Supplementary material

A new heterometallic multiligand 3D coordination polymer: synthesis and structure of $[Pb(OH)]_n[Ag(SCN)(CN)]_n$.

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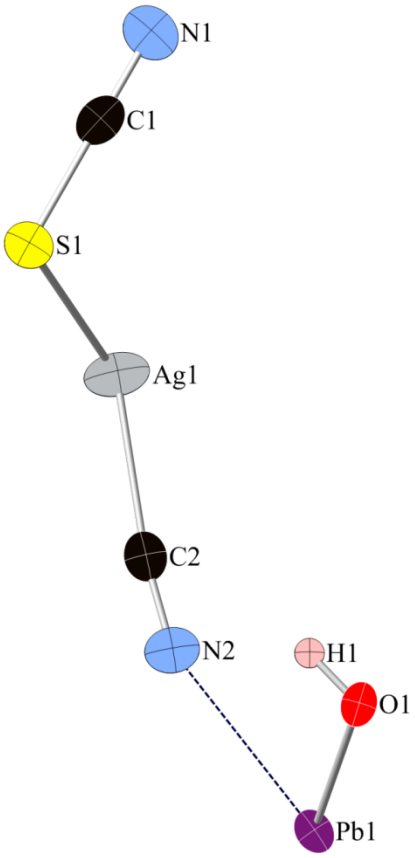

Figure S1. ORTEP plot (thermal ellipsoids at 50% of probability) of asymmetric unit with atom labeling.

Table S1. Crystal data and structure refinement for $[Pb(OH)]_n[Ag(SCN)(CN)]_n$.	
Empirical formula	C_2 H Ag N_2 O Pb S
Formula weight	416.17
Temperature	293(2) K
Wavelength	0.71073 Å 0 0.71073 Å
Crystal system, space group	orthorhombic, Pnma
Unit cell dimensions .	a = 21.8268(5) Å b = 3.9863 (1) Å c = 7.1628(2) Å
Volume	623.22(3) $Å^3$
Z, Calculated density	4, 4.435 g/cm^3
Absorption coefficient	30.350 mm^{-1}
F(000)	720
Crystal size	0.04 x 0.05 x 0.21 mm
Theta range for data collection	3.40 to 32.67 deg.
Limiting indices	-32<=h<=32, -5<=k<=6, -10<=l<=10
Reflections collected / unique	12721 / 1241 [R(int) = 0.0547]
Completeness to theta = 32.67	96.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1241 / 1 / 53
Goodness-of-fit on F2	1.092
Final R indices [I>2σ(I)]	R1 = 0.0245, wR2 = 0.0578
R indices (all data)	R1 = 0.0302, wR2 = 0.0608
Extinction coefficient	0.0019(2)
Largest diff. peak and hole	1.370 and -1.638 e $Å^3$

Table S2. Bond lengths [Å] and angles [deg]		
	Exper.	Computed
Pb(1)-O(1)	2.390(4)	2.404
Pb(1)-O(1)#1	2.419(3)	2.452
Pb(1)-O(1)#2	2.419(3)	2.452
Pb(1)-N(2)	2.639(7)	2.598
Ag(1)-C(2)	2.118(8)	2.106
Ag(1)-S(1)	2.6077(14)	2.643
Ag(1)-S(1)#3	2.6077(14)	2.643
Ag(1)-S(1)#4	2.712(2)	2.891
S(1)-C(1)	1.654(8)	1.667
S(1)-Ag(1)#5	2.6077(14)	2.643
S(1)-Ag(1)#6	2.712(2)	2.891
C(1)-N(1)	1.159(10)	1.168
C(2)-N(2)	1.119(9)	1.162
O(1)-Pb(1)#1	2.419(3)	2.452
O(1)-Pb(1)#2	2.419(3)	2.452
O(1)-H(1)	0.817(10)	0.968
O(1)-Pb(1)-O(1)#1	71.35(12)	71.85
O(1)-Pb(1)-O(1)#2	71.35(12)	71.85
O(1)#1-Pb(1)-O(1)#2	110.99(19)	108.15
O(1)-Pb(1)-N(2)	113.75(19)	109.20
O(1)#1-Pb(1)-N(2)	72.59(13)	70.84
O(1)#2-Pb(1)-N(2)	72.59(13)	70.84
C(2)-Ag(1)-S(1)	124.05(8)	127.46
C(2)-Ag(1)-S(1)#3	124.05(8)	127.46
S(1)-Ag(1)-S(1)#3	99.70(7)	97.55
C(2)-Ag(1)-S(1)#4	102.07(19)	102.27
S(1)-Ag(1)-S(1)#4	101.28(4)	100.10

S(1)#3-Ag(1)-S(1)#4	101.28(4)	100.10
C(1)-S(1)-Ag(1)	103.75(16)	102.27

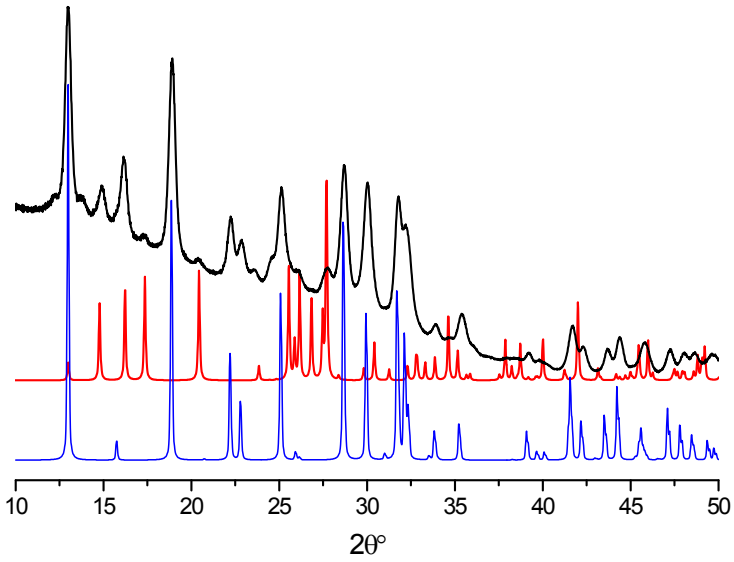

Figure S2. XRPD patterns for compounds **1** (black, experimental; red, simulated) and of Pb(OH)(NCS) (blue, simulated)

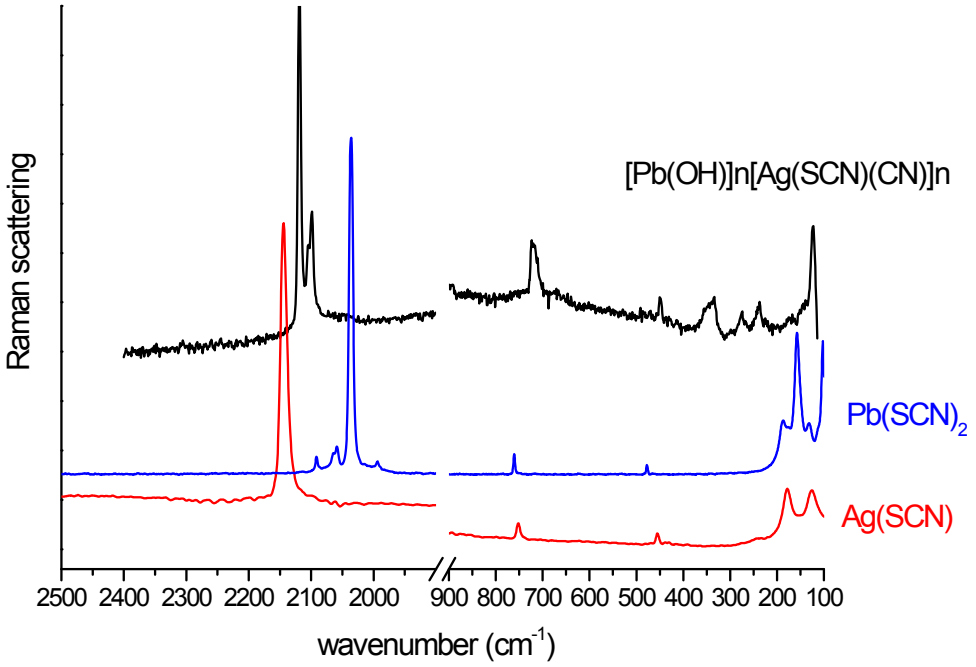

Fig. S3 Raman spectra of crystalline **1** compared with spectra of $Pb(SCN)_2$ and Ag(SCN)

computed frequency		computed intensities	assignment	Infrared (exp.)	raman (exp.)
3782	(B_{1u})	(407.14)	ν(O-H)	3557 s	3563 vw
3782	(B_{3g})	(0.00)	ν(O-H)		
3782	(B_{2u})	(314.26)	ν(O-H)		
3781	(A_g)	(0.00)	ν(O-H)		
2236	(B_{1u})	(186.97)	ν(CN)	2111 vs	2122 vs
2236	(A_g)	(0.00)	ν(CN)		
2235	(B_{3g})	(0.00)	ν(CN)		
2232	(B_{2u})	(572.95)	ν(CN)		
2201	(B_{3g})	(0.00)	νS(CN)	2085 vs	2092 s
2190	(A_g)	(0.00)	νS(CN)		
2190	(B_{1u})	(755.04)	νS(CN)		
2189	(B_{2u})	(2714.73)	νS(CN)		
793,0	(B_{3g})	(0.00)	ρ(OH)	740 w	750 m
792,5	(A_g)	(0.00)	ρ(OH)		
790,6	(B_{1u})	(417.32)	ρ(OH)		
789,0	(B_{2u})	(156.33)	ρ(OH)		
743,0	(A_g))	(0.00)	ν(SC)N	726 m	735 w
742,0	(B_{1u})	(0.07)	ν(SC)N		
740,3	(B_{2u})	(38.67)	ν(SC)N		
740,0	(B_{3g})	(0.00)	ν(SC)N		
708,8	(B_{2g})	(0.00)	δ(OH)	682 w	

708,8	(B_{1g})	(0.00)	δ(OH)	648 w	
705,2	(B_{3u})	(1054.99)	δ(OH)		
705,1	(A_u)	(0.00)	δ(OH)		
466,3	(B_{3u})	(45.33)	δ(SCN)	480 m 448 m	460 m 490 m
466,2	(B_{2g})	(0.00)	δ(SCN)		
465,4	(A_u)	(0.00)	δ(SCN)		
465,4	(B_{1g})	(0.00)	δ(SCN)		
459,9	(B_{1u})	(30.22)	δ(SCN)		
459,5	(A_g)	(0.00)	δ(SCN)		
458,0	(B_{2u})	(13.31)	δ(SCN)		
457,7	(B_{3g})	(0.00)	δ(SCN)		
401,5	(B_{1u})	(9.53)	ν(Ag-CN-Pb)	380 m 364 m	380 m 345 m-w
384,5	(B_{2u})	(508.38)	ν(Ag-CN-Pb)		
378,3	(A_g)	(0.00)	ν(Ag-CN-Pb)		
377,7	(B_{3g})	(0.00)	ν(Ag-CN-Pb)		
349,6	(A_g)	(0.00)	ν(Ag-CN-Pb)		
349,2	(B_{3g})	(0.00)	ν(Ag-CN-Pb)		
331,2	(B_{1u})	(52.84)	ν(O-Pb)	310 m 292 m	294 w
329,9	(B_{1g})	(0.00)	ν(O-Pb)		
329,8	(B_{2g})	(0.00)	ν(O-Pb)		
325,9	(B_{2u})	(170.32)	ν(O-Pb)		
317,3	(B_{1u})	(451.73)	ν(O-Pb)		
315,9	(B_{2u})	(55.61)	ν(O-Pb)		
281,9	(A_u)	(0.00)	ν(O-Pb)		
281,6	(B_{3u})	(410.41)	ν(O-Pb)		
276,8	(B_{3g})	(0.00)	ν(O-Pb)		
276,7	(A_g)	(0.00)	ν(O-Pb)		
251,5	(B_{3g})	(0.00)	δ(CN)	236 m	
248,5	(A_g)	(0.00)	δ(CN)		
246,4	(B_{1g})	(0.00)	δ(CN)		
245,2	(B_{2g})	(0.00)	δ(CN)		
240,9	(B_{2u})	(4.23)	δ(CN)		
237,2	(B_{1u})	(82.30)	δ(CN)		
233,1	(A_u)	(0.00)	δ(CN)		
232,3	(B_{3u})	(103.11)	δ(CN)		
197,3	(B_{3g})	(0.00)	ν(S-Ag)		
192,4	(B_{2u})	(30.98)	ν(S-Ag)		
179,7	(A_g)	(0.00)	ν(S-Ag)		
171,1	(B_{1g})	(0.00)	ν(S-Ag)		
170,8	(B_{1u})	(0.14)	ν(S-Ag)		
168,4	(B_{3g})	(0.00)	ν(S-Ag)		
163,8	(B_{2g})	(0.00)			
161,1	(A_g)	(0.00)			
159,0	(A_u)	(0.00)	ν(S-Ag)		
142,4	(B_{1u})	(30.47)	ν(S-Ag)		147 s (sh)
142,1	(B_{2u})	(3.70)	ν(S-Ag)		

139,5	(B_{3u})	(70.97)			
137,3	(B_{3g})	(0.00)			
137,2	(A_g)	(0.00)			
132,8	(B_{1g})	(0.00)			
126,9	(B_{3g})	(0.00)			
124,2	(B_{2u})	(14.67)			
123,3	(B_{2g})	(0.00)			
122,9	(B_{1u})	(179.53)			
118,7	(B_{3u})	(159.11)			
116,2	(B_{2u})	(75.71)			
113,5	(A_u)	(0.00)			
113,3	(B_{3g})	(0.00)			
113,0	(A_g)	(0.00)			
99,72	(B_{1u})	(293.21)			
97,75	(B_{1g})	(0.00)			
95,04	(A_g)	(0.00)			
90,64	(A_u)	(0.00)			
89,90	(A_g)	(0.00)			
88,46	(B_{2g})	(0.00)			
81,26	(B_{1u})	(0.00)			
78,80	(B_{3u})	(697.40)			
78,65	(B_{2u})	(120.32)			
77,43	(B_{3g})	(0.00)			
61,30	(B_{1g})	(0.00)			
61,27	(B_{2g})	(0.00)			
57,31	(B_{2u})	(1.21)			
53,98	(B_{3g})	(0.00)			
53,46	(B_{1u})	(4.83)			
49,86	(B_{3g})	(0.00)			
42,90	(A_g)	(0.00)			
37,31	(B_{1u})	(0.36)			
36,60	(A_g)	(0.00)			
26,48	(B_{3u})	(2.75)			
25,30	(B_{2u})	(0.26)			
21,47	(A_u)	(0.00)			
20,41	(B_{1g})	(0.00)			
19,98	(B_{2g})	(0.00)			
18,74	(A_u)	(0.00)			

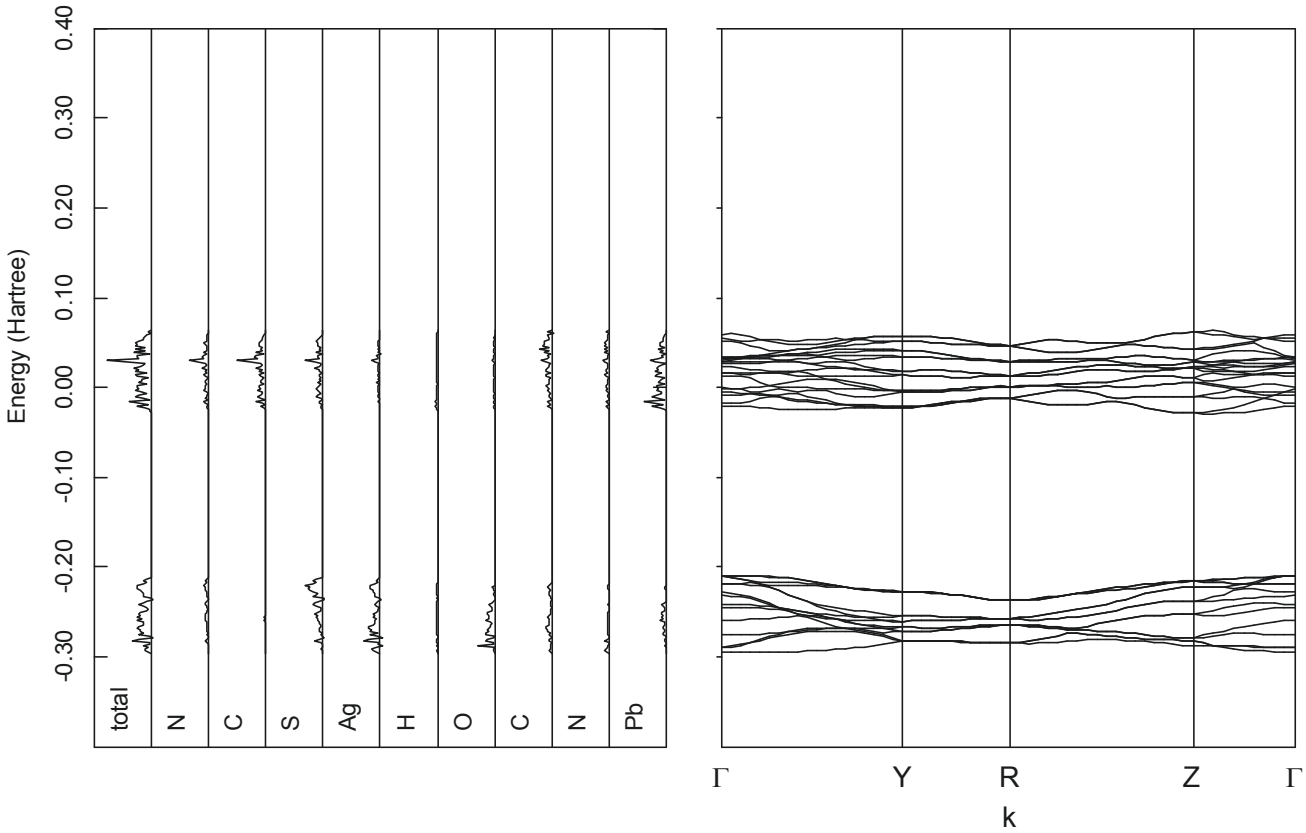

Figure S4: computed density of states of **1**, along the path Γ→Y→R→Z→Γ in the Brillouin zone

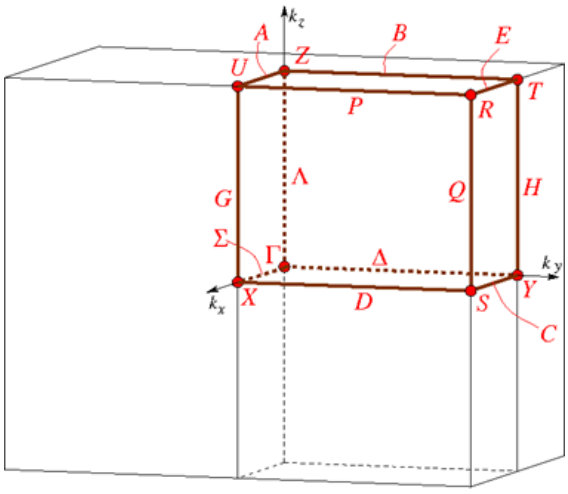

Figure S5: the Brillouin zone of **1**.