.784169	0.487939
C	-3.291449	-1.887906	-0.291877
H	-3.978316	1.283143	0.598468
H	-3.708009	0.676633	-1.091431
H	-3.394087	-0.898520	1.570308
H	-3.293947	-2.882638	0.143028
H	-3.277831	-1.825333	-1.378119
C	-2.064388	2.417242	-0.057569
H	-2.850038	2.767744	-0.718754
H	-1.087526	2.710998	-0.457343
H	-2.199357	2.738996	0.972620

E + ZPVE = -512.6624 Hartrees
Imaginary Frequency = -258.2427 cm^{-1}

(D3) $AgCuI^+$ + $[C_4H_8]$

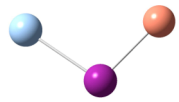


Ag	-0.982989	-0.404594	-0.156804
Cu	2.960084	-0.903689	0.403849
I	1.417281	0.902765	-0.201375
C	-4.210242	0.344474	0.049400
C	-3.363961	-0.848331	0.392930
C	-2.842960	-1.741623	-0.504600
H	-5.238904	0.073969	0.333594
H	-4.218231	0.503900	-1.035144

H	-3.268668	-1.075262	1.457510
H	-2.431754	-2.693172	-0.170831
H	-3.038328	-1.639167	-1.571528
C	-3.816703	1.631027	0.792562
H	-4.524356	2.432584	0.563357
H	-3.816140	1.483846	1.878324
H	-2.818267	1.976406	0.493994

E + ZPVE = -512.7513 Hartrees

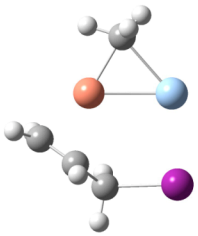
AgCuI$^+$



Ag	-1.431193	-1.287645	0.000000
Cu	2.319520	0.197921	0.000000
I	0.000000	1.033577	0.000000

E + ZPVE = -355.58576 Hartrees

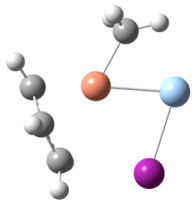
(B4) $CH_3AgCu^+ + C_3H_5I$ (coupling on Cu)



C	-2.771664	-1.047093	0.057041
Cu	-1.823152	0.736082	-0.028914
Ag	-0.487652	-1.387169	0.012330
C	-1.361411	2.785762	0.098492
C	-0.234476	2.203337	-0.424743
C	1.001588	1.952647	0.377087
I	2.010069	-0.017851	-0.024737
H	-1.437472	3.032254	1.156976
H	-2.113932	3.215302	-0.561606
H	-0.131737	2.128329	-1.507503
H	1.791705	2.651187	0.092749
H	0.846654	1.970931	1.454906
H	-2.867195	-1.762970	0.880612
H	-3.074532	-1.512623	-0.884177
H	-3.560298	-0.293653	0.290852

E + ZPVE = -512.6971 Hartrees

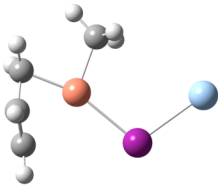
(TS(B4-C4)) $CH_3AgCu^+ + C_3H_5I$ (coupling on Cu) (TS)



Cu	-1.504678	0.115593	-0.159223
Ag	0.320779	-1.611665	0.080286
I	1.678334	0.758022	-0.044777
C	-2.869092	1.587515	0.337948
C	-1.783606	2.225695	-0.284253
C	-0.580137	2.541390	0.388521
H	-3.807259	1.466277	-0.196532
H	-2.908142	1.470871	1.420468
H	-1.868474	2.501342	-1.334668
H	0.129788	3.213839	-0.076204
H	-0.490982	2.401363	1.461934
C	-2.149565	-1.773258	-0.077336
H	-1.613683	-2.744099	-0.042465
H	-2.734548	-1.806809	-1.002227
H	-2.804917	-1.769918	0.797636

E + ZPVE = -512.6726 Hartrees
Imaginary Frequency = -137.0966 cm^{-1}

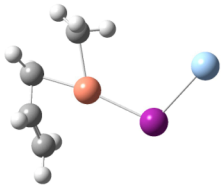
(C4) $AgCuI^{+}$ +[C_4H_8](coupling on Cu)



Cu	1.685128	0.490746	0.007611
Ag	-2.535864	0.530858	-0.006782
I	-0.387068	-1.106176	-0.009389
C	3.544137	1.152598	0.053697
C	3.701165	-0.198871	-0.441547
C	3.371036	-1.288950	0.319116
H	3.786571	1.978911	-0.606029
H	3.706752	1.347641	1.113617
H	3.899001	-0.335954	-1.503640
H	3.353810	-2.287889	-0.105620
H	3.216405	-1.210720	1.394404
C	1.069882	2.343482	0.076916
H	0.330804	2.302048	0.882622
H	0.608114	2.488944	-0.904055
H	1.812747	3.112858	0.275280

E + ZPVE = -512.6974 Hartrees

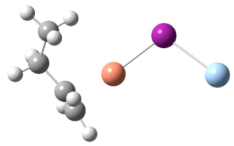
(TS(C4-D4)) $AgCuI^+$ + [C_4H_8] (coupling on Cu) (TS)



Cu	-1.683072	0.338649	-0.013289
Ag	2.604887	0.583269	0.035011
I	0.473222	-1.068430	-0.026942
C	-3.540061	1.164066	-0.034062
C	-3.688685	-0.199845	0.523210
C	-3.580744	-1.333905	-0.218370
H	-3.911244	1.951792	0.611936
H	-3.838653	1.284992	-1.074066
H	-3.809222	-0.283874	1.602523
H	-3.650765	-2.314124	0.243129
H	-3.503600	-1.308132	-1.304183
C	-1.731376	2.372625	-0.160387
H	-2.426836	3.078071	-0.605429
H	-0.858309	2.286299	-0.819231
H	-1.457559	2.679668	0.850766

E + ZPVE = -512.6914 Hartrees
Imaginary Frequency = -270.5801cm^{-1}

(D4) $AgCuI^+$ + [C_4H_8] (coupling on Cu)

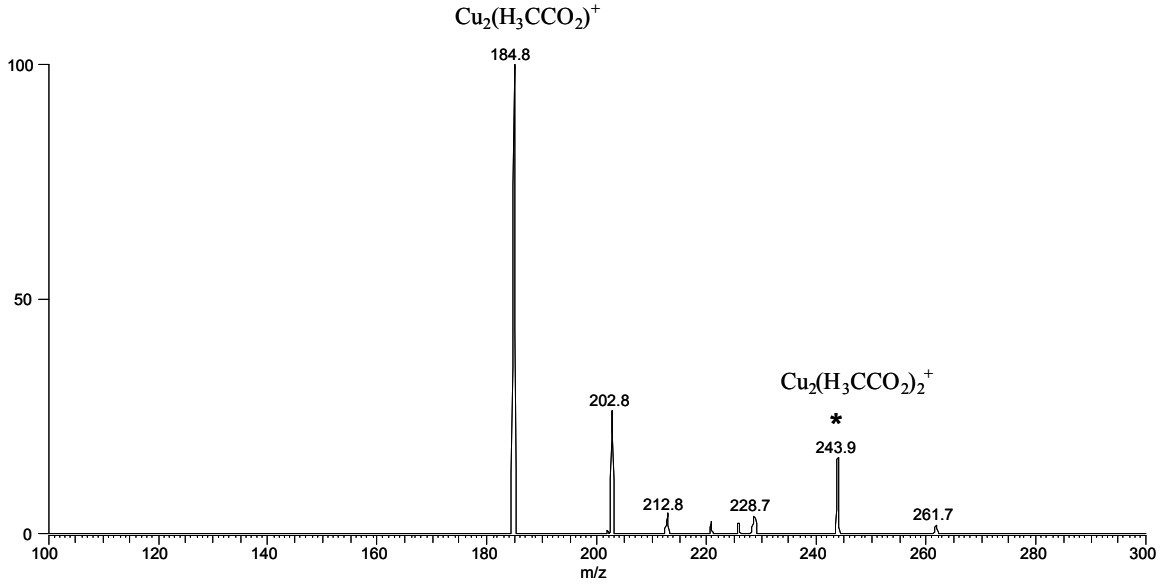


Cu	1.379750	0.408507	-0.342147
Ag	-2.625805	0.671663	0.352761
I	-0.661451	-1.063166	-0.305227
C	4.367661	0.024229	0.318220
C	3.375340	1.153128	0.248809
C	2.889080	1.720638	-0.902826
H	5.332500	0.489790	0.572593
H	4.494800	-0.429743	-0.671605
H	3.144189	1.641558	1.199034
H	2.361376	2.673659	-0.876885
H	3.216496	1.369549	-1.881585
C	4.038942	-1.041130	1.376125
H	4.843984	-1.779073	1.431525
H	3.923848	-0.595388	2.370495

H 3.113658 -1.578615 1.133989

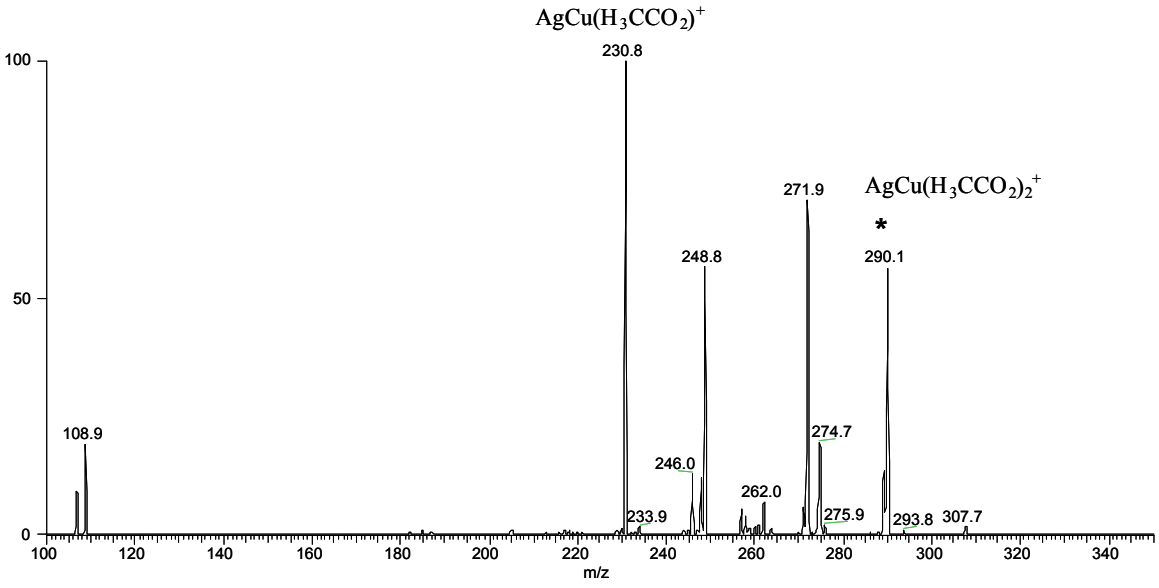
E + ZPVE = -512.7632 Hartrees

Figure S1



CID spectrum of $Cu_2(H_3CCO_2)_2^+$ (m/z 244)

Figure S2



CID spectrum of $AgCu(H_3CCO_2)_2^+$ (m/z 290)