Supplementary Material (ESI) for Chemical Communications

A New 2D Network Built from Potassium Sandwiches $\{K[Cu^{II}_3(bdap)_3]_2\}$ and $\{(\mu_{1,3}\text{-}SCN)_3Cu^{I}(NCS)\}$ Anions: Structure and Magnetic behaviour.

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Electronic Supplementary Information:

1 Magnetic measurements for **1** were carried out on polycrystalline sample, at the "Servei de Magnetoquímica of the Universitat de Barcelona", with Quantum Design SQUID MPMS-XL susceptometer apparatus working in the range 2-300 K under magnetic field of approximately 10000 G from 300 to 30 K and 500 G from 29 to 2 K. Diamagnetic corrections were estimated from Pascal Tables.

2 Complex **1** with empirical formula $C_{26}H_{54}Cu_7KN_{20}O_6S_8$, crystallizes in the orthorhombic system, space group $Pbc2_1$, with unit cell parameters a = 10.531(1) Å, b = 21.440(1) Å, c = 22.895(1) Å, $\alpha = \beta = \gamma = 90.0$, Z = 4. Good quality crystals of **1**, were selected and mounted on a MAR345 diffractometer with an image plate detector. The accurate unit-cell parameters were determined from automatic centring of 7843 ($3 < \theta < 31^{o}$) and refined by least-squares method. Intensities were collected with graphite monochromated Mo-K_α radiation. 15271 reflections were measured in the range $2.10 \leq \theta \leq 31.79$. 7514 reflections were assumed as observed applying the condition $I > 2\sigma(I)$. Lorentz polarization and absorption corrections were made. The structures were solved by direct methods using the SHELXS computer program and refined by full-matrix least-squares method, using the SHELX97 computer program using 8234 reflections. (Very negative intensities were not assumed). The functions minimised were $\Sigma w\ [|F_o|^2 - |F_c|^2\ ]^2$, where $w = [\sigma^2(I) + (0.0423 \cdot P)^2 + 1.0028\ P]^{-1}$ and $P = (\ |F_o\ |^2 + 2\ |F_c\ |^2)/3$. f, f', and f'' were taken from International Tables of X-Ray Crystallography. All H atoms were computed and refined, using a riding model, with an isotropic temperature factor equal to 1.2 time the equivalent temperature factor of the atom which are linked. The nitrogen atom labelled N(26) corresponding to the thiocyanate ligand is found in disordered position. An occupancy factor of 0.5 was assigned to each position according to the high of the peaks of the Fourier syntheses, and was refined with an overall isotropic temperature factor. The final *R* (on *F*) factor was 0.048; *wR* (on $|Fo\ |^2$) was 0.0865. The number of refined parameters was 622. The maximum and

the minimum peaks in final difference synthesis were 0.411 and –0.394 respectively.