Electronic Supplementary Information

for

Metallic Cyanoacetylides of Copper, Silver and Gold: Generation and Structural Characterization

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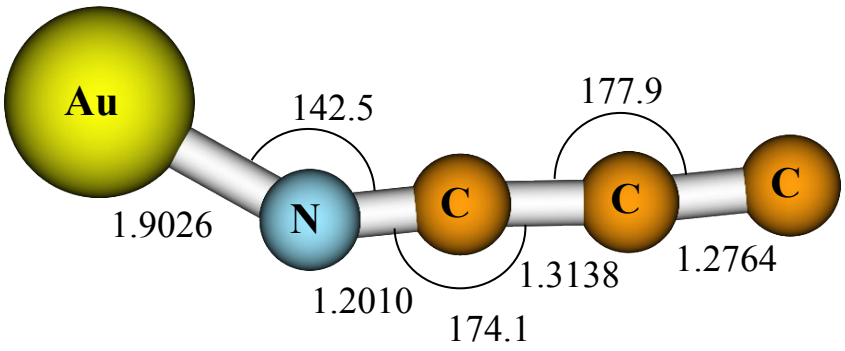
Figure S1. Geometrical parameters obtained at the MP2/aug-cc-pVTZ+PP level for the bent structure of AuNCCC. Distances are given in Ångstroms and angles in degrees.



Rotational constants (MHz): A = 67404.7; B = 851.6; C = 841.0

Figure S2. Contour maps of the Laplacian distribution of the electron density for the MCCCN and MNCCC isomers. Red dashed lines indicate regions of electronic charge concentration ($\nabla^2\rho(r) < 0$), and blue continuous lines denote regions of electronic charge depletion ($\nabla^2\rho(r) > 0$). Small red spheres represent bond critical points

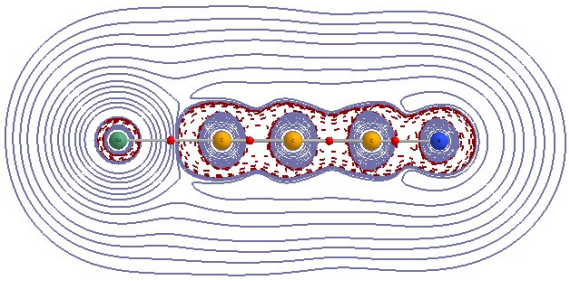
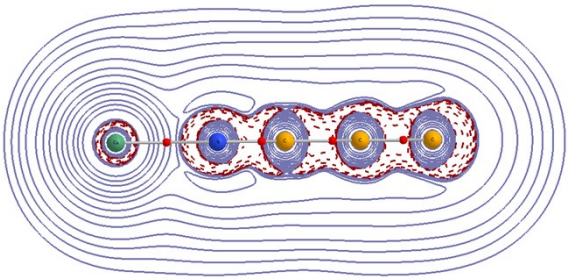
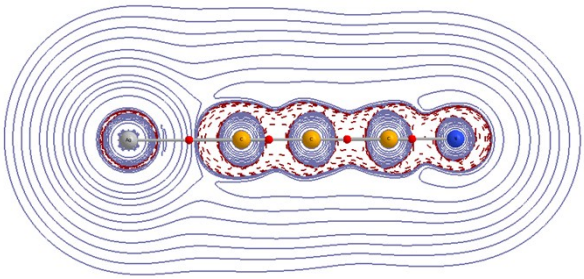
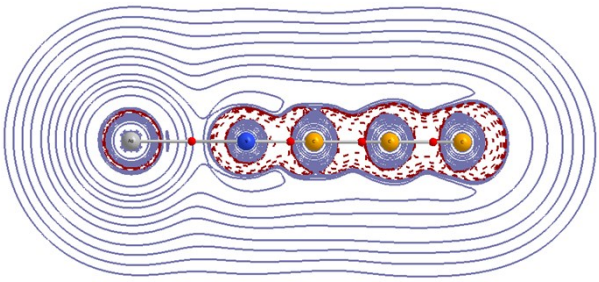
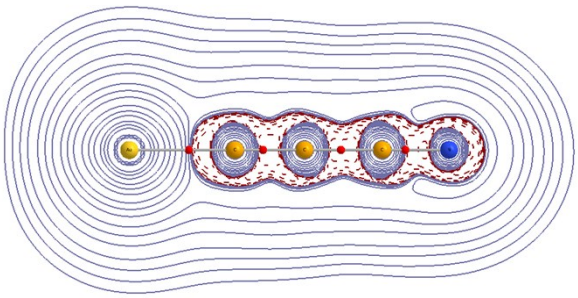
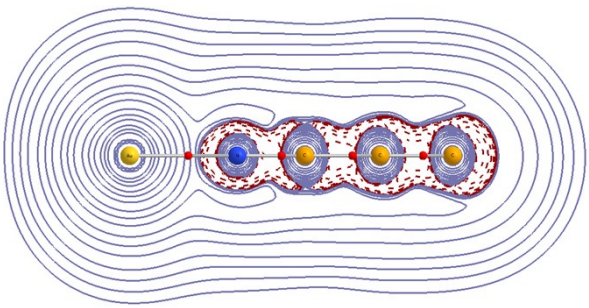
M	MCCCN	MNCCC
Cu		
Ag		
Au		

Table S1. Measured frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of ^{63}CuCCCN.

J′	J′′	F'_1	F''_1	F′	F′′	$\nu_{obs.}$	$\nu_{obs.}-\nu_{cal.}$
2	1	1.5	1.5	1.5	1.5	4020.15931	0.00136
		1.5	1.5	0.5	1.5	4020.46279	0.00144
		1.5	1.5	2.5	2.5	4021.36651	0.00100
		1.5	1.5	1.5	0.5	4021.81008	0.00236
		2.5	1.5	2.5	1.5	4024.00925	0.00264
		2.5	1.5	1.5	1.5	4024.66140	0.00209
		3.5	2.5	2.5	1.5	4024.82305	0.00238
		3.5	2.5	3.5	2.5	4024.89298	0.00236
		3.5	2.5	4.5	3.5	4025.13962	0.00119
		2.5	1.5	3.5	2.5	4025.29901	0.00288
		0.5	0.5	0.5	0.5	4025.35099	-0.00150
		0.5	0.5	1.5	0.5	4025.48506	0.00112
		0.5	0.5	0.5	1.5	4025.54958	0.00195
		0.5	0.5	1.5	1.5	4025.68126	0.00218
		1.5	2.5	2.5	1.5	4026.14535	0.00245
		2.5	1.5	1.5	0.5	4026.31000	0.00092
		3.5	0.5	2.5	1.5	4030.01772	0.00178
		2.5	2.5	3.5	3.5	4030.45826	0.00076
		1.5	0.5	1.5	0.5	4030.90452	0.00199
		2.5	2.5	2.5	2.5	4031.04658	0.00068
		1.5	0.5	2.5	1.5	4031.34056	0.00239
3	2	3.5	2.5	3.5	2.5	6037.70176	0.00060
		4.5	3.5	4.5	3.5	6037.95566	0.00075
		4.5	3.5	5.5	4.5	6038.06743	0.00119
		3.5	2.5	4.5	3.5	6038.12795	0.00126
		3.5	2.5	2.5	1.5	6038.15966	0.00342
		4.5	3.5	3.5	2.5	6038.19728	0.00210
4	3	4.5	3.5	4.5	3.5	8050.74166	-0.00311
		5.5	4.5	5.5	4.5	8050.83673	-0.00294
		5.5	4.5	4.5	3.5	8050.89875	-0.00135
		4.5	3.5	5.5	4.5	8050.92701	-0.00353
		3.5	2.5	3.5	2.5	8051.31578	-0.00222
		2.5	1.5	2.5	1.5	8051.35634	-0.00226
		3.5	2.5	4.5	3.5	8051.53611	-0.00300
		3.5	2.5	2.5	1.5	8051.55281	-0.00263
		2.5	1.5	3.5	2.5	8051.60586	-0.00316

Table S2. Measured frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of ^{65}CuCCCN.

J′	J′′	F'_1	F''_1	F′	F′′	$\nu_{obs.}$	$\nu_{obs.}-\nu_{cal.}$
2	1	2.5	2.5	1.5	1.5	3980.29978	0.00113
		3.5	2.5	2.5	1.5	3981.09002	0.00098
		3.5	3.5	2.5	2.5	3981.18809	0.00129
		3.5	4.5	2.5	3.5	3981.43499	0.00220
		2.5	3.5	1.5	2.5	3981.59012	0.00127
3	2	3.5	3.5	2.5	2.5	5972.11233	0.00074
		4.5	4.5	3.5	3.5	5972.36547	0.00153
		4.5	5.5	3.5	4.5	5972.47704	0.00269
		3.5	4.5	2.5	3.5	5972.53681	0.00284
		4.5	3.5	3.5	2.5	5972.62303	0.00198
		3.5	2.5	2.5	2.5	5973.21119	0.00084
		2.5	3.5	1.5	2.5	5973.63758	0.00266
		1.5	2.5	0.5	1.5	5973.85015	0.00303
4	3	4.5	4.5	3.5	3.5	7963.27920	-0.00189
		5.5	5.5	4.5	4.5	7963.36814	-0.00247
		5.5	4.5	4.5	3.5	7963.43214	-0.00277
		4.5	5.5	3.5	4.5	7963.45817	-0.00236
		3.5	3.5	2.5	2.5	7963.80080	-0.00151
		2.5	2.5	1.5	1.5	7963.84181	-0.00185
		2.5	1.5	1.5	0.5	7963.89431	-0.00103
		3.5	4.5	2.5	3.5	7964.01075	-0.00069
		2.5	3.5	1.5	2.5	7964.09106	-0.00110

Table S3. Measured frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of ^{107}AgCCCN.

J´	J´´	F´	F´´	$\nu_{obs.}$	$\nu_{obs.}$-$\nu_{cal.}$
2	1	2	1	3135.61171	-0.00099
		3	2	3135.69994	-0.00021
3	2	2	1	4703.21351	0.00000
		3	2	4703.41725	-0.00026
		4	3	4703.46585	-0.00024
4	3	3	2	6271.13337	0.00036
		4	3	6271.22124	0.00079
		5	4	6271.25228	0.00091
5	4	4	3	7838.97155	-0.00079
		5	4	7839.02106	0.00014
		6	5	7839.04210	-0.00022

Table S4. Measured frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of ^{109}AgCCCN.

J´	J´´	F´	F´´	$\nu_{obs.}$	$\nu_{obs.}$-$\nu_{cal.}$
2	1	2	1	3120.17763	0.00007
		3	2	3120.26521	0.00040
3	2	2	1	4680.06176	0.00050
		3	2	4680.26385	-0.00098
		4	3	4680.31349	0.00019
4	3	3	2	6240.26284	-0.00020
		4	3	6240.35028	-0.00001
		5	4	6240.38118	0.00004
5	4	4	3	7800.38389	-0.00097
		5	4	7800.43482	0.00148
		6	5	7800.45430	-0.00039

Table S5. Measured frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of ^{197}AuCCCN.

J′	J′′	F'_1	F''_1	F′	F′′	$\nu_{obs.}$	$\nu_{obs.}-\nu_{cal.}$
2	1	3.5	2.5	3.5	2.5	2897.73394	-0.00018
		3.5	2.5	2.5	1.5	2897.79371	0.00019
		3.5	2.5	4.5	3.5	2897.99412	0.00047
3	2	3.5	2.5	3.5	2.5	4347.25679	0.00000
		4.5	3.5	4.5	3.5	4347.51576	0.00034
		4.5	3.5	5.5	4.5	4347.63294	0.00021
		4.5	3.5	3.5	2.5	4347.67957	0.00047
		3.5	2.5	4.5	3.5	4347.69957	0.00021
		3.5	2.5	2.5	1.5	4347.75014	-0.00004
		2.5	1.5	3.5	2.5	4349.87919	-0.00005
		1.5	0.5	2.5	1.5	4349.99278	0.00030
		2.5	1.5	1.5	0.5	4350.20599	-0.00040
4	3	3.5	3.5	3.5	3.5	5793.71245	0.00050
		3.5	3.5	4.5	4.5	5793.87118	-0.00085
		3.5	3.5	2.5	2.5	5793.91658	-0.00068
		4.5	3.5	4.5	3.5	5796.93079	-0.00009
		5.5	4.5	5.5	4.5	5797.04057	0.00017
		5.5	4.5	4.5	3.5	5797.08627	0.00059
		4.5	3.5	3.5	2.5	5797.10559	0.00025
		4.5	3.5	5.5	4.5	5797.13905	0.00017
		3.5	2.5	3.5	2.5	5797.92081	0.00032
		2.5	1.5	2.5	1.5	5797.96236	0.00038
		2.5	1.5	1.5	0.5	5798.03104	-0.00031
		3.5	2.5	2.5	1.5	5798.18409	-0.00128
		3.5	2.5	4.5	3.5	5798.19051	0.00028
		2.5	1.5	3.5	2.5	5798.22602	0.00000
5	4	5.5	4.5	5.5	4.5	7246.42065	0.00075
		6.5	5.5	5.5	4.5	7246.49106	-0.00004
		5.5	4.5	4.5	3.5	7246.49484	0.00053
		4.5	3.5	4.5	3.5	7247.01431	-0.00026
		3.5	2.5	3.5	2.5	7247.04482	-0.00072
		3.5	2.5	2.5	1.5	7247.06058	0.00020
		4.5	3.5	3.5	2.5	7247.12257	-0.00052
		4.5	3.5	5.5	4.5	7247.15272	-0.00060
		3.5	2.5	4.5	3.5	7247.17246	-0.00058
6	5	6.5	5.5	5.5	4.5	8695.87030	0.00085
		5.5	4.5	5.5	4.5	8696.23236	-0.00124
		4.5	3.5	4.5	3.5	8696.25296	-0.00046
		5.5	4.5	4.5	3.5	8696.28676	0.00078
		4.5	3.5	5.5	4.5	8696.32741	0.00083