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## Supporting Information

**TABLE S1**

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

| | Cu (wt. %) | S (wt. %) | Se (wt. %) | Cu/(S+Se) mole ratio | Se/(S+Se) |
|---|---|---|---|---|---|
| βCuSCN | 50 | 28.1 | | 0.9 | 0 |
| αCuSeCN | 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. %

**TABLE S2**

**Crystallographic Data for the Sludge and Reference Samples**

| Sample | Phase[1] | Unit-cell parameters (Å) | hkl reflections [3] |
|---|---|---|---|
| βCuSCN | βCuSCN | a=b=3.85$_7$ (σ=0.005)[2] | 003, 101, 006, 104, |
| | trace of αCuSCN | c=16.45 (σ=0.02)[2] | 015, 110, 107, 113, |
| | | α=β=90°, γ=120° | 018, 021, 116, 024, |
| | | | 1010, 0111, 027 |
| αCuSeCN | αCuSeCN | a=7.62 (σ=0.02) | 020, 120, 121, 002, |
| | | b=11.26 (σ=0.02) | 211, 112, 213 |
| | | c=6.95$_6$ (σ=0.007) | |
| | | α=β=γ=90° | |
| $CuS_{0.95}Se_{0.05}CN$[4] | αCu(S,Se)CN | a=7.28$_7$ (σ=0.008) | 020, 120, 121, 211, |
| | βCu(S,Se)CN | b=11.06 (σ=0.01) | 141, 321, 004 |
| | | c=6.68$_0$ (σ=0.005) | |
| | | α=β=γ=90° | |
| Sludge | αCu(S,Se)CN | a=7.31 (σ=0.01) | 020, 120, 002, 211, |
| | | b=11.09 (σ=0.01) | 112, 140, 141, 132, |
| | | c=6.73 (σ=0.01) | 321 |
| | | α=β=γ=90° | |

1- Nature of phases identified by XRD

2- Theoretical values: a = b = 3.857Å, c = 16.449 Å (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 | βCuSCN (Å) | αCuSCN (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 |