Table S1. Crystal data and structure refinement for the compound.

Compound	
Empirical Formula	$[C_{34}H_{34}ClCuN_6O_2S_2].CH_3CN$
Formula weight	762.84
Temperature (K)	293(2)
Radiation; λ (Å)	λ=0.71073
Crystal system	Triclinic ($P\bar{1}$)
Unit cell dimensions	
a (Å)	11.2752(3)
b (Å)	11.3929(3)
c (Å)	14.6176(4)
α (o)	104.335(2)
β (o)	97.823(2)
γ (o)	98.988(2)
Volume ($Å^3$)	1778.57(8)
Z / density calculated ($g.cm^{-3}$)	1.424
Absorption coefficient (mm^{-1})	0.850
F(000)	792
Crystal size (mm)	0.671 x 0.331 x 0.179
Range for data collection θ (°)	1.46 to 27.19
Index ranges	-14<=h<=12 -14<=k<=14 -18<=l<=18
Reflections collected	47786
Reflections unique	7879
Completeness to theta max.	99.5 %
Absorption correction	Gaussian
Max. and min. transmission	0.9980 and 0.8965
Data/restraints/parameters	7879 / 2 / 442
Goodness-of-fit F^2	1.024
Final *R* indices [$I>2\sigma(I)$]	R1 = 0.0308, wR2 = 0.0701
R indices (all data)	R1 = 0.0435, wR2 = 0.0752
Largest diff. peak and hole	0.440 to -0.325 (e)/$Å^{-3}$

$R1 = \Sigma||Fo|-|Fc||/\Sigma|Fo|$; $wR_2 = \Sigma[w(Fo^2-Fc^2)^2/\Sigma(wFo^2)]^{-1/2}$

Table S2. Hydrogen bonds [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3A)...Cl(1)#1	0.86	2.6300	3.2447(17)	128.8
N(3)-H(3B)...Cl(1)	0.86	2.3700	3.2230(18)	170.9
N(6)-H(6B)...Cl(1)	0.86	2.3700	3.2224(18)	170.1

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z+2

Appendix A.

CCDC 1500585 contains the supplementary crystallographic data for the copper(I) complex. These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB12 1EZ UK; fax: (+44) 1223 336 033.