

Supporting Information

To the paper entitled

Geometrically unprecedented 3-, 5- and 7-membered Hg(II)-Cu(I) and Hg(II)-Ag(I) thiolate clusters : Precursors to intermetallics

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Table S1: Atomic coordinates of optimized structure of 2.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	15	4.849268	1.293220	-1.392761
2	29	3.528041	-0.020680	-0.032194
3	6	3.800894	2.293448	-2.590755
4	6	5.964880	0.175373	-2.403106
5	6	6.560055	-0.539160	1.613946
6	15	4.888225	-1.323414	1.308973
7	16	1.977864	-1.148239	-1.245127
8	16	1.938230	1.063321	1.169793
9	6	4.103829	-1.578887	2.994256
10	6	5.174127	-3.031826	0.597032
11	6	2.736063	-1.852896	3.106014
12	6	2.158230	-2.115526	4.352294
13	6	2.945495	-2.093917	5.508652
14	80	0.000600	-0.093784	-0.030583
15	6	4.943451	-4.180261	1.366279
16	6	5.208308	-5.450430	0.842371
17	6	5.718733	-5.583835	-0.453452
18	16	-1.967319	1.041920	-1.192211
19	6	6.649834	0.600091	2.423224
20	16	-1.928666	-1.346751	1.066088
21	6	7.890559	1.188209	2.690039
22	6	9.058144	0.631311	2.156820
23	29	-3.513405	-0.200225	-0.083003
24	6	5.450574	-0.544443	-3.490577
25	6	6.267636	-1.407001	-4.229750
26	15	-4.544806	-1.551239	-1.646669
27	6	-5.438394	-3.044427	-0.960115
28	15	-5.145229	0.952369	1.084639
29	6	-5.640511	-0.459804	-2.698065
30	6	-4.789657	1.160090	2.911903
31	6	-5.382733	2.691735	0.426223
32	6	7.615134	-1.563654	-3.886056
33	6	4.028556	3.667562	-2.756881
34	6	3.251468	4.425609	-3.639741
35	6	2.222571	3.818905	-4.367810
36	6	5.879954	2.558502	-0.472061
37	6	7.018365	3.117084	-1.073115
38	6	7.767646	4.098841	-0.415627

39	6	7.363978	4.561024	0.841973
40	6	-6.484983	-3.644393	-1.674744
41	6	-7.133699	-4.778064	-1.172511
42	6	-6.714469	-5.346731	0.035551
43	6	-5.049012	0.428372	-3.608595
44	6	-5.838757	1.276833	-4.391961
45	6	-7.232108	1.255876	-4.259636
46	6	-3.228565	-2.320684	-2.746948
47	6	-2.139091	-2.983460	-2.166622
48	6	-1.144455	-3.562321	-2.961715
49	6	-1.244391	-3.506552	-4.356223
50	6	-5.352188	3.805784	1.275893
51	6	-5.577331	5.091547	0.771844
52	6	-5.853527	5.275865	-0.587108
53	6	-3.598577	1.764486	3.327398
54	6	-3.368576	2.040655	4.678590
55	6	-4.327845	1.693469	5.636064
56	6	-6.793097	0.072436	0.954668
57	6	-6.914999	-1.234136	1.442389
58	6	-8.136841	-1.911218	1.372645
59	6	-9.257603	-1.273657	0.828424
60	6	8.979902	-0.528947	1.378725
61	6	7.736682	-1.117307	1.119874
62	6	5.950183	-4.442195	-1.228028
63	6	5.670962	-3.177014	-0.702961
64	6	4.316925	-1.835827	5.406457
65	6	4.892860	-1.596686	4.153563
66	6	8.137392	-0.853773	-2.799467
67	6	7.314572	0.007240	-2.065017
68	6	6.204477	4.043167	1.428981
69	6	5.470262	3.051302	0.770605
70	6	1.985912	2.448866	-4.212623
71	6	2.774313	1.696450	-3.335384
72	6	-2.355311	-2.892896	-4.945611
73	6	-3.347012	-2.315807	-4.143771
74	6	-5.628946	-4.791130	0.722343
75	6	-4.987005	-3.656439	0.214747
76	6	-7.828301	0.385875	-3.339936
77	6	-7.034582	-0.465285	-2.562995
78	6	-9.152764	0.045158	0.371706
79	6	-7.926604	0.716808	0.441382
80	6	-5.898328	4.168290	-1.440275
81	6	-5.661103	2.888584	-0.930552
82	6	-5.519260	1.082476	5.231924
83	6	-5.753631	0.832648	3.875405
84	6	1.980344	-2.943954	-1.192451
85	6	1.374672	-3.668338	-0.156053
86	6	1.347583	-5.067257	-0.185262
87	6	1.906263	-5.758557	-1.265203
88	6	1.884274	2.847173	0.914666
89	6	1.532956	3.421493	-0.313712
90	6	1.488172	4.812128	-0.462322
91	6	1.794632	5.646065	0.617746
92	6	-1.995952	-1.290830	2.860601
93	6	-0.975111	-0.706185	3.624205
94	6	-1.008349	-0.757954	5.022641
95	6	-2.065598	-1.395967	5.678846
96	6	-2.014540	2.819964	-0.925512
97	6	-1.623444	3.406417	0.285172
98	6	-1.644273	4.795686	0.446191
99	6	-2.026735	5.618522	-0.617661

100	6	2.492333	-5.042815	-2.314710
101	6	2.530019	-3.644484	-2.276408
102	6	2.131560	5.081497	1.852524
103	6	2.166720	3.690198	2.000519
104	6	-2.392899	5.043210	-1.839108
105	6	-2.390565	3.651845	-1.989805
106	6	-3.091488	-1.978166	4.926634
107	6	-3.050420	-1.931343	3.528939
108	1	2.114745	-1.888213	2.206033
109	1	1.089441	-2.354758	4.420781
110	1	2.493281	-2.304060	6.487506
111	1	4.559818	-4.092687	2.390064
112	1	5.020628	-6.344638	1.452370
113	1	5.929060	-6.580775	-0.864063
114	1	5.737712	1.023349	2.862992
115	1	7.948285	2.082786	3.324464
116	1	10.033387	1.092470	2.364175
117	1	4.392685	-0.457300	-3.760082
118	1	5.845887	-1.974227	-5.070743
119	1	8.255236	-2.249559	-4.457480
120	1	4.815318	4.173920	-2.186189
121	1	3.439752	5.502403	-3.749598
122	1	1.601741	4.414228	-5.050978
123	1	7.316037	2.799200	-2.080813
124	1	8.659689	4.522822	-0.896729
125	1	7.943415	5.339345	1.356973
126	1	-6.791673	-3.235374	-2.645696
127	1	-7.959712	-5.232859	-1.736259
128	1	-7.215984	-6.241983	0.427718
129	1	-3.955686	0.475525	-3.693834
130	1	-5.362769	1.974295	-5.094526
131	1	-7.853622	1.932371	-4.861999
132	1	-2.065373	-3.067960	-1.076503
133	1	-0.294430	-4.073665	-2.490919
134	1	-0.468796	-3.967149	-4.983223
135	1	-5.162442	3.681598	2.348443
136	1	-5.545560	5.957773	1.446821
137	1	-6.033865	6.284776	-0.982412
138	1	-2.850143	2.044250	2.580270
139	1	-2.434117	2.528951	4.986022
140	1	-4.147676	1.904506	6.698926
141	1	-6.044724	-1.720371	1.897768
142	1	-8.217495	-2.937709	1.754444
143	1	-10.219449	-1.801566	0.774196
144	1	9.895316	-0.981981	0.973822
145	1	7.692752	-2.034953	0.521602
146	1	6.344563	-4.536462	-2.248895
147	1	5.853499	-2.286079	-1.309756
148	1	4.946397	-1.847063	6.306926
149	1	5.976716	-1.442091	4.085144
150	1	9.190216	-0.981806	-2.513029
151	1	7.734994	0.540435	-1.205885
152	1	5.869511	4.412469	2.407768
153	1	4.564388	2.656833	1.239091
154	1	1.176578	1.963541	-4.774898
155	1	2.562787	0.627694	-3.230855
156	1	-2.456493	-2.876530	-6.039618
157	1	-4.226834	-1.869872	-4.623157
158	1	-5.272013	-5.251689	1.653661
159	1	-4.117997	-3.247637	0.742019
160	1	-8.919903	0.379565	-3.216600

161	1	-7.513156	-1.125886	-1.831946
162	1	-10.033677	0.554769	-0.042221
163	1	-7.861887	1.752881	0.088523
164	1	-6.117819	4.300566	-2.508359
165	1	-5.708365	2.022225	-1.594556
166	1	-6.281856	0.820211	5.978063
167	1	-6.713547	0.397404	3.572995
168	1	0.893501	-3.155381	0.684902
169	1	0.871669	-5.622692	0.634534
170	1	1.879023	-6.856467	-1.292492
171	1	1.268293	2.791283	-1.170487
172	1	1.195949	5.249625	-1.426000
173	1	1.753748	6.737600	0.500995
174	1	-0.122810	-0.209576	3.144964
175	1	-0.198602	-0.298311	5.606022
176	1	-2.092612	-1.435694	6.776332
177	1	-1.268939	2.786993	1.116833
178	1	-1.334159	5.240641	1.401453
179	1	-2.030034	6.710504	-0.497548
180	1	2.925965	-5.579482	-3.169814
181	1	2.989003	-3.099738	-3.113032
182	1	2.361473	5.730390	2.708966
183	1	2.425422	3.262627	2.979264
184	1	-2.687915	5.684828	-2.680864
185	1	-2.681921	3.217273	-2.955946
186	1	-3.926694	-2.480285	5.433992
187	1	-3.856102	-2.415835	2.962772

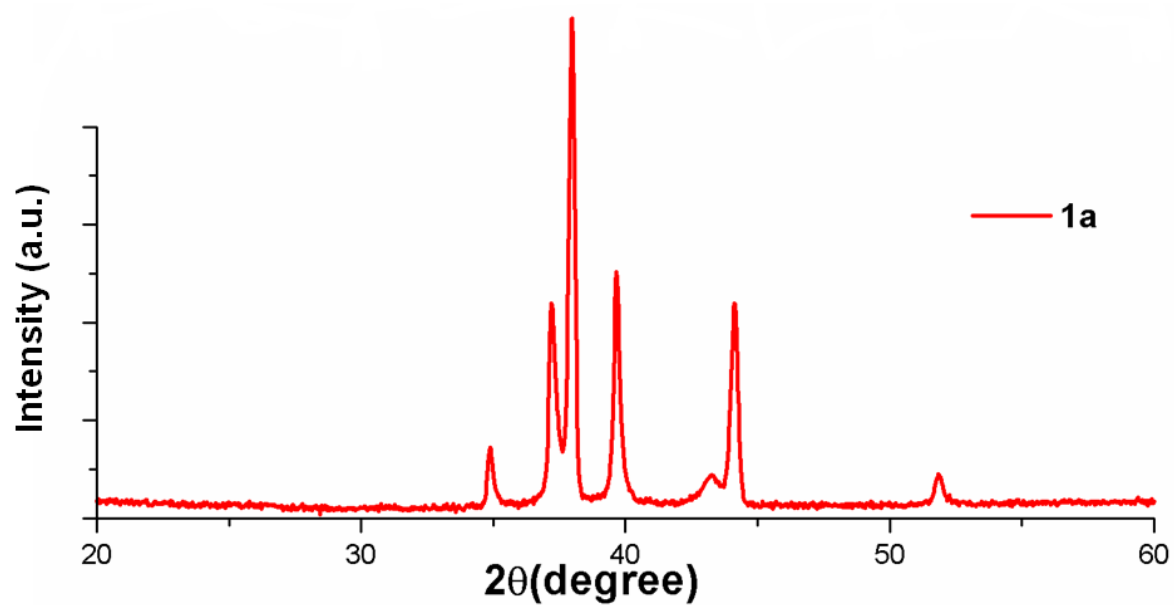


Figure S1: Powder XRD patterns of **1a**.

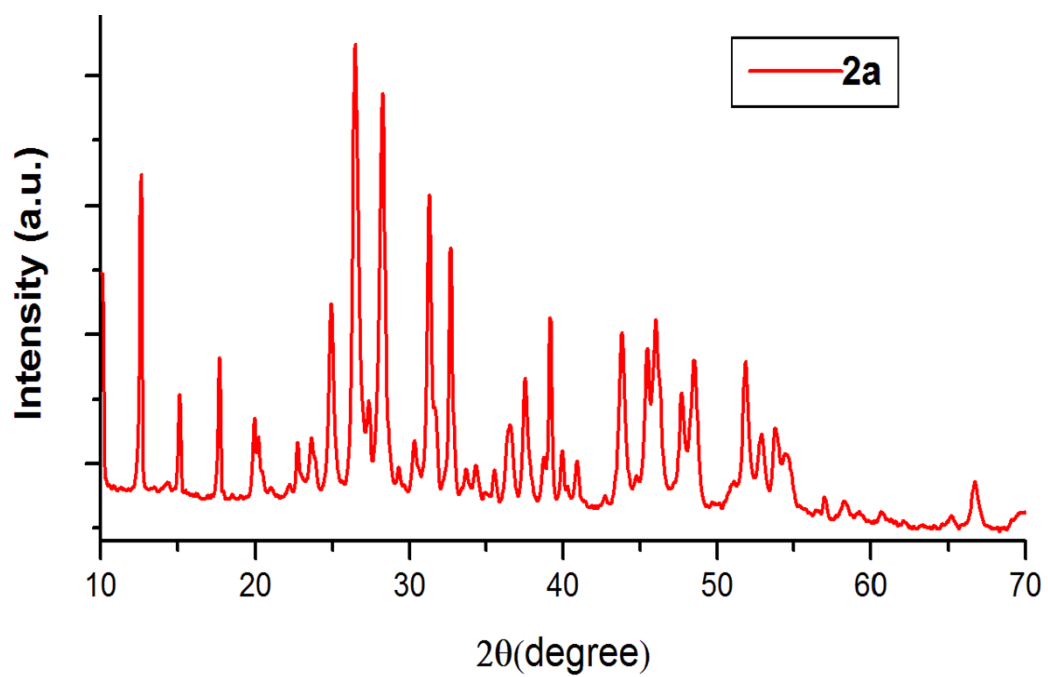


Figure S2: Powder XRD patterns of **2a**.

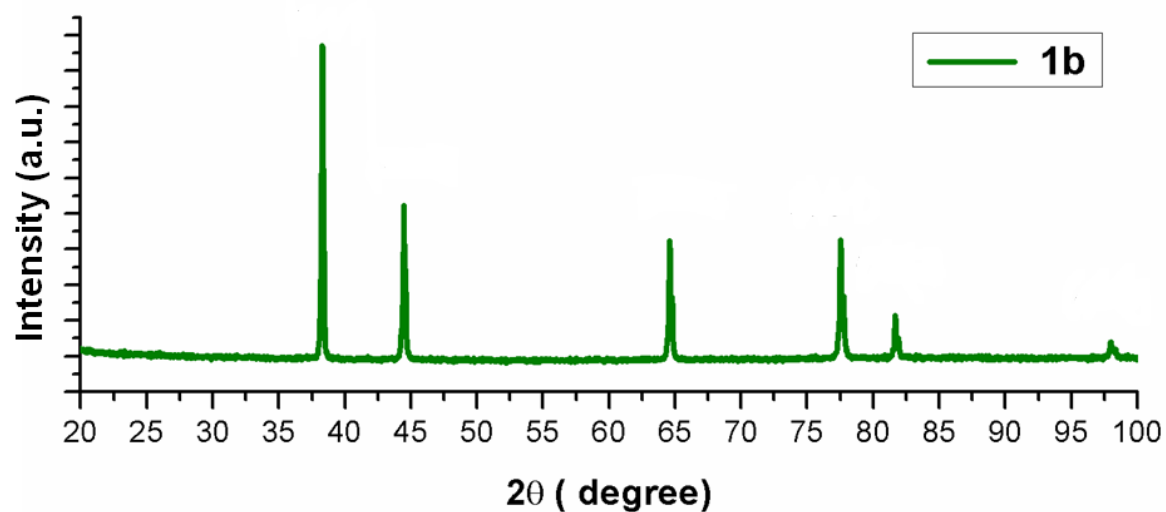


Figure S3: Powder XRD pattern of **1b**

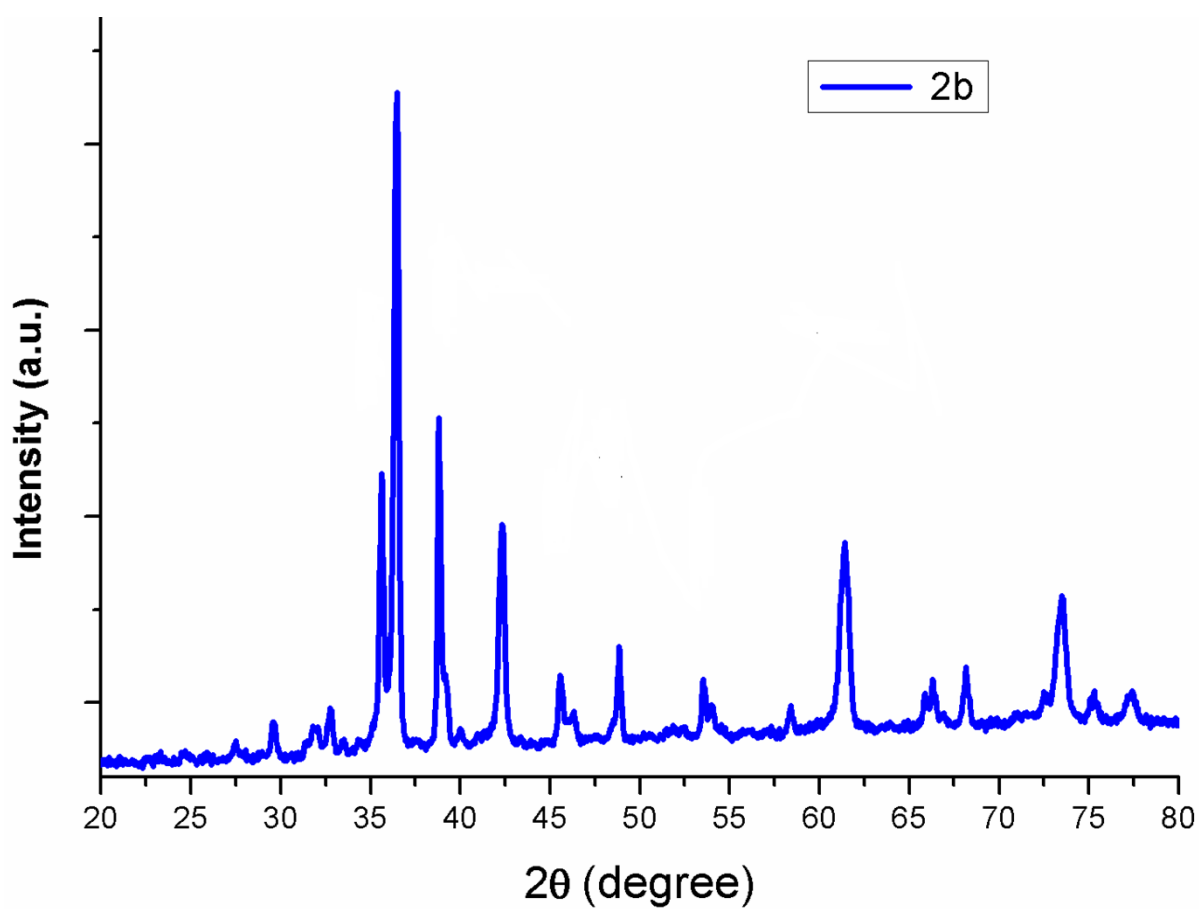


Figure S4: Powder XRD pattern of **2b**

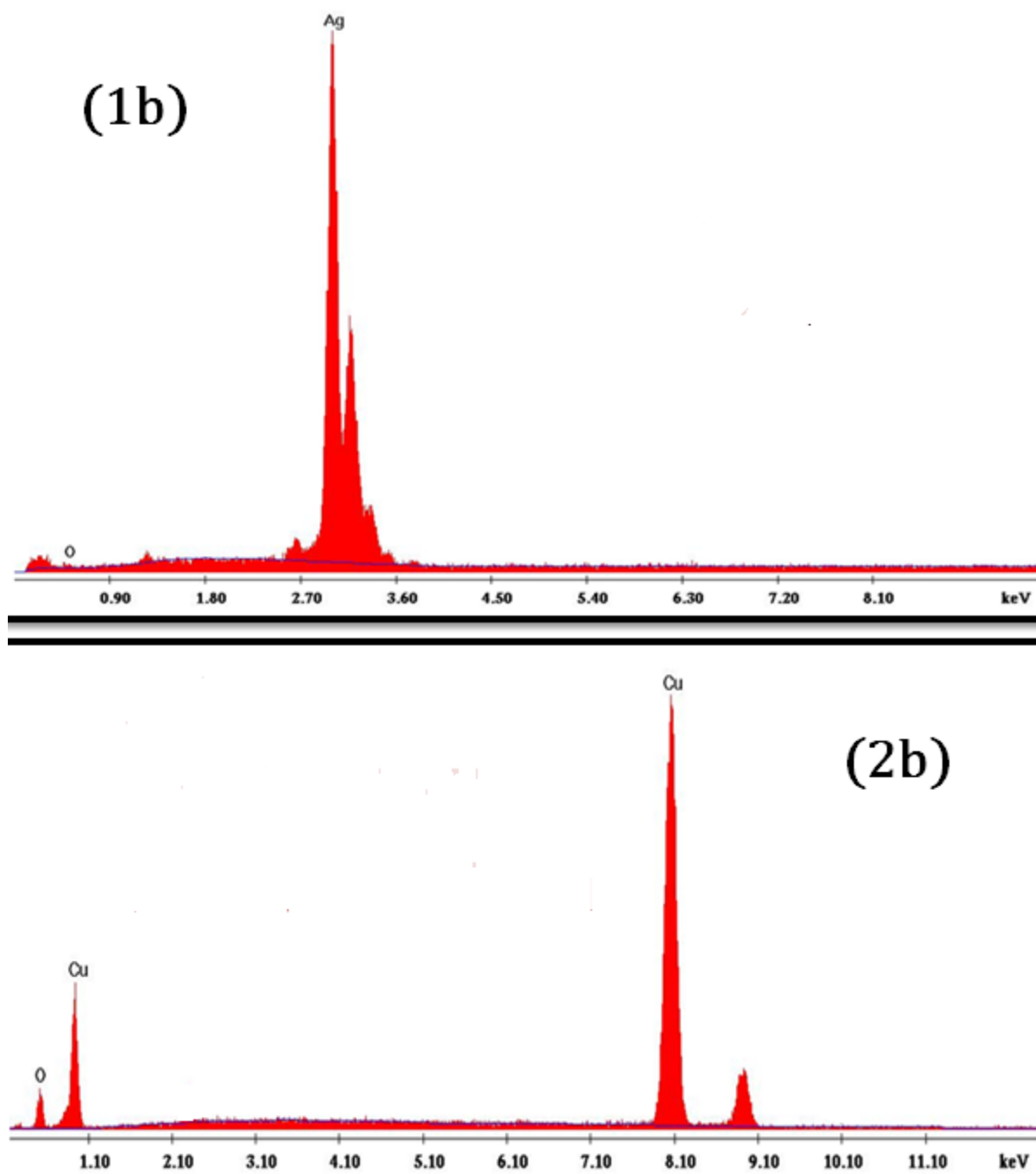


Figure S5: EDS images of 1b and 2b