Electronic Supplementary Material (ESI) for Dalton Transactions.
This journal is © The Royal Society of Chemistry 2021

Table S1. Summary of data collection and refinement parameters for reported crystal structures.

Crystal	[c]$Cu(2ip)_2Cl_2$	[c]$Cu(2ip)_2Cl_2$	[d]$Cu(2ip)_2Br_2$	[d]$Cu(2ip)_2Br_2$	Cu(2ip)2Cl2	Cu(2ip)2Br2
Formula	$C_{10}H_8Cl_2CuI_2N_2$	$C_{10}H_8Cl_2CuI_2N_2$	$C_{10}H_8Br_2CuI_2N_2$	$C_{10}H_8Br_2CuI_2N_2$	$C_{10}H_8Cl_2CuI_2N_2$	$C_{10}H_8Br_2CuI_2N_2$
M_r	544.42	544.42	633.34	633.34	544.42	633.34
ρ_{calc} (Mg/m^3)	2.509	2.539	2.774	2.822	2.500	2.760
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*C2/c*	*C2/c*	*C2/c*	*C2/c*	*C2/c*	*C2/c*
a (Å)	15.4157(9)	15.3782(17)	15.5405(17)	15.4484(14)	15.439(1)	15.561(1)
b (Å)	7.7608(4)	7.7571(9)	7.9511(9)	7.9306(7)	7.771(1)	7.963(1)
c (Å)	12.7242(6)	12.6701(14)	12.9193(14)	12.8457(11)	12.731(1)	12.949(1)
β(°)	108.754(3)	109.536(5)	108.214(4)	108.690(3)	108.73(1)	108.16(1)
V($Å^3$)	1441.48(13)	1424.4(3)	1516.4(3)	1490.8(2)	1446.44(7)	1524.46(15)
Temperature (K)	296(2)	150(2)	296(2)	150(2)	298	298
CCDC	2063248	2063249	2063250	2063251	2036457	2036456
ind. Reflections	1747	1724	1681	1671	1473	1538
Data/restraints/ paran	1747/0/80	1724/0/80	1681/0/80	1671/0/80	1473 / 0 / 80	1538 / 0 / 79
R(int)	0.0128	0.0213	0.0676	0.0532	0.0218	0.0223
Z	4	4	4	4	4	4
Goodness of fit	1.097	1.162	1.024	1.071	1.033	1.036
R_1[a] [I> 2σ]	0.0164	0.0117	0.0353	0.0303	0.0237	0.0320
wR_2[b] [I> 2σ]	0.0363	0.0259	0.0652	0.0614	0.0474	0.0706
μ, mm^{-1}	6.148	6.222	10.762	10.947	6.127	10.705
Largest diff. peak/hole / e $Å^{-3}$	0.47/-0.52	0.39/-0.33	0.78/-0.84	0.95/-1.49	0.505 and -0.36	0.559 and -0.944

[a] $R_1 = \Sigma||Fo| - |Fc||/| \Sigma |Fo|$.

[b] $wR_2 = \{ \Sigma w(Fo^2 - Fc^2)^2 / \Sigma w(Fo^2)^2 \}^{1/2}$.

[c] data set were collected using the same crystal.

[d] data set were collected using the same crystal.

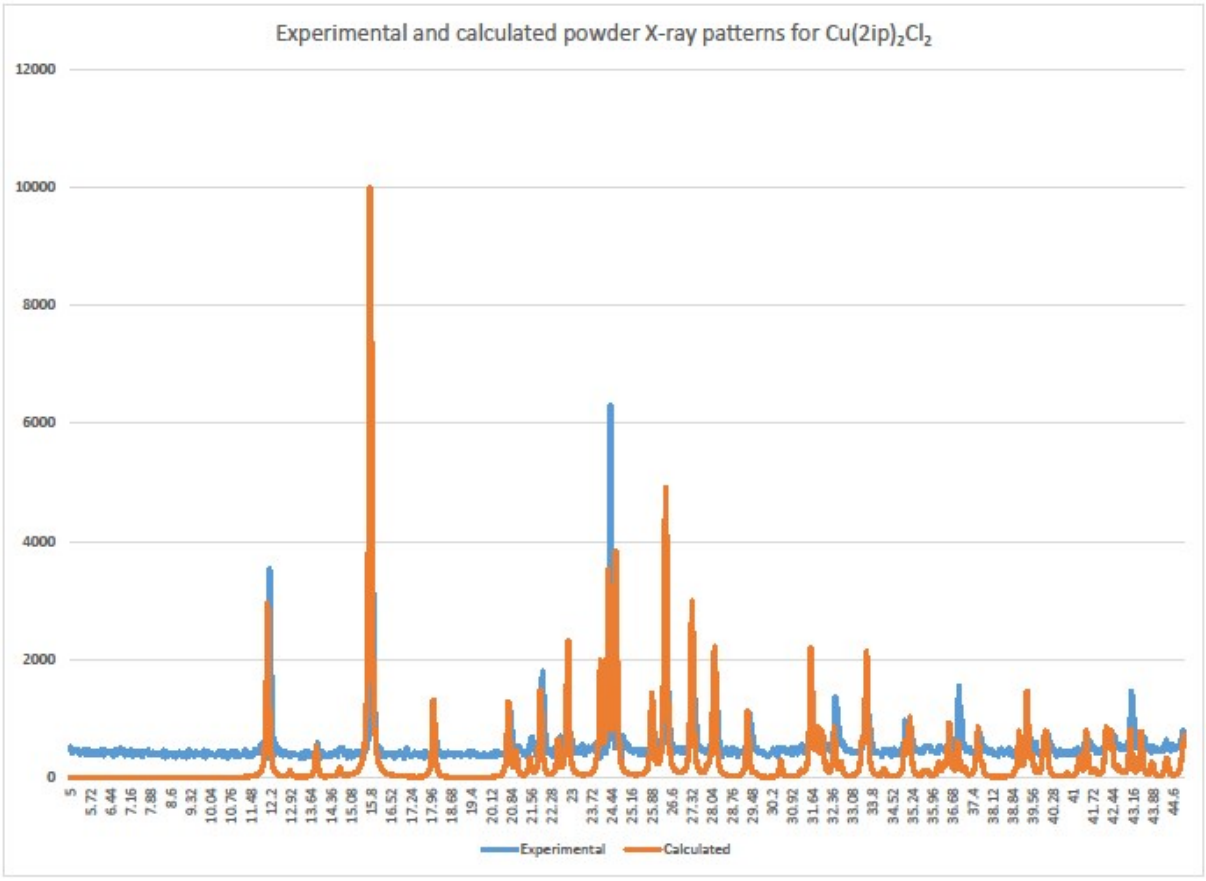

Figure S1. XRD diffraction pattern (Blue) of $Cu(2ip)_2Cl_2$ and the calculated one (Brown).

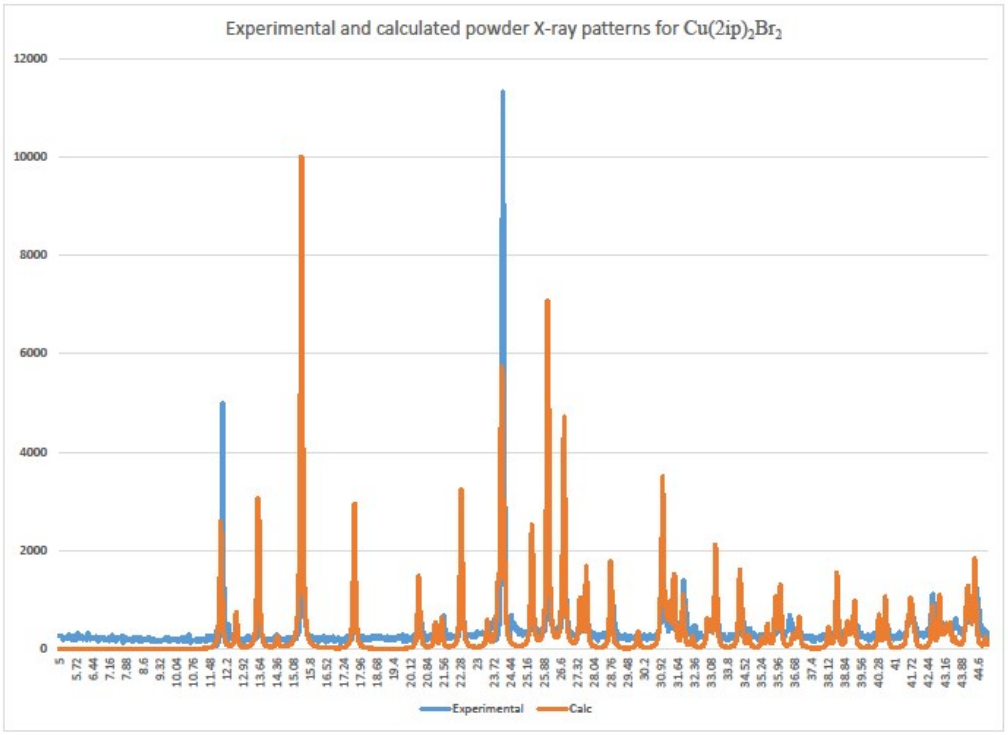

Figure S2. XRD diffraction pattern (Blue) of $Cu(2ip)_2Br_2$ and the calculated one (Brown).