Supplementary Material for Chemical Communications

Supplementary data

Table 1. Crystal data and structure refinement for $[Cu(IN)_2]\cdot I_2$

Formula	$C_{12}H_8N_2O_4CuI_2$
FW	561.54
Temperature	223(2) K
Wavelength	0.71073
Crystal system	Monoclinic
Space group	$P2_1/n$
Cell dimensions,?	5.795(1) x 12.646(1)x 10.816(1) ß =91.253(1)
V, Å^3	792.4(1)
Z,	2
$?_{calc,}$ gcm^{-3}	2.353
μ , mm^{-1}	5.288
F(000)	522
Crystal size,mm	0.40 x 0.30 x 0.18
Collected ? range	2.48 to 24.99
Index ranges	-6 = h = 6, 0 = k = 15, 0 = l = 12
Reflections collected	4160
Independent reflections	1468 [R(int) = 0.0266)
Refinement method	Full-matrix least-squares on F^2
Goodness-of-fit F^2	1.138
Final R indices [I>4s(I)]	R1 = 0.0232, wR2 = 0.0619
R indices (all data)	R1 = 0.0244, wR2 = 0.0634

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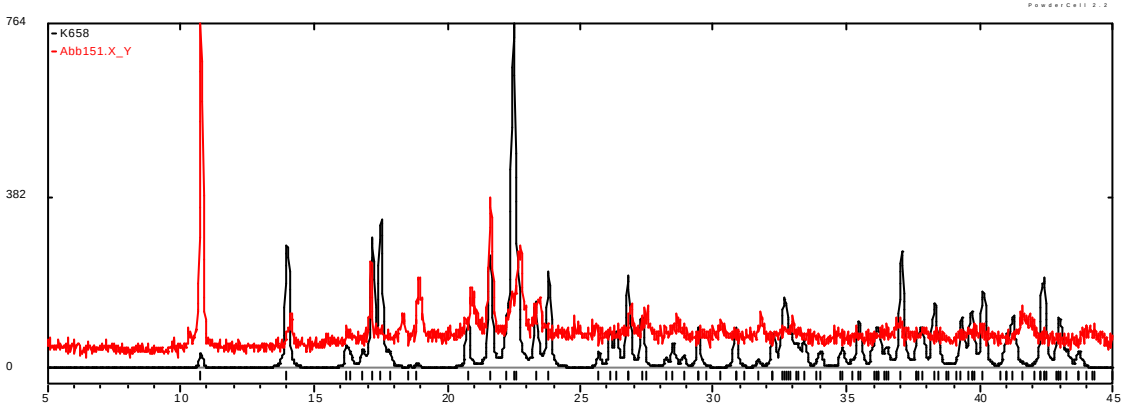
Black color: simulation from as-synthesized single crystal structure of $[Cu(IN)_2]\cdot I_2$; red color: from blue crystals.



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Black color: simulation from as-synthesized single crystal structure of $[Cu(IN)_2]\cdot I_2$; red color: simulation from iodine-removed single crystal structure of $[Cu(IN)_2]\cdot I_2$.