Electronic supplementary information

Two-dimensional copper thio- and seleno-cyanates

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Table S1 Fractional coordinates of atoms in the orthorhombic unit cell (a = 6.83 Å, b = 4.28 Å, c = 11.15 Å) of γ-CuSCN.

Atom	x	y	z
Cu	0.0000	0.5000	0.0000
Cu	0.5001	0.3503	1.0000
Cu	0.2497	0.3500	0.5000
Cu	0.7498	0.5004	0.4999
S	0.2192	0.1685	0.9182
S	0.7191	0.6819	0.9183
S	0.0307	0.6821	0.4183
S	0.5307	0.1685	0.4182
C	0.0246	0.6123	0.2716
C	0.5246	0.2381	0.2716
C	0.2251	0.2382	0.7716
C	0.7252	0.6122	0.7716
N	0.0195	0.5753	0.1674
N	0.5195	0.2751	0.1674
N	0.2302	0.2753	0.6674
N	0.7302	0.5753	0.6674

Table S2 Fractional coordinates of atoms in the unit cell of γ-CuSeCN. The lattice vectors are (expressed in Å): (6.74, 0.00, 0.00), (0.00, 4.94, -0.65), (0.00, -1.44, 11.48).

Atom	*x*	*y*	*z*
Cu	0.0000	0.5000	0.0000
Cu	0.5109	0.4353	0.9928
Cu	0.2392	0.4351	0.4927
Cu	0.7506	0.4997	0.4999
Se	0.2355	0.1987	0.8791
Se	0.7343	0.7533	0.9383
Se	0.0160	0.7535	0.4384
Se	0.5149	0.1986	0.3792
C	0.0147	0.6382	0.2740
C	0.5151	0.3140	0.2401
C	0.2354	0.3141	0.7400
C	0.7357	0.6380	0.7739
N	0.0117	0.5770	0.1695
N	0.5145	0.3721	0.1482
N	0.2359	0.3720	0.6481
N	0.7388	0.5767	0.6694

Table S3 Fractional coordinates of atoms in the unit cell of γ′-CuSeCN. The lattice vectors are (expressed in Å): (5.50, 0.00, 0.00), (0.00, 6.43, -0.66), (0.00, -1.74, 11.24).

Atom	*x*	*y*	*z*
Cu	0.0000	0.5000	0.0000
Cu	0.5007	0.4133	0.9872
Cu	0.2325	0.4135	0.4872
Cu	0.7332	0.5002	0.5000
Se	0.1850	0.1918	0.8684
Se	0.6848	0.7219	0.9447
Se	0.0484	0.7220	0.4446
Se	0.5482	0.1919	0.3685
C	0.0513	0.6432	0.2776
C	0.5508	0.2734	0.2248
C	0.1825	0.2734	0.7248
C	0.6820	0.6433	0.7776
N	0.0483	0.6009	0.1712
N	0.5476	0.3164	0.1308
N	0.1858	0.3164	0.6308
N	0.6850	0.6011	0.6712