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Supporting Information

TABLE S1

Concentration of Cu, S and Se in the References and Sample

	Cu	S	Se	Cu/(S+Se)	Se/(S+Se)
	(wt. %)	(wt. %)	(wt. %)	mole ratio	
β CuSCN	50	28.1	.	0.9	0
α CuSeCN	39		31.3	1.5	1
CuS _{0.95} Se _{0.05} CN	49	24.0	3.0	1.0	0.05
Sludge ¹	39	11.4	2.7	1.6	0.09

1- [C]=17.7; [N]=4.2; [Cl]=3.48; [H]=2.2 wt. %

Supporting Information

TABLE S2

Crystallographic Data for the Sludge and Reference Samples

Sample	Phase ¹	Unit-cell parameters (Å)	hkl reflections ³
β CuSCN	β CuSCN	$a=b=3.857$ ($\sigma=0.005$) ²	003, 101, 006, 104,
	trace of α CuSCN	$c=16.45$ ($\sigma=0.02$) ²	015, 110, 107, 113,
		$\alpha=\beta=90^\circ$, $\gamma=120^\circ$	018, 021, 116, 024,
			1010, 0111, 027
α CuSeCN	α CuSeCN	$a=7.62$ ($\sigma=0.02$)	020, 120, 121, 002,
		$b=11.26$ ($\sigma=0.02$)	211, 112, 213
		$c=6.95_6$ ($\sigma=0.007$)	
		$\alpha=\beta=\gamma=90^\circ$	
$\text{CuS}_{0.95}\text{Se}_{0.05}\text{CN}^4$	$\alpha\text{Cu}(\text{S},\text{Se})\text{CN}$	$a=7.287$ ($\sigma=0.008$)	020, 120, 121, 211,
	$\beta\text{Cu}(\text{S},\text{Se})\text{CN}$	$b=11.06$ ($\sigma=0.01$)	141, 321, 004
		$c=6.68_0$ ($\sigma=0.005$)	
		$\alpha=\beta=\gamma=90^\circ$	
Sludge	$\alpha\text{Cu}(\text{S},\text{Se})\text{CN}$	$a=7.31$ ($\sigma=0.01$)	020, 120, 002, 211,
		$b=11.09$ ($\sigma=0.01$)	112, 140, 141, 132,
		$c=6.73$ ($\sigma=0.01$)	321
		$\alpha=\beta=\gamma=90^\circ$	

1- Nature of phases identified by XRD

2- Theoretical values: $a = b = 3.857\text{\AA}$, $c = 16.449\text{\AA}$ (After JCPDS card 29-581)

3- Used to determine unit-cell parameters

4- Unit cell parameters for the α component

Supporting Information

TABLE S3

Interatomic Distances in Copper(I) Thiocyanates. From (21, 33).

Central atom	Atomic shell	Number of atoms	β CuSCN (Å)	α CuSCN (Å)
Cu	N	1	1.93	1.93
	S	3	2.34	2.35-2.37
	C	1	3.03	3.02
	C	3	3.30	3.19-3.23
	Cu	6	3.85	3.59-4.28
S	C	1	1.70	1.70
	Cu	3	2.34	2.35
	N	1	2.80	2.81
	N	3	3.47	3.43-3.62
	S	6	3.85	3.69-3.85