Electronic supplementary file

Exploring Coinage Bonding Interactions in $[Au(CN)_4]^-$ Assemblies with Silver and Zinc Complexes: A Structural and Theoretical Study

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1. Table S1

Table S1. Crystallographic Data and Details of Refinements for complexes **1 - 4**.

	1	**2**	**3**	**4**
empirical formula	$C_{34}H_{18}Ag_2Au_2N_{14}$	$C_{38}H_{24}Au_2N_{14}Zn$	$C_{44}H_{24}Au_2N_{14}Zn$	$C_{23}H_{17}Au_2N_{11}O_3Zn$
fw	1232.30	1136.01	1208.07	954.78
crystal system	Monoclinic	Triclinic	Triclinic	Orthorhombic
space group	$P\,2_1/c$	$P\,\bar{1}$	$P\,\bar{1}$	P bcn
a (Å)	9.4843(7)	8.9756(3)	11.2779(5)	27.7951(10)
b (Å)	8.6630(9)	11.2053(2)	11.4229(4)	19.2710(7)
c (Å)	20.9623(14)	41.1536(9)	16.8703(7)	7.8649(2)
α (°)	90	84.0567(17)	77.701(3)	90
β (°)	99.890(7)	88.165(2)	79.358(4)	90
γ (°)	90	80.659(2)	83.815(3)	90
V (Å^3)	1696.7(2)	4061.69(17)	2081.65(14)	4212.8(2)
Z	2	4	2	4
D_{calcd} (mg/m^3)	2.412	1.858	1.927	1.505
μ(Mo-Kα) (mm^{-1})	25.424	14.373	14.074	13.766
F(000)	1144	2152	1148	1776
θ range (°)	4.28 - 67.62	3.24 - 67.00	2.72 - 66.77	2.79 - 66.84
Collected reflections	9666	58197	16409	12823
Independent reflections	2899	14027	6837	3657
R_{int}	0.0929	0.0503	0.0439	0.1323
Observed refls $I > 2\sigma(I)$	2142	11815	5795	2492
Parameters	235	992	551	183
GOF on F^2	1.012	1.069	1.042	1.057
$R1$ ($I > 2\sigma(I)$) [a]	0.0540	0.0357	0.0310	0.0666
$wR2$ ($I > 2\sigma(I)$) [a]	0.1176	0.0780	0.0708	0.1844
residuals (e Å^{-3})	1.826, -1.794	1.637, -1.758	0.927, -0.809	2.465, -2.617

[a] $R1 = \Sigma\,||Fo|-|Fc||\,/\,\Sigma|Fo|$, $wR2 = \Sigma\,w\,(Fo^2 - Fc^2)^2\,/\,\Sigma w\,(Fo^2)^2\,]^{½}$

2. Figure S1

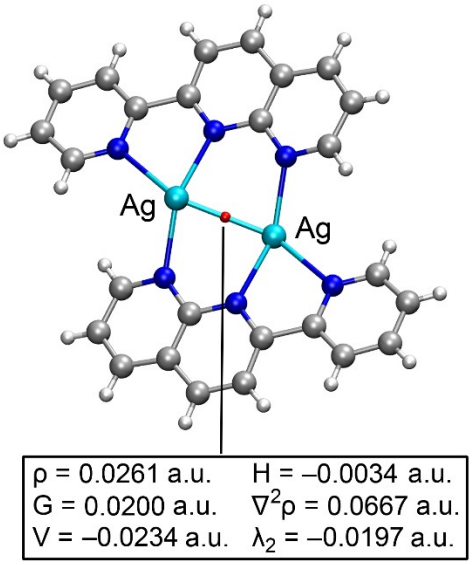

Fig. S1 QTAIM analysis of compound **1**. OnlyAg···Ag BCP is shown as a red sphere.

2. Cartesian Coordinates

Optimized dimers and trimers

Dimer T-shape

Au	7.2579695	2.5514463	3.8987006
N	10.3978511	2.7502659	3.7617065
N	7.4957105	0.1606345	5.9349320
N	4.1194100	2.3068659	3.9778300
N	7.0196112	4.8874913	1.8004392
C	9.2487561	2.6778724	3.8126168
C	7.4093848	1.0362878	5.1905623
C	5.2680661	2.3964936	3.9498357
C	7.1067030	4.0342057	2.5702447
Au	7.0625326	6.9413691	8.0666699
N	3.9313799	6.6552612	8.2164074
N	6.9323245	9.4077129	10.0173363
N	10.1939507	7.2255582	7.9188696
N	7.1932654	4.4774655	6.1148581
C	5.0775873	6.7602671	8.1615763
C	6.9798923	8.5051116	9.3025651
C	9.0475749	7.1216581	7.9723082
C	7.1453360	5.3784610	6.8303746

Antiparallel dimer

Au	4.4694027	6.6674168	19.1999962
N	6.1957343	4.0869285	18.6781704
N	5.0838106	6.4678274	22.2820356
N	2.7579336	9.2552789	19.7334907
N	3.8596662	6.8783136	16.1200238
C	5.5618318	5.0299697	18.8692970
C	4.8463110	6.5283912	21.1555132
C	3.3802669	8.3060007	19.5356857
C	4.0846260	6.8034918	17.2476843
Au	7.6420815	8.4902257	21.7277558
N	5.9149149	11.0711124	22.2447937
N	7.0291706	8.6859290	18.6451982
N	9.3556601	5.9029947	21.1977233
N	8.2527382	8.2855102	24.8080134
C	6.5489597	10.1278711	22.0552112
C	7.2661613	8.6263609	19.7718816
C	8.7327347	6.8520721	21.3946700
C	8.0270960	8.3581053	23.6803563

Trimer in Fig. 12 (left)

Au	7.2515016	2.4028093	3.8514274
N	10.3924093	2.5941542	3.7182229
N	7.4909381	0.1463596	6.0353833
N	4.1108720	2.2076480	3.9853680
N	7.0146828	4.6532181	1.6608654
C	9.2428126	2.5254932	3.7660269
C	7.4026527	0.9722293	5.2361898
C	5.2602921	2.2788794	3.9371926
C	7.1011777	3.8313559	2.4643173
Au	7.0621842	6.9544545	8.0733767
N	3.9314125	6.6653246	8.2218378
N	6.9292207	9.4115960	10.0365237
N	10.1938111	7.2392365	7.9343232
N	7.1986185	4.5035754	6.1044608
C	5.0775206	6.7712729	8.1662217
C	6.9774700	8.5122296	9.3177445
C	9.0471853	7.1354233	7.9834157

C	7.1478254	5.3995178	6.8269026
Au	7.3545109	-2.2318929	-0.3012965
N	10.4893275	-2.0038028	-0.4706759
N	7.2748250	0.2718064	1.6035441
N	4.2190154	-2.4601061	-0.1468156
N	7.4328194	-4.7429459	-2.1978224
C	9.3417730	-2.0872780	-0.4071639
C	7.3036279	-0.6435275	0.9044145
C	5.3669777	-2.3756567	-0.2006615
C	7.4049444	-3.8233872	-1.5039010

Trimer in Fig. 12 (right)

Au	7.2505960	2.7443144	4.0837430
N	10.3909497	2.9400454	3.9490608
N	7.4887714	0.3803879	6.1509375
N	4.1117157	2.4996608	4.1591472
N	7.0160196	5.0513219	1.9532589
C	9.2417105	2.8692008	3.9991608
C	7.4012580	1.2460792	5.3951640
C	5.2604250	2.5893111	4.1328667
C	7.1014421	4.2090342	2.7352988
Au	7.0263293	7.1621597	8.2090558
N	3.8953388	6.8641159	8.3389839
N	6.8758673	9.6571123	10.1191432
N	10.1579406	7.4491620	8.0743866
N	7.1820104	4.6772043	6.2872191
C	5.0413808	6.9743158	8.2923225
C	6.9308321	8.7429316	9.4211275
C	9.0114151	7.3457170	8.1243884
C	7.1237410	5.5848934	6.9933349
Au	6.7820991	11.6775474	12.2487435
N	9.9209645	11.9187466	12.1706830
N	6.5457137	14.0272741	10.1654329
N	3.6417052	11.4919140	12.3891387
N	7.0154575	9.3760798	14.3855961
C	8.7721706	11.8304476	12.1972457
C	6.6322758	13.1666246	10.9270696
C	4.7911453	11.5573167	12.3365508
C	6.9305619	10.2184123	13.6035922