3. Results

3.1 The studies on preparation of the crystals

The suitable conditions of synthesis complexes have been determined and are shown in Table 2. Some of their physical properties together with reacting ligand are summarized in Table 3.

Table 2 The suitable conditions of synthesis complexes.

Reactants	Mole Ratio	Solvent	Temperature(^{o}C)	Complexes
CuCl : ptu	1 : 3	Acetonitrile	50	$[Cu(ptu)_4]Cl$
CuBr : ptu	1 : 2.5	Acetonitrile	60	$[Cu_4(ptu)_6Br_4]_2$
CuI : ptu	1 : 3	Acetonitrile	60	$[Cu_4(ptu)_6I_4]_2$

Table 3 The Physical properties of ligands and compounds.

Compounds	Physical properties			
	Appearance	Colour	Melting point (^{o}C)	Solubility
Ligand ptu	Powder	White	145-150[a]	*
$[Cu(ptu)_4]Cl$	Needle	Colorless	161	**
$[Cu_4(ptu)_6I_4]_2$	Plate	Colorless	189-192(mwd)	**
$[Cu_4(ptu)_6Br_4]_2$	Plate	Colorless	205-207(mwd)	**

mwd = melt with decomposition, * = ethanol, acetone, acetonitrile, ** = acetone, acetonitrile, [a] The Merck Index, 1996: 80.

3.2 X-ray Fluorescence Spectrometry (XRF)

X-ray fluorescence spectra of all complexes were focused on 3 elements ; Cu, S and X (X= Cl, Br and I) as shown in Figure 16 – 24.

3.3 Infrared Spectroscopy

The present infrared absorption study of ptu and its metal complexes; $[Cu(ptu)_4]Cl$, $[Cu_4(ptu)_6Br_4]_2$ and $[Cu_4(ptu)_6I_4]_2$ are shown in Figure 25 – 28.

3.4 Elemental Analysis

Table 4 The partial elemental analyses of the compound.

Compound	%C Found (Calcd.)	%H Found (Calcd.)	%N Found (Calcd.)	%S Found (Calcd.)
$[Cu(ptu)_4]Cl$	46.68 (47.47)	4.40 (4.52)	14.36 (15.82)	21.71 (18.08)
$[Cu_4(ptu)_6Br_4]_2$	31.61 (33.89)	2.65 (3.23)	9.54 (11.30)	19.07 (12.91)
$[Cu_4(ptu)_6I_4]_2$	29.29 (30.09)	2.33 (2.87)	9.34 (10.03)	12.62 (11.46)

3.5 Crystal structure determination

3.5.1 X-ray Photography

$[Cu_4(ptu)_6I_4]_2$ was studied. The oscillation and Weissenberg photographs are shown in Figure 29 – 30.

3.5.2 Crystal Structure

The results from crystal structure determination using Xtal program System of complex 1, 2 and 3 are shown in Table 5 , 8 and 11, respectively, and Figure 31 – 40.

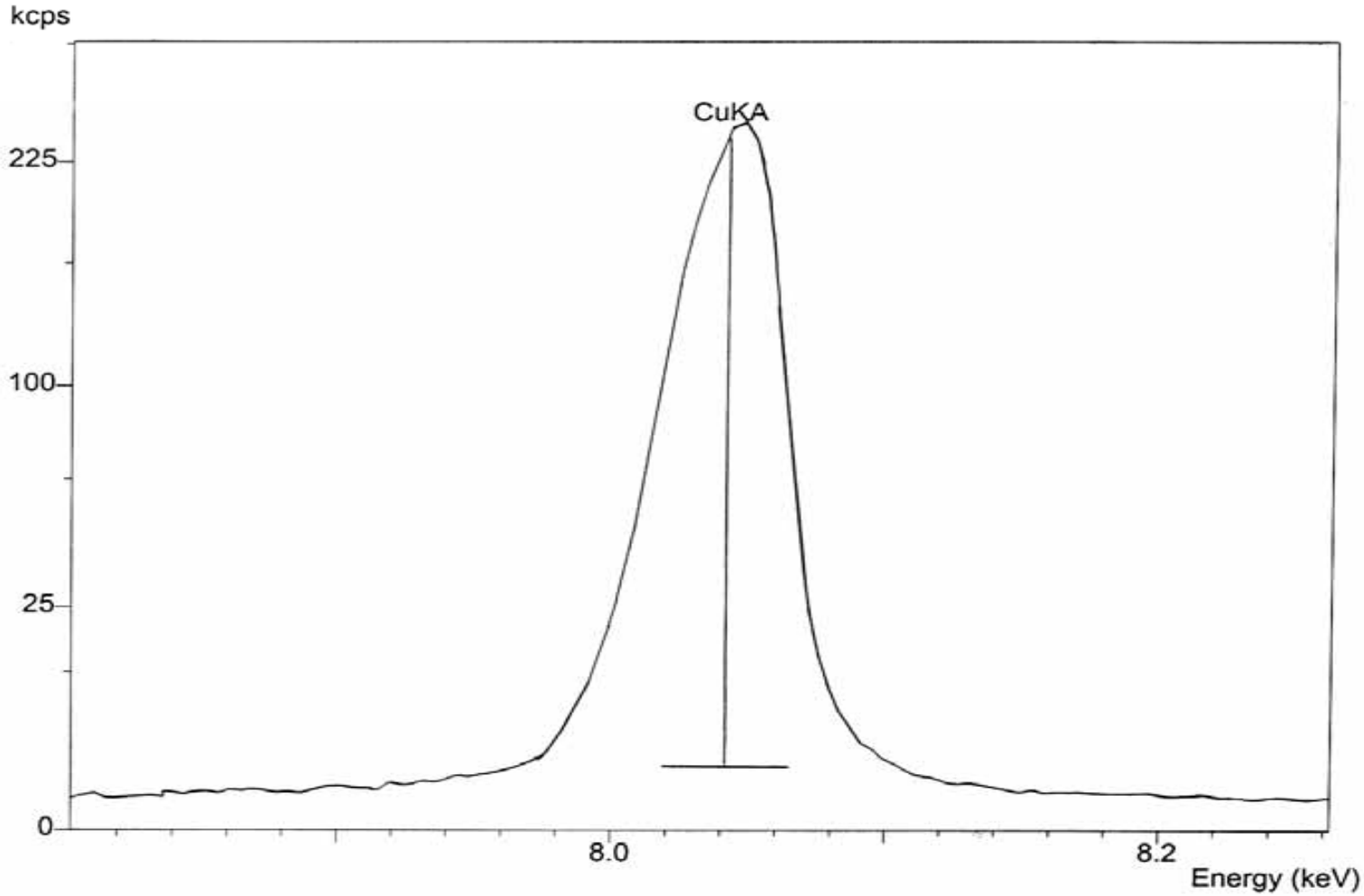

Figure 16 The X-ray fluorescence spectrum of $[Cu(ptu)_4]Cl$ (Cu atom).

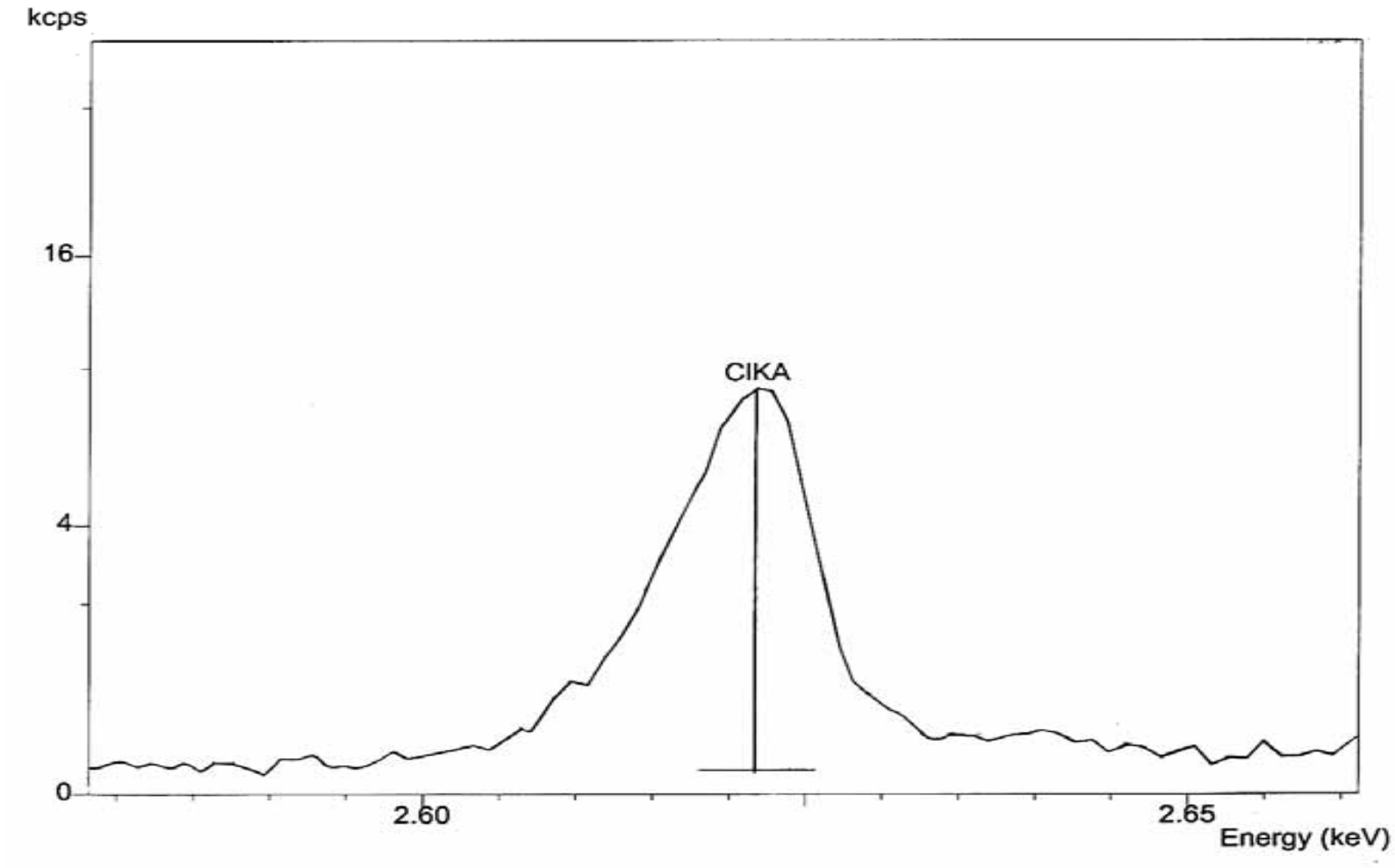

Figure 17 The X-ray fluorescence spectrum of $[Cu(ptu)_4]Cl$ (Cl atom).

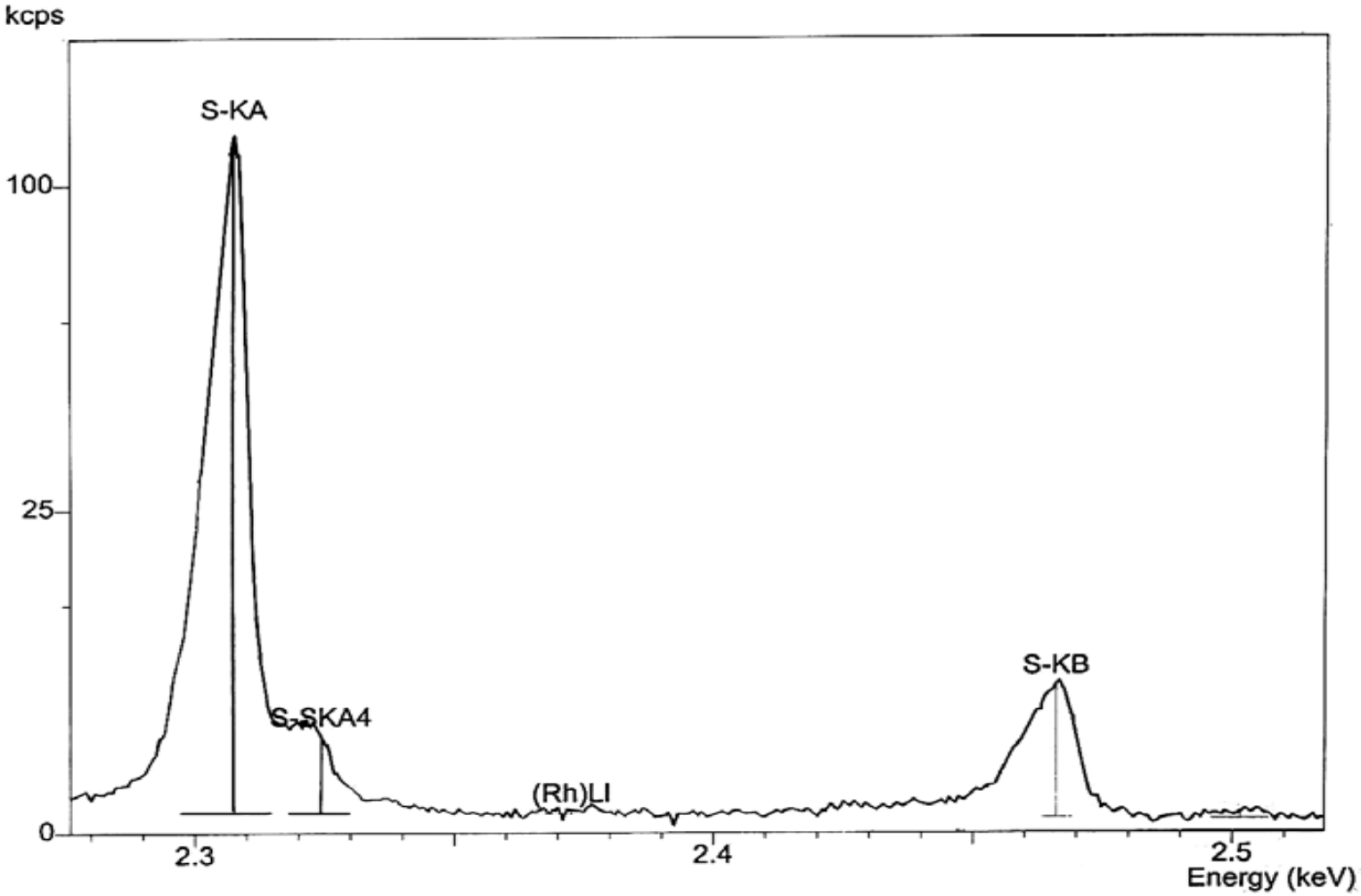

Figure 18 The X-ray fluorescence spectrum of $[Cu(ptu)_4]Cl$ (S atom).

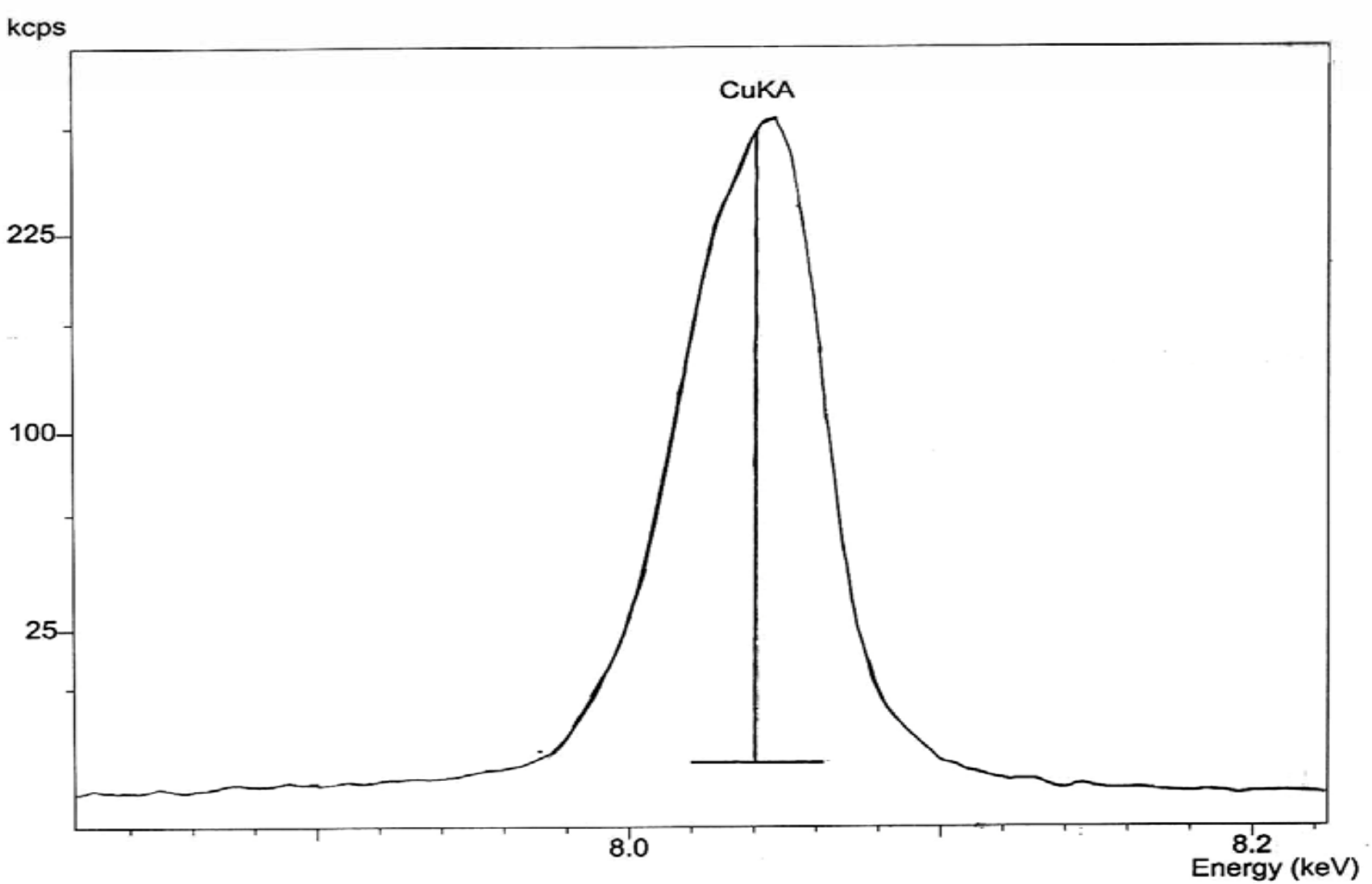

Figure 19 The X-ray fluorescence spectrum of $[Cu_4(ptu)_6Br_4]_2$ (Cu atom).

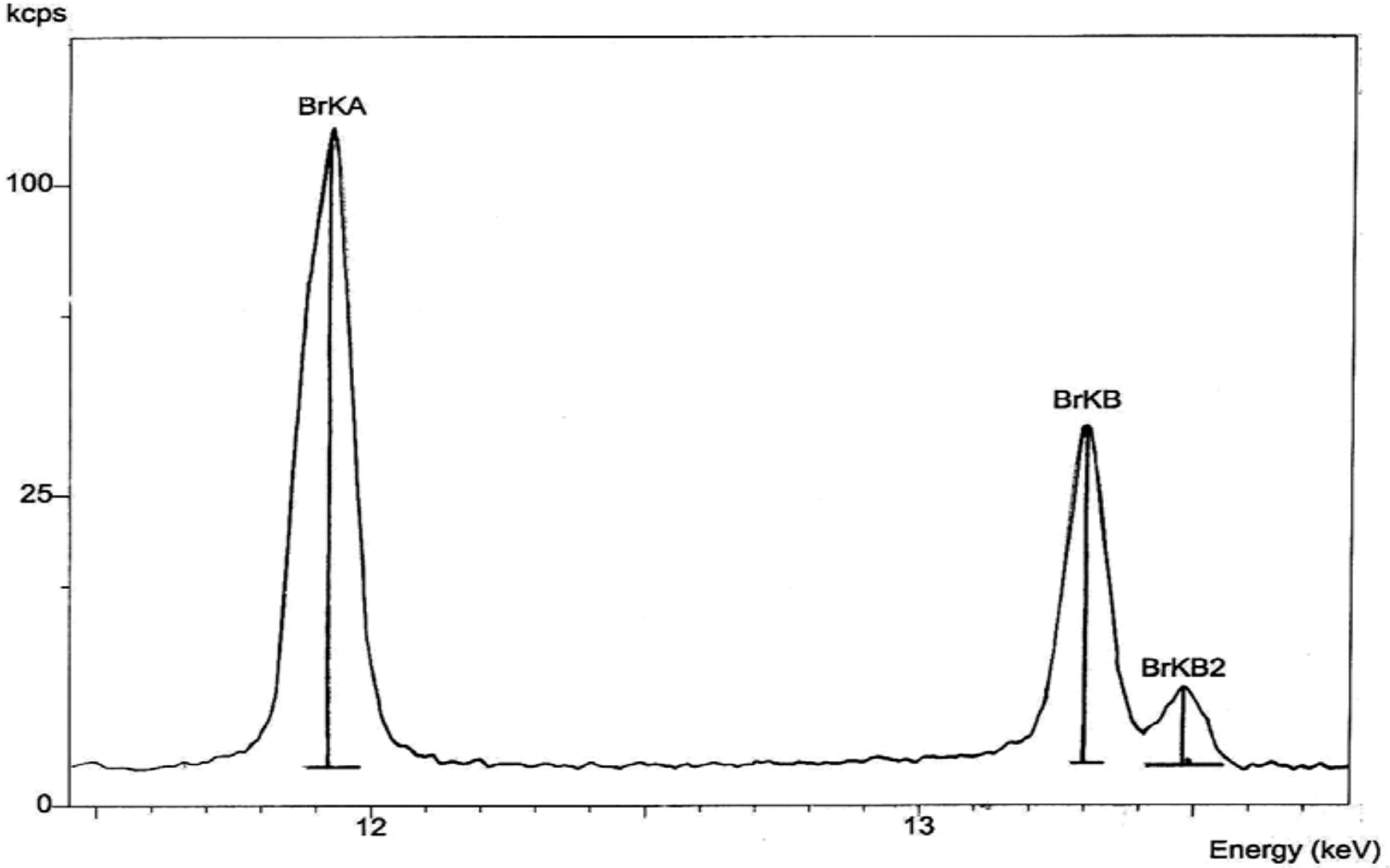

Figure 20 The X-ray fluorescence spectrum of $[Cu_4(ptu)_6Br_4]_2$ (Br atom).

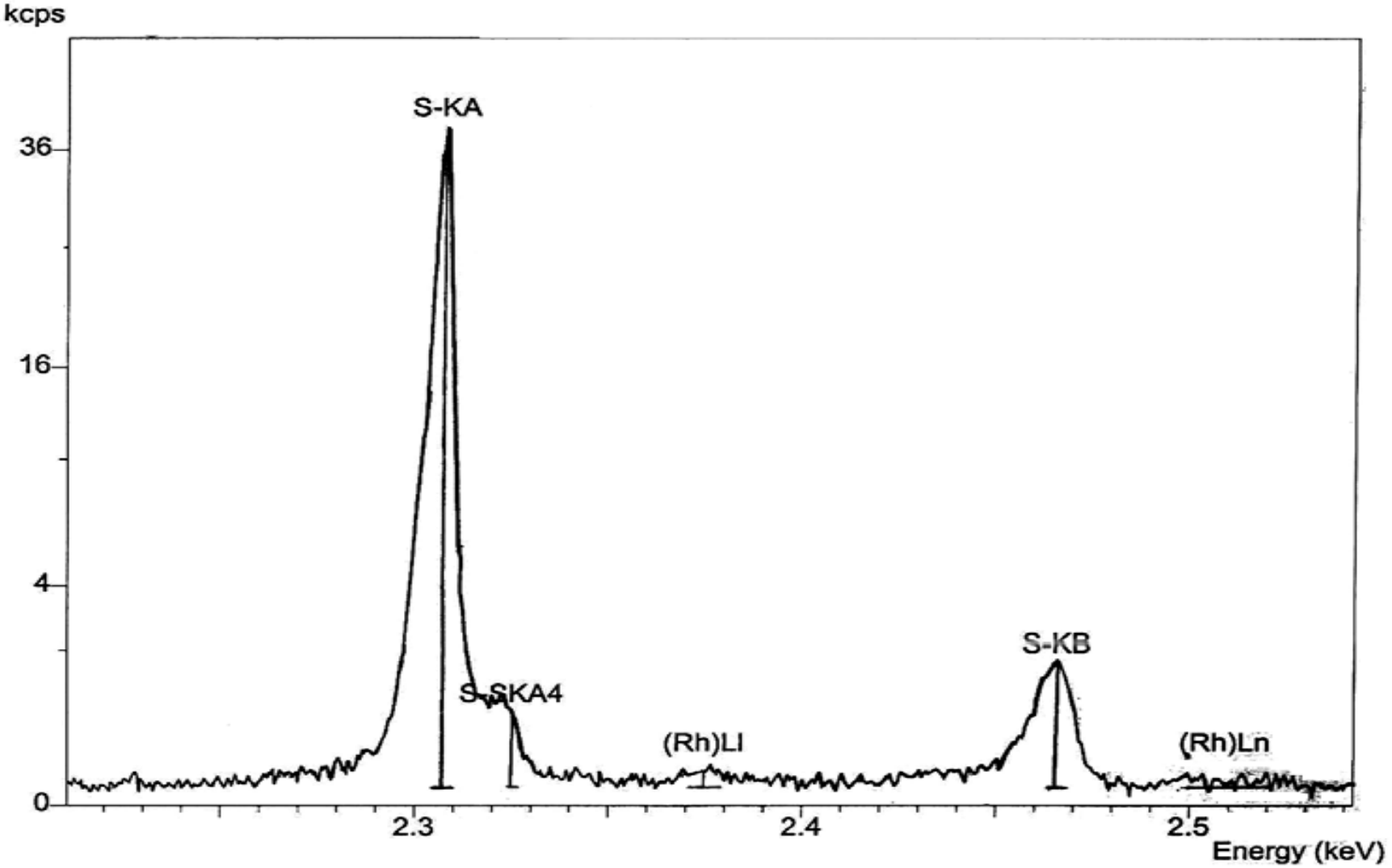

Figure 21 The X-ray fluorescence spectrum of $[Cu_4(ptu)_6Br_4]_2$ (S atom).

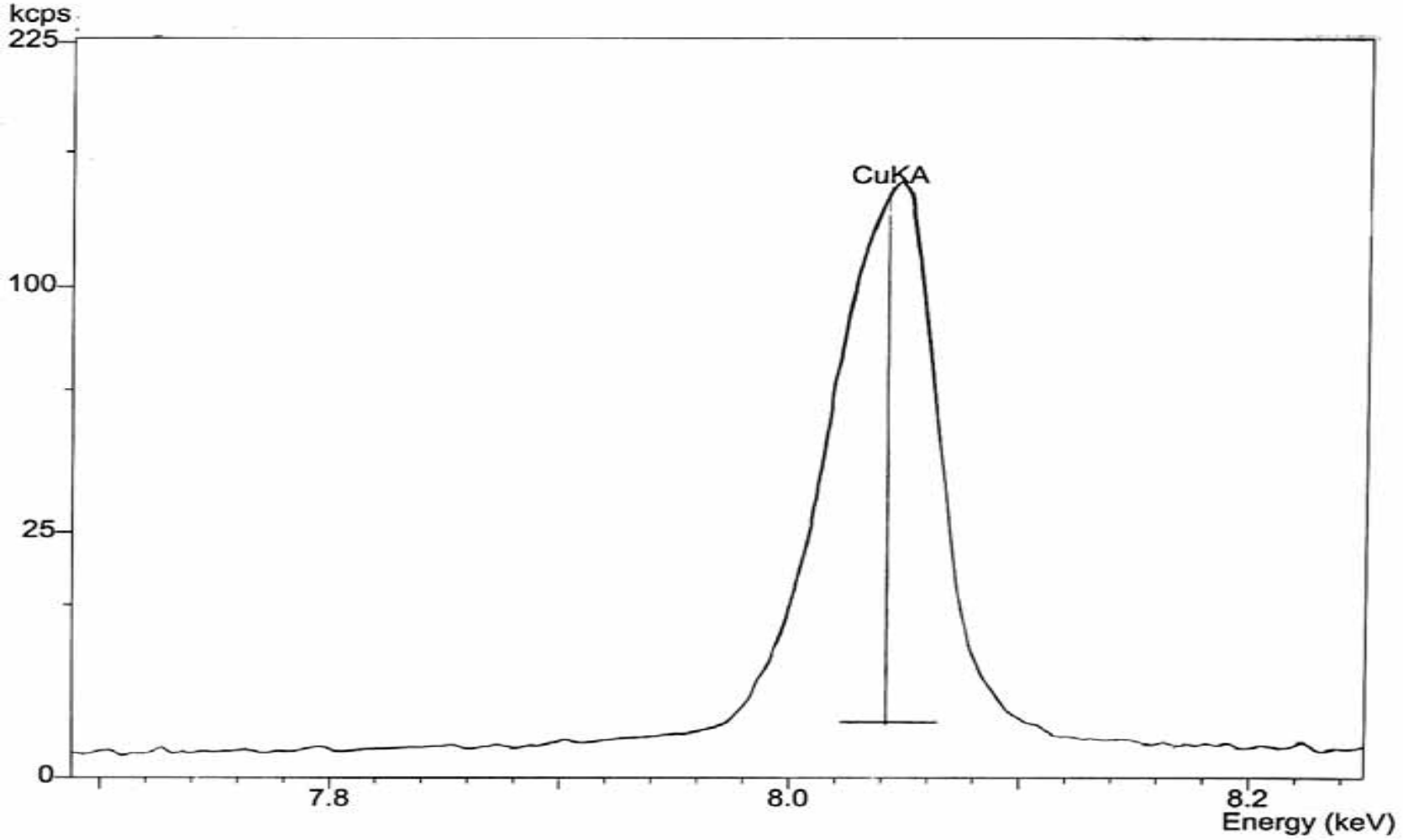

Figure 22 The X-ray fluorescence spectrum of $[Cu_4(ptu)_6I_4]_2$ (Cu atom).

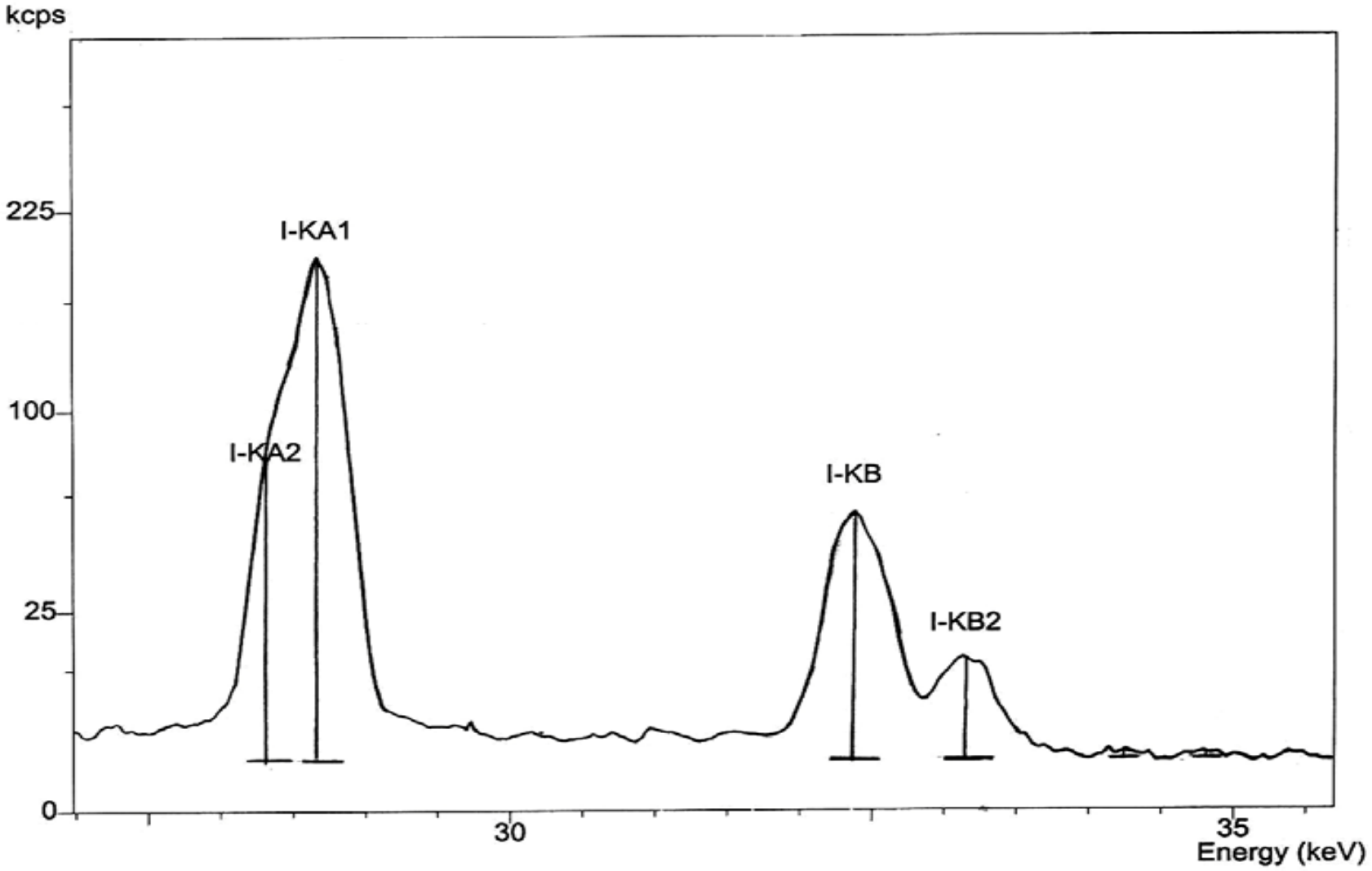

Figure 23 The X-ray fluorescence of $[Cu_4(ptu)_6I_4]_{2=}$(I atom).

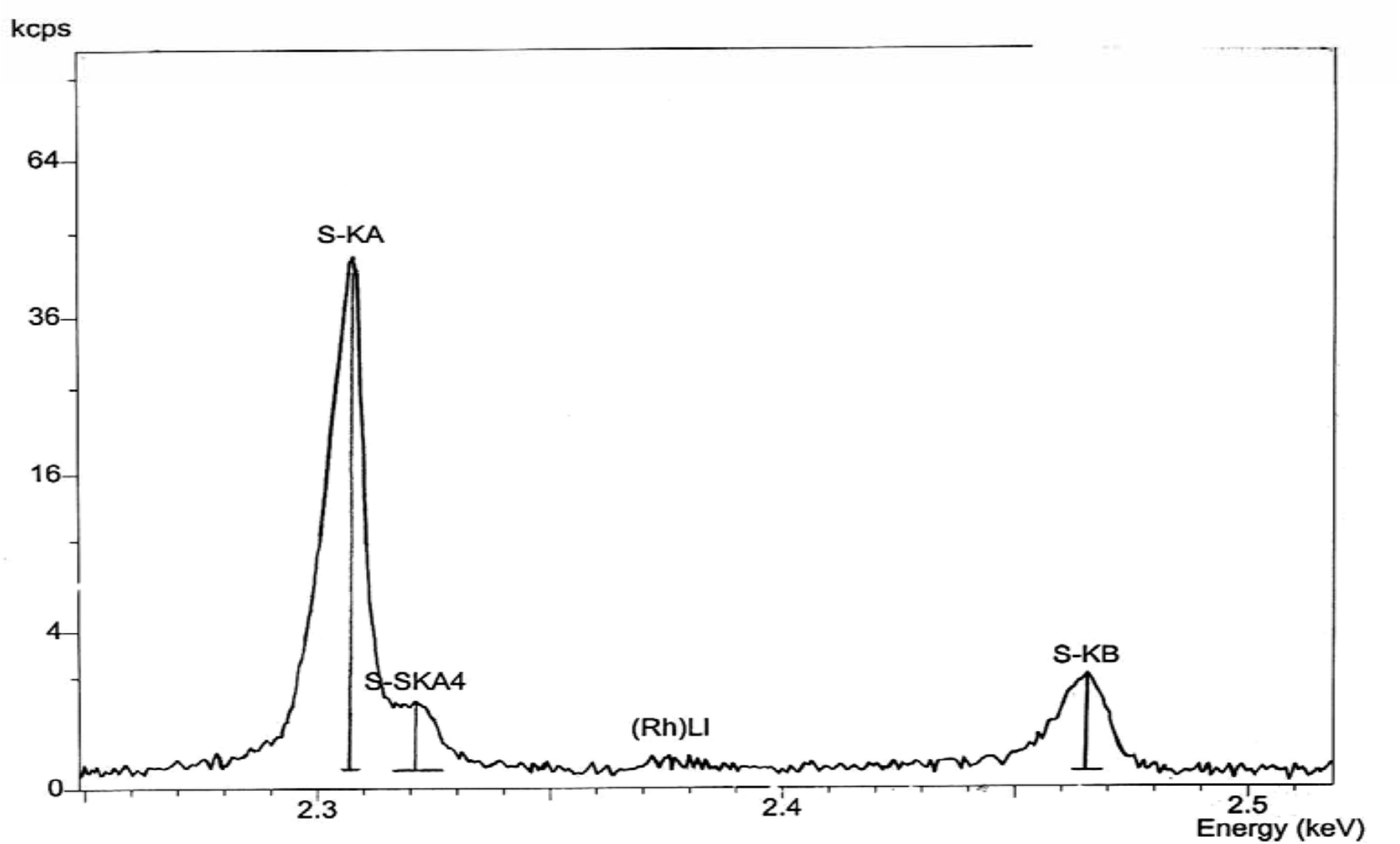

Figure 24 The X-ray fluorescence of $[Cu_4(ptu)_6I_4]_{2=}$(S atom).

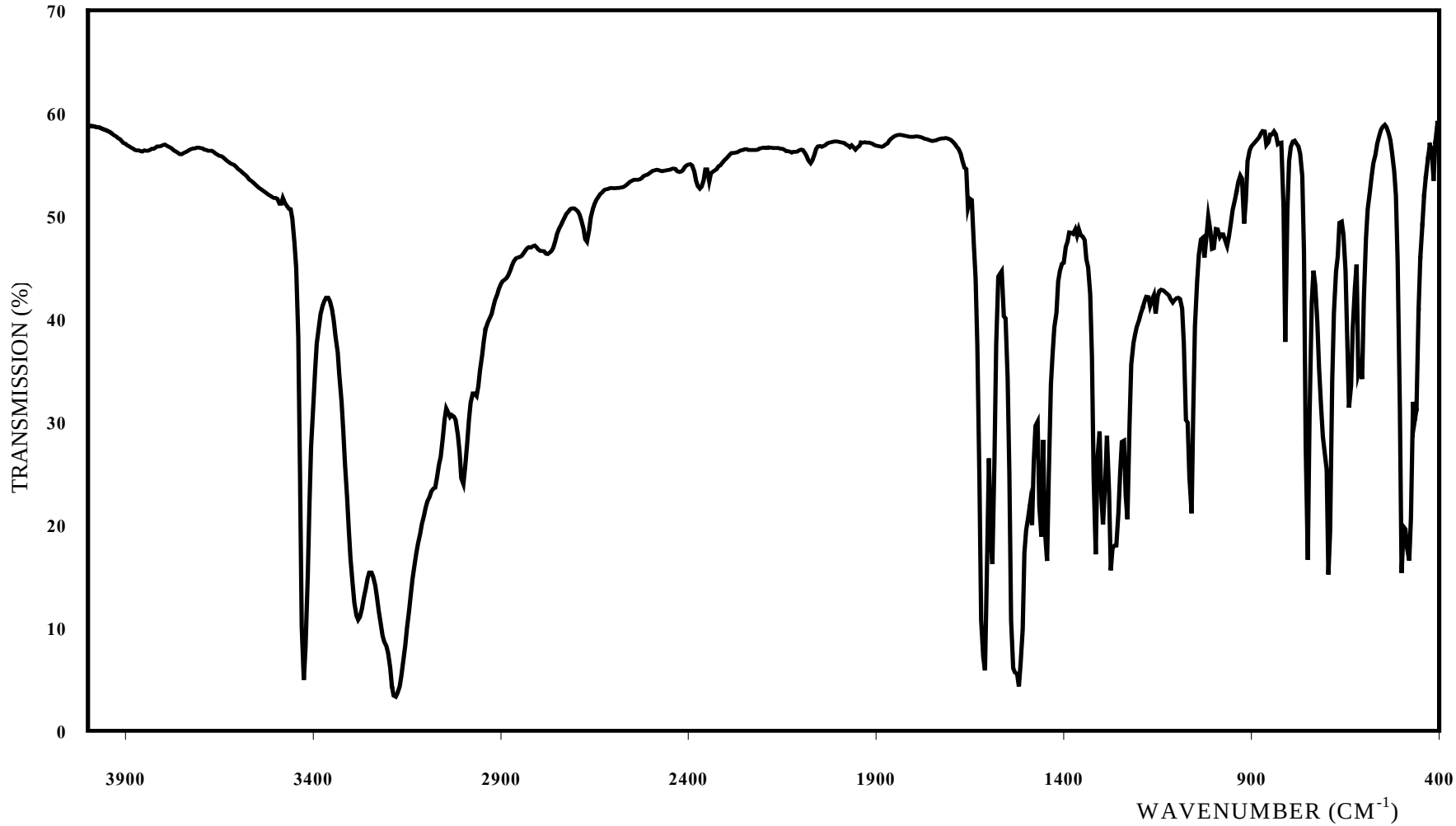

Figure 25 The infrared spectrum of ligand *N*-phenylthiourea.

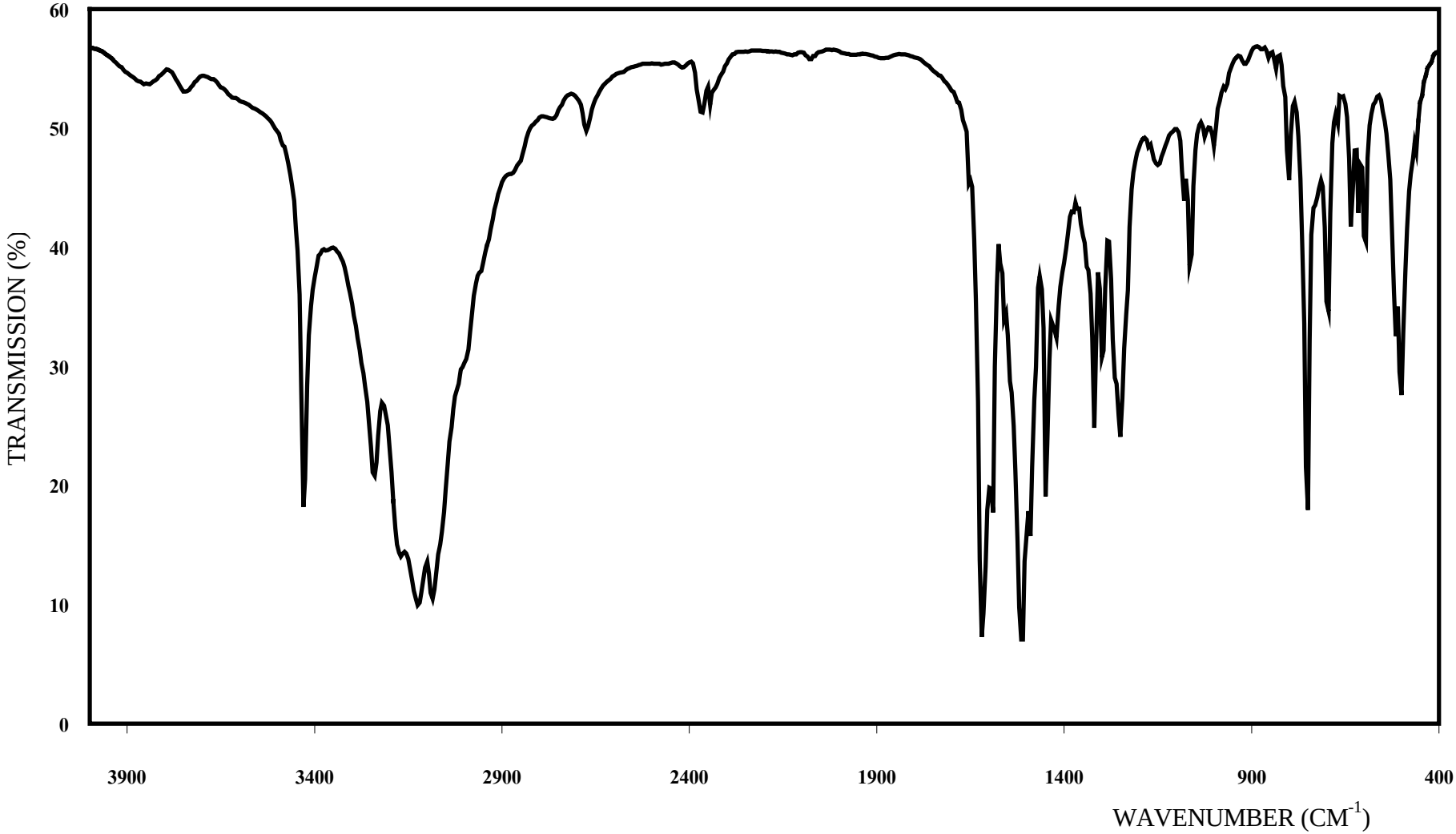

Figure 26 Infrared spectrum of $[Cu(ptu)_4]Cl$.

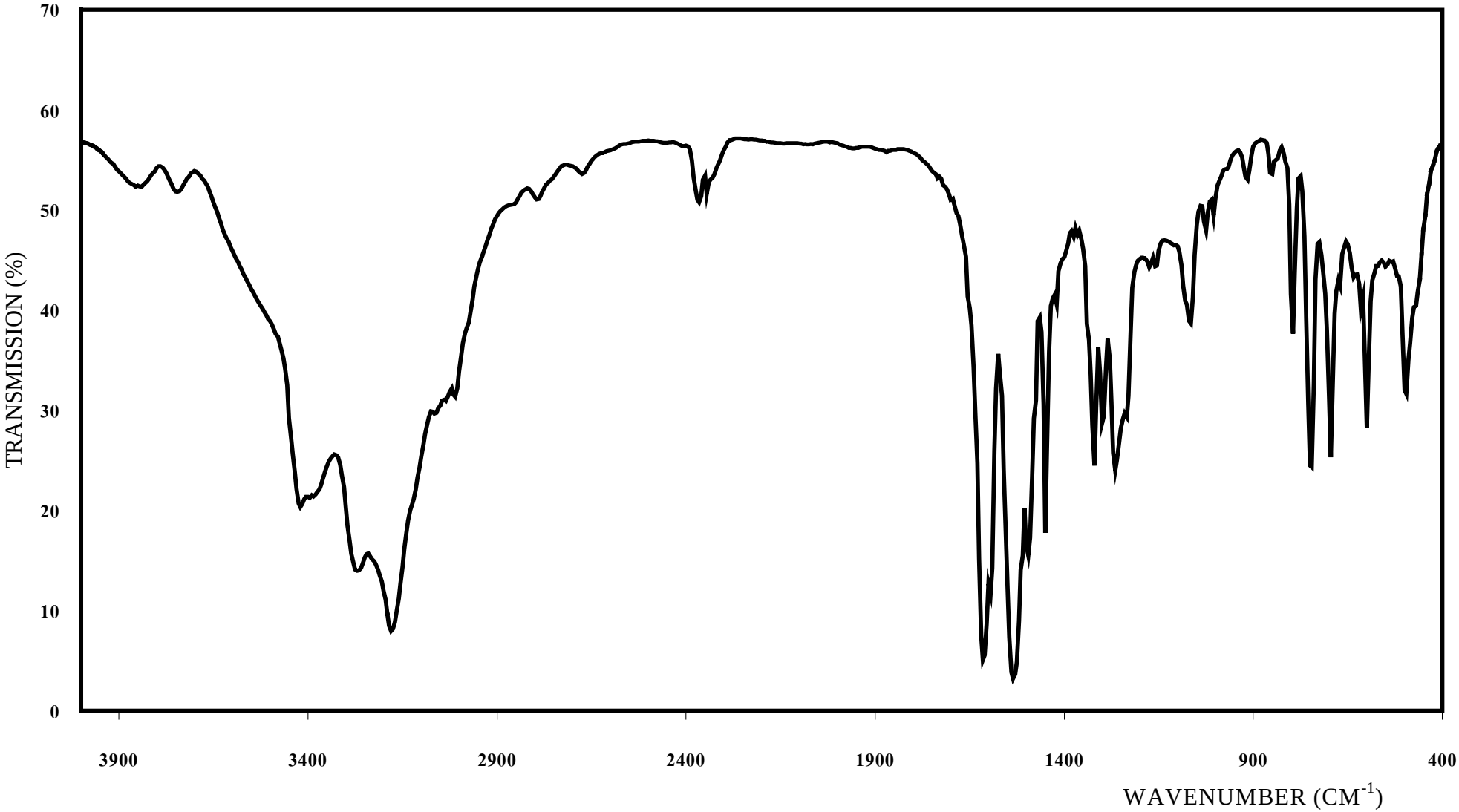

Figure 27 Infrared spectrum of $[Cu_4(ptu)_6Br_4]_2$.

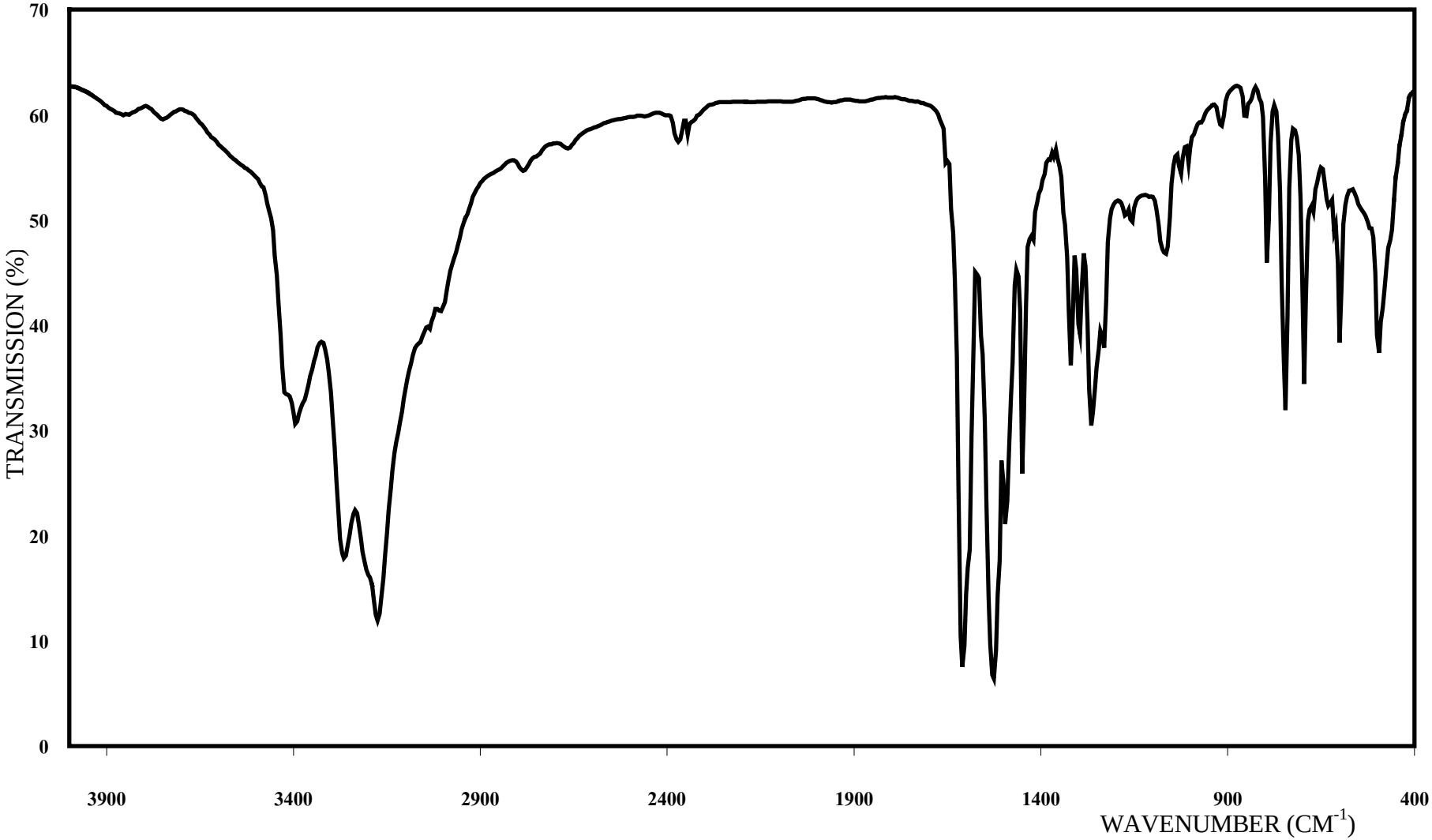

Figure 28 The infrared spectrum of $[Cu_4(ptu)_6I_4]_2$.

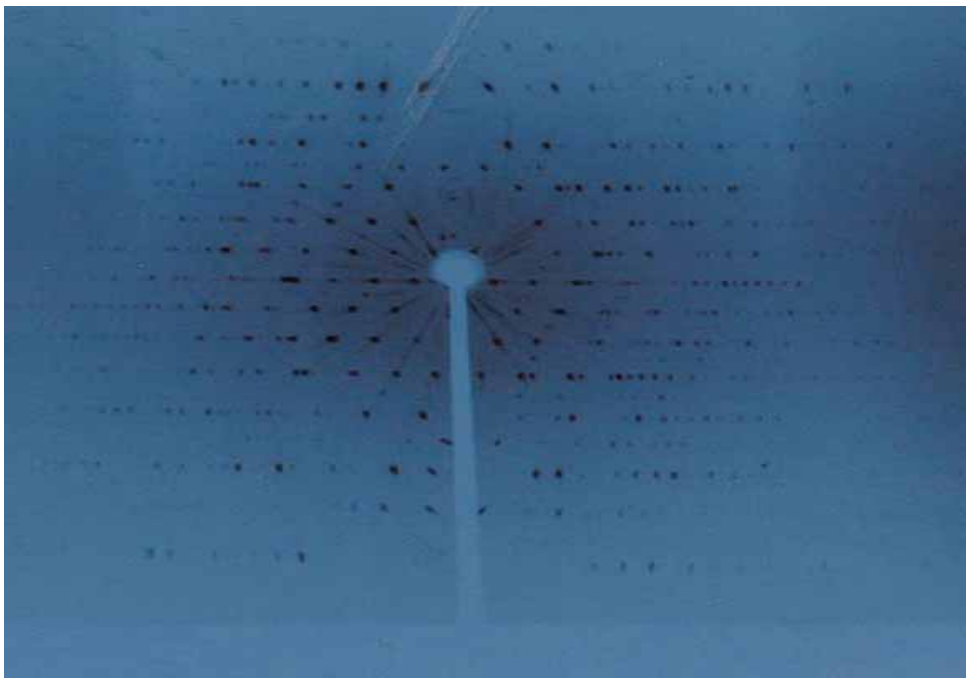

Figure 29 The oscillation photograph of $[Cu_4(ptu)_6I_4]_2$.

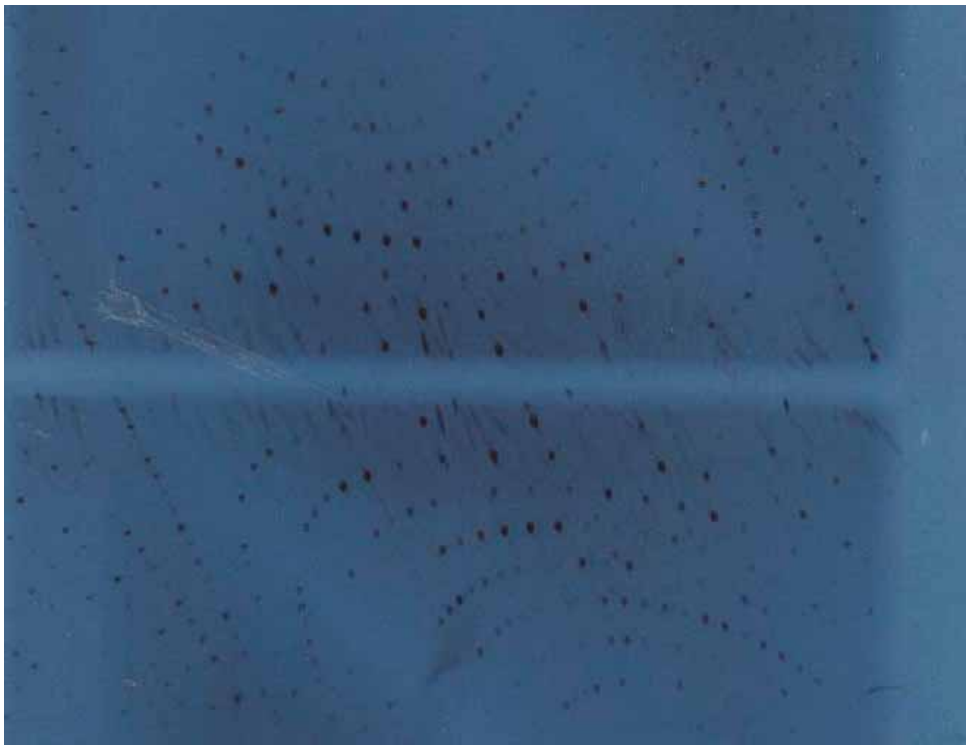

Figure 30 The zero layer Weissenberg photograph of $[Cu_4(ptu)_6I_4]_2$.

Table 5 Crystallographic data for $[Cu(ptu)_4]Cl$.

Chemical formula	$CuClS_4N_8C_{28}H_{32}$
Formula weight	707.9
Color; habit	Colorless, needle
Crystal system	Tetragonal
Space group	$I\bar{4}$ (No. 82)
Unit cell dimensions	
a (Å)	11.5084(2)
b (Å)	11.5084(2)
c (Å)	12.8895(3)
α (^{o})	90.00(0)
β (^{o})	90.00(0)
γ (^{o})	90.00(0)
V (Å^3)	1707.1(1)
Z	2
Density (calc.)(g cm^{-3})	1.377
F(000)	732
Measured reflections	1305
Observed reflections	1059
Condition for observed reflections	$F>4\sigma(F)$
R	0.0452
R_w	0.0555

Table 6 Non-hydrogen interatomic distances of $[Cu(ptu)_4]Cl$.

Bond	Distances(Angstroms)
Cu-S(1)	2.335(1)
Cu-S(1)'	2.335(1)
Cu-S(1)"	2.335(1)
Cu-S(1)"'	2.335(1)
S(1)-C(1)	1.707(4)
N(1)-C(11)	1.434(6)
N(1)-C(1)	1.338(5)
N(2)-C(1)	1.311(7)
C(11)-C(12)	1.380(8)
C(11)-C(16)	1.372(7)
C(12)-C(13)	1.38(1)
C(13)-C(14)	1.39(1)
C(14)-C(15)	1.37(1)
C(15)-C(16)	1.40(1)

Transformations of the asymmetric unit :

(') = (-x, -y, +z)

(") = (½ +y, ½ -x, ½ -z)

("') = (½ -y, ½ +x, ½ -z)

Table 7 Non-hydrogen interatomic angles of $[Cu(ptu)_4]Cl$.

Bond	Angles(degrees)
S(1)-Cu-S(1)'	117.26(4)
S(1)-Cu-S(1)''	105.72(4)
S(1)-Cu-S(1)'''	105.72(4)
S(1)'-Cu-S(1)''	105.72(4)
S(1)'-Cu-S(1)'''	105.72(4)
S(1)''-Cu-S(1)'''	117.26(4)
Cu-S(1)-C(1)	106.7(1)
C(11)-N(1)-C(1)	125.7(4)
N(1)-C(11)-C(12)	118.7(4)
N(1)-C(11)-C(16)	121.7(4)
C(12)-C(11)-C(16)	119.6(5)
C(11)-C(12)-C(13)	120.8(6)
C(12)-C(13)-C(14)	119.1(7)
C(13)-C(14)-C(15)	120.5(7)
C(14)-C(15)-C(16)	119.8(6)
C(11)-C(16)-C(15)	120.2(6)
S(1)-C(1)-N(1)	120.5(3)
S(1)-C(1)-N(2)	120.1(4)
N(1)-C(1)-N(2)	119.4(4)

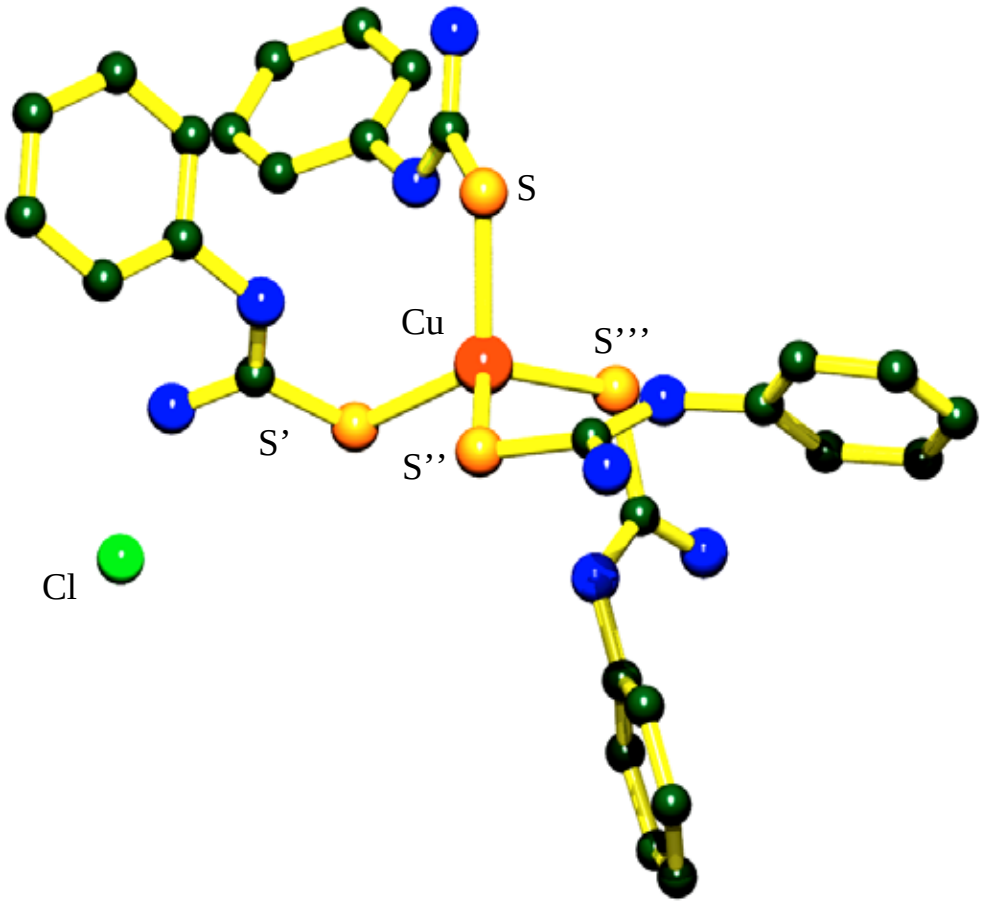

Figure 31 The structure of $[Cu(ptu)_4]Cl$ (H atom omitted for clarity).

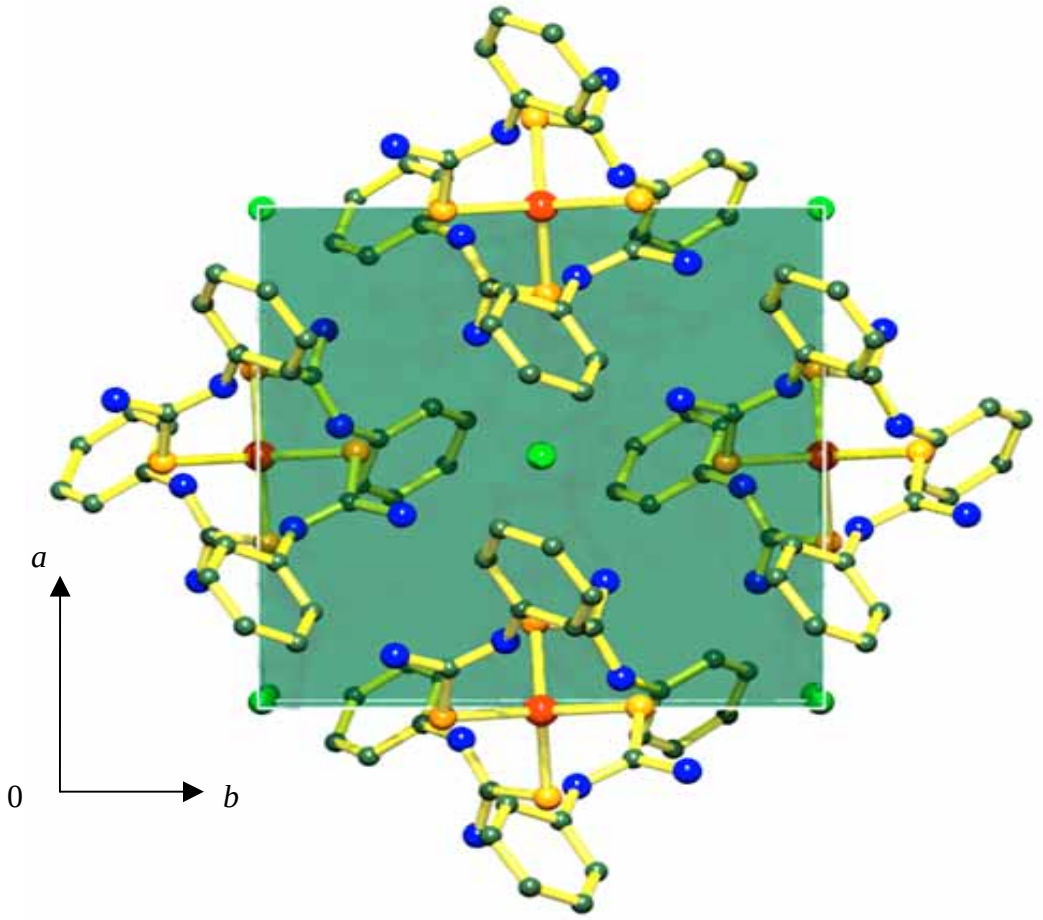

Figure 32 Unit cell contents of $[Cu(ptu)_4]Cl$ projected down *c*.

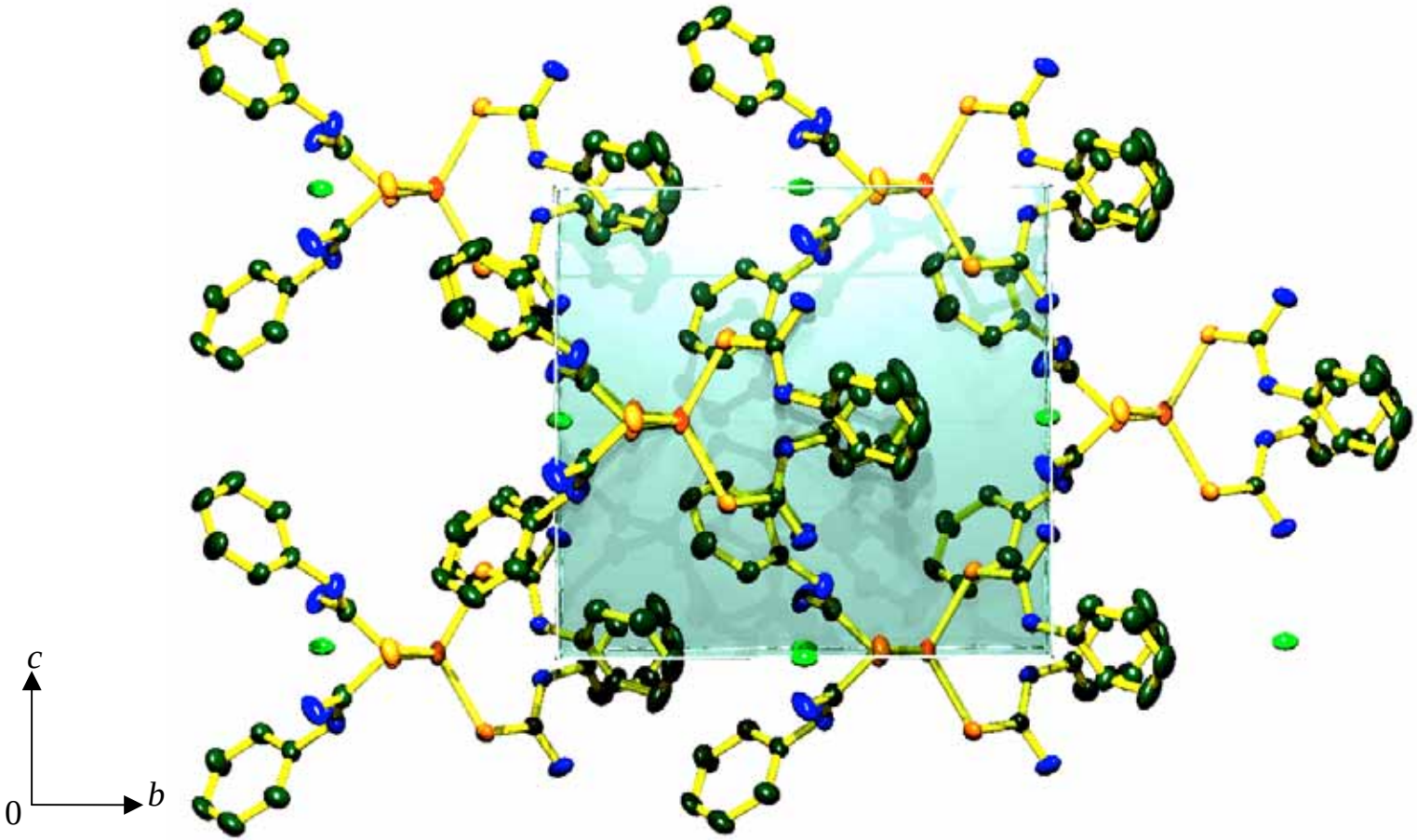

Figure 33 Unit cell contents of $[Cu(ptu)_4]Cl$ projected down *a*.

Table 8 Crystallographic data for $[Cu_4(ptu)_6Br_4]_2$.

Chemical formula	$Cu_8Br_8S_{12}N_{24}C_{48}H_{96}$
Formula weight	2974.25
Color; habit	Colorless, plate
Crystal system	Triclinic
Space group	$P\bar{1}$ (No.2)
Unit cell dimensions	
a (Å)	11.987(1)
b (Å)	19.891(2)
c (Å)	25.213(2)
α (^{o})	111.58(1)
β (^{o})	95.91(1)
γ (^{o})	97.45(1)
V (Å^3)	5468.7(1)
Z	2
Density (calc.)(g cm^{-3})	1.806
F(000)	2944
Measured reflections	24918
Observed reflections	18904
Condition for observed reflections	$F>4\sigma(F)$
R	0.049
R_w	0.039

Table 9 Non-Hydrogen interatomic distances of $[Cu_4(ptu)_6Br_4]_2$.

Bond	Angstroms
Molecule A	
Br(1A)-Cu(1A)	2.4937(9)
Br(2A)-Cu(2A)	2.521(1)
Br(3A)-Cu(3A)	2.7262(8)
Br(4A)-Cu(4A)	2.4779(7)
Cu(1A)-S(1A)	2.291(2)
Cu(1A)-S(4A)	2.320(1)
Cu(1A)-S(5A)	2.318(1)
Cu(2A)-S(1A)	2.283(2)
Cu(2A)-S(2A)	2.352(1)
Cu(2A)-S(6A)	2.261(1)
Cu(3A)-S(2A)	2.295(2)
Cu(3A)-S(3A)	2.261(1)
Cu(3A)-S(5A)	2.262(2)
Cu(4A)-S(3A)	2.342(1)
Cu(4A)-S(4A)	2.293(2)
Cu(4A)-S(6A)	2.330(2)
S(6A)-C(6A)	1.723(6)

Table 9 Non-Hydrogen interatomic distances of $[Cu_4(ptu)_6Br_4]_2$ (cont).

Bond	Angstroms
S(2A)-C(2A)	1.717(5)
S(1A)-C(1A)	1.730(6)
S(5A)-C(5A)	1.723(6)
S(4A)-C(4A)	1.722(5)
S(3A)-C(3A)	1.731(6)
N(61A)-C(6A)	1.321(7)
N(61A)-C(61A)	1.426(8)
N(41A)-C(4A)	1.330(8)
N(41A)-C(41A)	1.434(7)
N(51A)-C(5A)	1.331(8)
N(51A)-C(51A)	1.425(8)
N(12A)-C(1A)	1.329(8)
N(52A)-C(5A)	1.318(8)
N(11A)-C(1A)	1.312(9)
N(11A)-C(11A)	1.426(7)
N(62A)-C(6A)	1.319(7)
C(4A)-N(42A)	1.319(6)
N(32A)-C(3A)	1.321(7)

Table 9 Non-Hydrogen interatomic distances of $[Cu_4(ptu)_6Br_4]_2$ (cont).

Bond	Angstroms
C(31A)-C(36A)	1.381(8)
C(31A)-C(32A)	1.387(9)
N(31A)-C(31A)	1.429(7)
N(31A)-C(3A)	1.326(6)
C(41A)-C(46A)	1.382(8)
C(41A)-C(42A)	1.378(7)
C(46A)-C(45A)	1.394(8)
C(36A)-C(35A)	1.396(9)
N(21A)-C(2A)	1.328(8)
N(21A)-C(21A)	1.435(7)
C(66A)-C(61A)	1.382(8)
C(66A)-C(65A)	1.387(9)
C(51A)-C(56A)	1.385(9)
C(51A)-C(52A)	1.391(8)
N(22A)-C(2A)	1.326(8)
C(56A)-C(55A)	1.38(1)
C(33A)-C(32A)	1.393(8)
C(33A)-C(34A)	1.376(8)

Table 9 Non-Hydrogen interatomic distances of $[Cu_4(ptu)_6Br_4]_2$ (cont).

Bond	Angstroms
C(42A)-C(43A)	1.379(8)
C(43A)-C(44A)	1.369(9)
C(35A)-C(34A)	1.39(1)
C(61A)-C(62A)	1.378(9)
C(52A)-C(53A)	1.38(1)
C(62A)-C(63A)	1.39(1)
C(45A)-C(44A)	1.374(9)
C(63A)-C(64A)	1.379(9)
C(55A)-C(54A)	1.373(9)
C(65A)-C(64A)	1.37(1)
C(11A)-C(12A)	1.382(8)
C(11A)-C(16A)	1.383(9)
C(12A)-C(13A)	1.389(9)
C(54A)-C(53A)	1.38(1)
C(16A)-C(15A)	1.38(1)
C(26A)-C(21A)	1.372(7)
C(26A)-C(25A)	1.386(8)
C(21A)-C(22A)	1.390(9)

Table 9 Non-Hydrogen interatomic distances of $[Cu_4(ptu)_6Br_4]_2$ (cont).

Bond	Angstroms
C(22A)-C(23A)	1.389(8)
C(23A)-C(24A)	1.355(9)
C(14A)-C(13A)	1.37(1)
C(14A)-C(15A)	1.40(1)
C(24A)-C(25A)	1.38(1)
Molecule B	
Br(1B)-Cu(1B)	2.5241(8)
Br(2B)-Cu(2B)	2.4756(7)
Br(3B)-Cu(3B)	2.4945(9)
Br(4B)-Cu(4B)	2.4957(9)
Cu(1B)-S(1B)	2.332(1)
Cu(1B)-S(4B)	2.300(2)
Cu(1B)-S(5B)	2.289(2)
Cu(2B)-S(6B)	2.359(2)
Cu(2B)-S(1B)	2.349(1)
Cu(2B)-S(2B)	2.288(2)
Cu(3B)-S(3B)	2.288(2)
Cu(3B)-S(5B)	2.343(1)

Table 9 Non-Hydrogen interatomic distances of $[Cu_4(ptu)_6Br_4]_2$ (cont).

Bond	Angstroms
Cu(3B)-S(2B)	2.314(1)
Cu(4B)-S(3B)	2.299(2)
Cu(4B)-S(4B)	2.292(1)
Cu(4B)-S(6B)	2.325(1)
S(3B)-C(3B)	1.721(5)
S(6B)-C(6B)	1.721(6)
S(4B)-C(4B)	1.729(4)
S(1B)-C(1B)	1.721(6)
S(5B)-C(5B)	1.729(6)
S(2B)-C(2B)	1.717(5)
N(21B)-C(2B)	1.333(8)
N(21B)-C(21B)	1.430(7)
N(31B)-C(3B)	1.339(8)
N(31B)-C(31B)	1.426(8)
N(32B)-C(3B)	1.313(7)
N(22B)-C(2B)	1.323(7)
N(12B)-C(1B)	1.328(7)
N(51B)-C(5B)	1.330(8)

Table 9 Non-Hydrogen interatomic distances of $[Cu_4(ptu)_6Br_4]_2$ (cont).

Bond	Angstroms
N(51B)-C(51B)	1.424(8)
N(11B)-C(11B)	1.419(8)
N(11B)-C(1B)	1.327(6)
N(42B)-C(4B)	1.324(8)
C(11B)-C(16B)	1.392(9)
C(11B)-C(12B)	1.394(8)
N(52B)-C(5B)	1.317(8)
N(41B)-C(4B)	1.325(8)
N(41B)-C(41B)	1.423(6)
C(21B)-C(22B)	1.375(7)
C(21B)-C(26B)	1.382(8)
N(61B)-C(61B)	1.424(8)
N(61B)-C(6B)	1.335(7)
N(62B)-C(6B)	1.322(6)
C(16B)-C(15B)	1.389(9)
C(52B)-C(51B)	1.385(9)
C(52B)-C(53B)	1.37(1)
C(42B)-C(41B)	1.397(7)

Table 9 Non-Hydrogen interatomic distances of $[Cu_4(ptu)_6Br_4]_2$ (cont).

Bond	Angstroms
C(42B)-C(43B)	1.382(7)
C(51B)-C(56B)	1.382(8)
C(32B)-C(31B)	1.388(6)
C(32B)-C(33B)	1.389(9)
C(61B)-C(66B)	1.377(8)
C(61B)-C(62B)	1.384(8)
C(15B)-C(14B)	1.386(9)
C(12B)-C(13B)	1.381(9)
C(56B)-C(55B)	1.39(1)
C(31B)-C(36B)	1.400(8)
C(14B)-C(13B)	1.37(1)
C(34B)-C(33B)	1.377(9)
C(34B)-C(35B)	1.379(7)
C(41B)-C(46B)	1.393(9)
C(22B)-C(23B)	1.373(9)
C(53B)-C(54B)	1.384(8)
C(54B)-C(55B)	1.365(9)
C(46B)-C(45B)	1.377(7)

Table 9 Non-Hydrogen interatomic distances of $[Cu_4(ptu)_6Br_4]_2$ (cont).

Bond	Angstroms
C(43B)-C(44B)	1.39(1)
C(36B)-C(35B)	1.381(9)
C(44B)-C(45B)	1.374(8)
C(26B)-C(25B)	1.380(9)
C(23B)-C(24B)	1.36(1)
C(24B)-C(25B)	1.38(1)
C(66B)-C(65B)	1.38(1)
C(62B)-C(63B)	1.38(1)
C(65B)-C(64B)	1.37(1)
C(64B)-C(63B)	1.390(9)

Table 10 Non-Hydrogen interatomic angles of $[Cu_4(ptu)_6Br_4]_2$.

Bond	Degrees
Molecule A	
Br(1A)-Cu(1A)-S(1A)	112.35(5)
Br(1A)-Cu(1A)-S(5A)	114.80(5)
Br(1A)-Cu(1A)-S(4A)	111.44(5)
Br(2A)-Cu(2A)-S(6A)	112.56(5)
Br(2A)-Cu(2A)-S(2A)	107.62(5)
Br(2A)-Cu(2A)-S(1A)	108.50(4)
Br(3A)-Cu(3A)-S(2A)	103.10(4)
Br(3A)-Cu(3A)-S(5A)	101.95(4)
Br(3A)-Cu(3A)-S(3A)	108.59(4)
Br(4A)-Cu(4A)-S(6A)	106.70(5)
Br(4A)-Cu(4A)-S(4A)	120.77(4)
Br(4A)-Cu(4A)-S(3A)	112.22(4)
Cu(2A)-S(6A)-Cu(4A)	113.47(7)
Cu(2A)-S(6A)-C(6A)	107.4(2)
Cu(4A)-S(6A)-C(6A)	111.1(2)
Cu(2A)-S(2A)-Cu(3A)	103.27(6)
Cu(2A)-S(2A)-C(2A)	99.8(2)

Table 10 Non-Hydrogen interatomic angles of $[Cu_4(ptu)_6Br_4]_2$ (cont).

Bond	Degrees
Cu(3A)-S(2A)-C(2A)	104.1(2)
Cu(2A)-S(1A)-Cu(1A)	111.20(6)
Cu(2A)-S(1A)-C(1A)	109.7(2)
Cu(1A)-S(1A)-C(1A)	112.2(2)
Cu(3A)-S(5A)-Cu(1A)	106.47(6)
Cu(3A)-S(5A)-C(5A)	110.7(2)
Cu(1A)-S(5A)-C(5A)	108.3(2)
Cu(4A)-S(4A)-Cu(1A)	118.26(6)
Cu(4A)-S(4A)-C(4A)	113.1(2)
Cu(1A)-S(4A)-C(4A)	115.7(2)
Cu(4A)-S(3A)-Cu(3A)	105.09(6)
Cu(4A)-S(3A)-C(3A)	109.7(2)
Cu(3A)-S(3A)-C(3A)	104.5(1)
S(6A)-Cu(2A)-S(2A)	104.96(5)
S(6A)-Cu(2A)-S(1A)	115.34(6)
S(2A)-Cu(2A)-S(1A)	107.43(6)
S(6A)-Cu(4A)-S(4A)	107.91(6)
S(6A)-Cu(4A)-S(3A)	113.73(5)

Table 10 Non-Hydrogen interatomic angles of $[Cu_4(ptu)_6Br_4]_2$ (cont).

Bond	Degrees
S(4A)-Cu(4A)-S(3A)	95.46(6)
S(2A)-Cu(3A)-S(5A)	111.98(6)
S(2A)-Cu(3A)-S(3A)	112.72(6)
S(5A)-Cu(3A)-S(3A)	116.90(5)
S(1A)-Cu(1A)-S(5A)	96.34(5)
S(1A)-Cu(1A)-S(4A)	117.61(6)
S(5A)-Cu(1A)-S(4A)	103.18(5)
C(6A)-N(61A)-C(61A)	129.2(5)
C(4A)-N(41A)-C(41A)	128.3(4)
C(5A)-N(51A)-C(51A)	129.5(5)
C(1A)-N(11A)-C(11A)	125.2(5)
S(1A)-C(1A)-N(12A)	119.3(5)
S(1A)-C(1A)-N(11A)	120.0(4)
N(12A)-C(1A)-N(11A)	120.7(5)
S(5A)-C(5A)-N(51A)	117.7(4)
S(5A)-C(5A)-N(52A)	120.6(5)
N(51A)-C(5A)-N(52A)	121.6(6)
S(4A)-C(4A)-N(41A)	118.8(3)

Table 10 Non-Hydrogen interatomic angles of $[Cu_4(ptu)_6Br_4]_2$ (cont).

Bond	Degrees
S(4A)-C(4A)-N(42A)	120.0(4)
N(41A)-C(4A)-N(42A)	121.2(5)
S(6A)-C(6A)-N(61A)	118.7(4)
S(6A)-C(6A)-N(62A)	119.3(5)
N(61A)-C(6A)-N(62A)	122.0(6)
C(31A)-N(31A)-C(3A)	127.1(5)
N(31A)-C(31A)-C(36A)	117.7(6)
N(31A)-C(31A)-C(32A)	121.6(5)
C(36A)-C(31A)-C(32A)	120.7(5)
N(41A)-C(41A)-C(46A)	117.3(4)
N(41A)-C(41A)-C(42A)	121.6(5)
C(46A)-C(41A)-C(42A)	121.1(5)
S(3A)-C(3A)-N(32A)	119.1(4)
S(3A)-C(3A)-N(31A)	118.0(4)
N(32A)-C(3A)-N(31A)	122.9(5)
C(41A)-C(46A)-C(45A)	119.3(5)
C(31A)-C(36A)-C(35A)	119.6(6)
C(2A)-N(21A)-C(21A)	125.4(5)

Table 10 Non-Hydrogen interatomic angles of $[Cu_4(ptu)_6Br_4]_2$ (cont).

Bond	Degrees
C(61A)-C(66A)-C(65A)	119.9(6)
N(51A)-C(51A)-C(56A)	117.8(5)
N(51A)-C(51A)-C(52A)	122.5(6)
C(56A)-C(51A)-C(52A)	119.6(6)
C(51A)-C(56A)-C(55A)	120.5(5)
C(32A)-C(33A)-C(34A)	120.4(6)
C(41A)-C(42A)-C(43A)	118.8(5)
C(31A)-C(32A)-C(33A)	119.3(5)
C(42A)-C(43A)-C(44A)	120.9(5)
C(36A)-C(35A)-C(34A)	119.8(6)
S(2A)-C(2A)-N(21A)	120.2(4)
S(2A)-C(2A)-N(22A)	119.7(5)
N(21A)-C(2A)-N(22A)	120.1(5)
C(33A)-C(34A)-C(35A)	120.2(6)
N(61A)-C(61A)-C(66A)	122.0(6)
N(61A)-C(61A)-C(62A)	118.1(5)
C(66A)-C(61A)-C(62A)	119.7(6)
C(51A)-C(52A)-C(53A)	119.1(6)

Table 10 Non-Hydrogen interatomic angles of $[Cu_4(ptu)_6Br_4]_2$ (cont).

Bond	Degrees
C(61A)-C(62A)-C(63A)	119.8(6)
C(62A)-C(63A)-C(64A)	120.5(6)
C(46A)-C(45A)-C(44A)	119.4(6)
C(56A)-C(55A)-C(54A)	120.2(6)
C(66A)-C(65A)-C(64A)	120.6(6)
N(11A)-C(11A)-C(12A)	119.9(5)
N(11A)-C(11A)-C(16A)	119.6(5)
C(12A)-C(11A)-C(16A)	120.5(6)
C(63A)-C(64A)-C(65A)	119.5(6)
C(11A)-C(12A)-C(13A)	119.9(6)
C(55A)-C(54A)-C(53A)	119.5(7)
C(43A)-C(44A)-C(45A)	120.6(6)
C(11A)-C(16A)-C(15A)	119.4(6)
C(52A)-C(53A)-C(54A)	121.1(6)
C(21A)-C(26A)-C(25A)	119.5(6)
N(21A)-C(21A)-C(26A)	119.8(5)
N(21A)-C(21A)-C(22A)	119.2(4)
C(26A)-C(21A)-C(22A)	121.0(5)

Table 10 Non-Hydrogen interatomic angles of $[Cu_4(ptu)_6Br_4]_2$ (cont).

Bond	Degrees
C(21A)-C(22A)-C(23A)	119.0(5)
C(22A)-C(23A)-C(24A)	119.6(7)
C(13A)-C(14A)-C(15A)	119.6(6)
C(23A)-C(24A)-C(25A)	121.8(6)
C(26A)-C(25A)-C(24A)	119.1(6)
C(12A)-C(13A)-C(14A)	120.2(6)
C(16A)-C(15A)-C(14A)	120.3(7)
Molecule B	
Br(1B)-Cu(1B)-S(4B)	109.14(4)
Br(1B)-Cu(1B)-S(1B)	110.27(4)
Br(1B)-Cu(1B)-S(5B)	114.66(5)
S(4B)-Cu(1B)-S(1B)	104.38(6)
S(4B)-Cu(1B)-S(5B)	109.02(6)
S(1B)-Cu(1B)-S(5B)	108.86(5)
Br(4B)-Cu(4B)-S(3B)	108.56(4)
Br(4B)-Cu(4B)-S(6B)	113.23(5)
Br(4B)-Cu(4B)-S(4B)	110.00(4)
S(3B)-Cu(4B)-S(6B)	103.83(5)

Table 10 Non-Hydrogen interatomic angles of $[Cu_4(ptu)_6Br_4]_2$ (cont).

Bond	Degrees
S(3B)-Cu(4B)-S(4B)	118.02(6)
S(6B)-Cu(4B)-S(4B)	103.09(5)
Br(3B)-Cu(3B)-S(3B)	112.15(5)
Br(3B)-Cu(3B)-S(5B)	118.80(5)
Br(3B)-Cu(3B)-S(2B)	109.98(5)
S(3B)-Cu(3B)-S(5B)	96.29(5)
S(3B)-Cu(3B)-S(2B)	117.04(6)
S(5B)-Cu(3B)-S(2B)	101.99(5)
Br(2B)-Cu(2B)-S(6B)	108.62(5)
Br(2B)-Cu(2B)-S(1B)	112.99(4)
Br(2B)-Cu(2B)-S(2B)	118.19(4)
S(6B)-Cu(2B)-S(1B)	112.64(5)
S(6B)-Cu(2B)-S(2B)	108.93(6)
S(1B)-Cu(2B)-S(2B)	95.01(6)
Cu(4B)-S(3B)-Cu(3B)	113.23(6)
Cu(4B)-S(3B)-C(3B)	108.1(2)
Cu(3B)-S(3B)-C(3B)	111.7(2)
Cu(4B)-S(6B)-Cu(2B)	113.70(7)

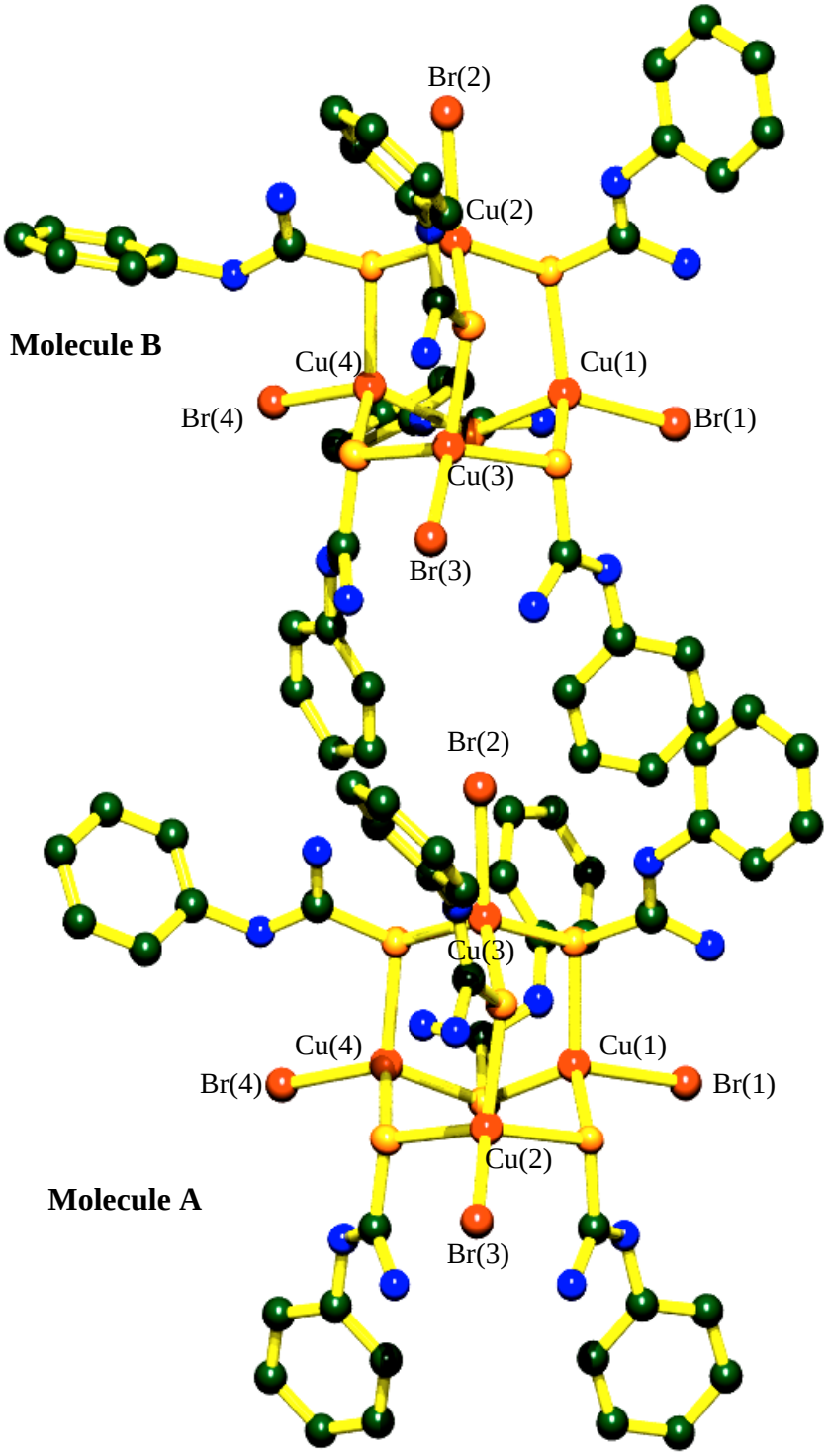

Figure 34 The structure of $[Cu_4(ptu)_6Br_4]_2$ (H atoms omitted for clarity).

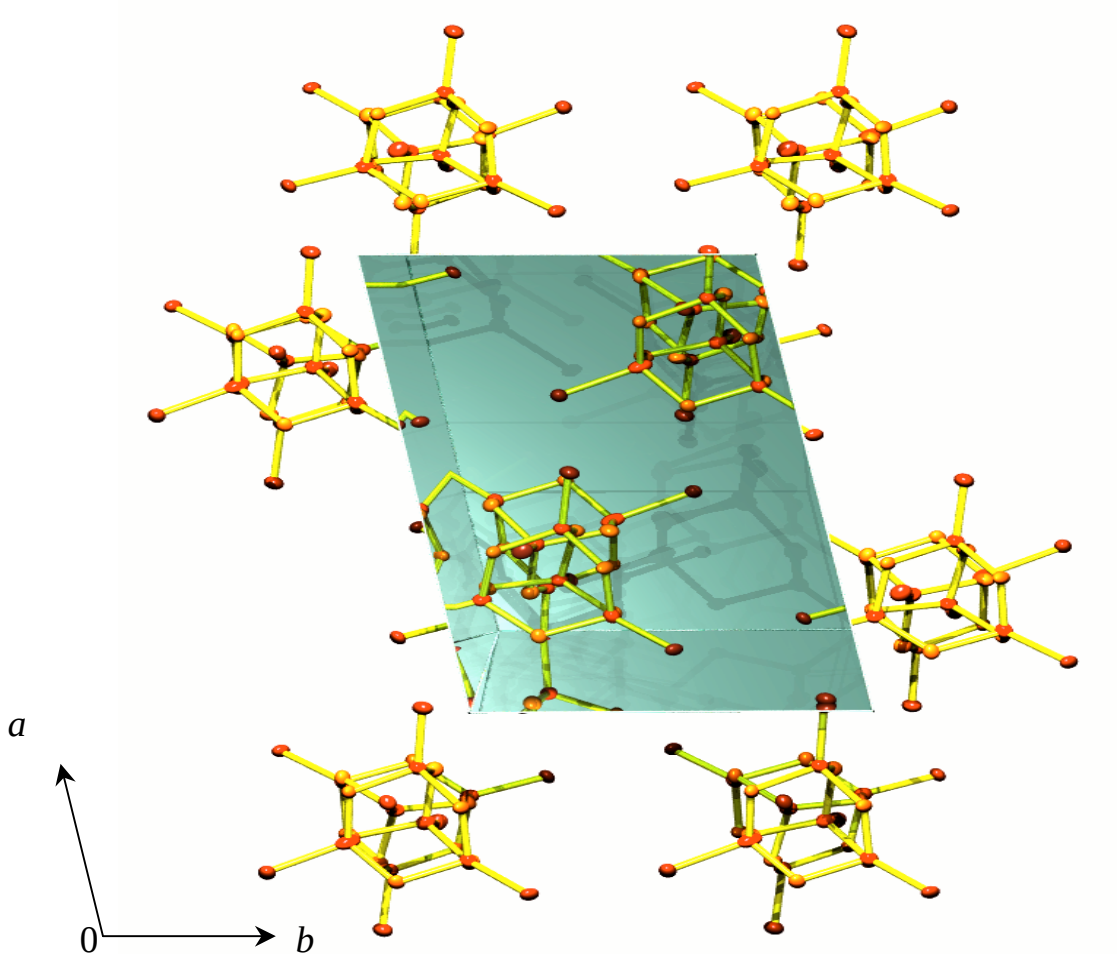

Figure 35 The unit cell contents of $[Cu_4(ptu)_6Br_4]_2$ projected down *c*.

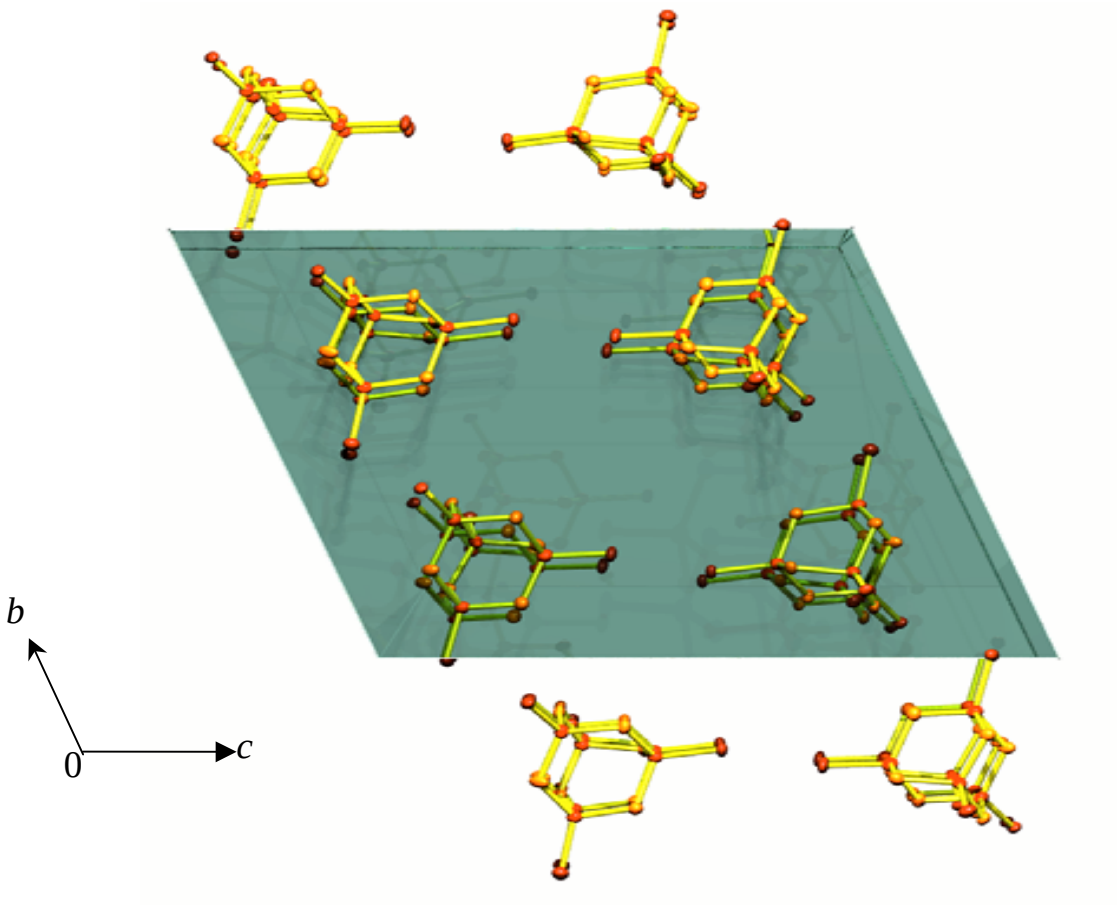

Figure 36 The unit cell contents of $[Cu_4(ptu)_6Br_4]_2$ projected down *a*.

Table 11 Crystallographic data for $[Cu_4(ptu)_6I_4]_2$.

Chemical formula	$Cu_8I_8S_{12}N_{24}C_{48}H_{96}$
Formula weight	3349.64
Color; habit	Colorless, plate
Crystal system	Triclinic
Space group	$P\bar{1}$ (No. 2)
Unit cell dimensions	
a (Å)	12.1943(1)
b (Å)	20.8855(4)
c (Å)	23.5722(4)
α (^{o})	82.121(1)
β (^{o})	89.217(1)
γ (^{o})	84.367(1)
V (Å^3)	5918.0(2)
Z	2
Density (calc.)(g cm^{-3})	1.88
F(000)	3232
Measured reflections	31688
Observed reflections	14959
Condition for observed reflections	$F>4\sigma(F)$
R	0.044
R_w	0.042

Table 12 Non-hydrogen interatomic distances of $[Cu_4(ptu)_6I_4]_2$.

Bond	Angstroms
Molecule A	
I(1A)-CU(1A)	2.6335(9)
I(2A)-CU(2A)	2.7466(9)
I(3A)-CU(3A)	2.6705(8)
I(4A)-CU(4A)	2.6261(9)
CU(1A)-S(1A)	2.421(2)
CU(1A)-S(4A)	2.310(2)
CU(1A)-S(5A)	2.376(1)
CU(2A)-S(1A)	2.283(2)
CU(2A)-S(2A)	2.312(2)
CU(2A)-S(6A)	2.311(2)
CU(3A)-S(2A)	2.368(2)
CU(3A)-S(3A)	2.313(2)
CU(3A)-S(5A)	2.306(2)
CU(4A)-S(3A)	2.340(1)
CU(4A)-S(4A)	2.352(2)
CU(4A)-S(6A)	2.325(2)
S(1A)-C(1A)	1.713(8)
S(2A)-C(2A)	1.724(6)
S(3A)-C(3A)	1.714(7)
S(4A)-C(4A)	1.717(6)

Table 12 Non-hydrogen interatomic distances of $[Cu_4(ptu)_6I_4]_2$ (cont).

Bond	Angstroms
S(5A)-C(5A)	1.715(8)
S(6A)-C(6A)	1.720(5)
N(11A)-C(1A)	1.331(9)
N(11A)-C(11A)	1.42(1)
N(12A)-C(1A)	1.30(1)
N(21A)-C(2A)	1.32(1)
N(21A)-C(21A)	1.41(1)
N(22A)-C(2A)	1.31(1)
N(31A)-C(3A)	1.331(9)
N(31A)-C(31A)	1.44(1)
N(32A)-C(3A)	1.317(8)
N(41A)-C(4A)	1.31(1)
N(41A)-C(41A)	1.428(9)
N(42A)-C(4A)	1.33(1)
N(51A)-C(5A)	1.342(7)
N(51A)-C(51A)	1.436(9)
N(52A)-C(5A)	1.29(1)
N(61A)-C(6A)	1.329(9)
N(61A)-C(61A)	1.432(8)
N(62A)-C(6A)	1.311(9)
C(11A)-C(12A)	1.35(1)

Table 12 Non-hydrogen interatomic distances of $[Cu_4(ptu)_6I_4]_2$ (cont).

Bond	Angstroms
C(11A)-C(16A)	1.38(1)
C(12A)-C(13A)	1.40(1)
C(13A)-C(14A)	1.35(1)
C(14A)-C(15A)	1.37(1)
C(15A)-C(16A)	1.40(2)
C(21A)-C(22A)	1.38(2)
C(21A)-C(26A)	1.37(2)
C(22A)-C(23A)	1.38(2)
C(23A)-C(24A)	1.43(4)
C(24A)-C(25A)	1.26(4)
C(25A)-C(26A)	1.33(3)
C(31A)-C(32A)	1.36(1)
C(31A)-C(36A)	1.36(1)
C(32A)-C(33A)	1.41(2)
C(33A)-C(34A)	1.34(2)
C(34A)-C(35A)	1.34(3)
C(35A)-C(36A)	1.43(2)
C(41A)-C(42A)	1.37(1)
C(41A)-C(46A)	1.37(1)
C(42A)-C(43A)	1.42(1)
C(43A)-C(44A)	1.37(2)

Table 12 Non-hydrogen interatomic distances of $[Cu_4(ptu)_6I_4]_2$ (cont).

Bond	Angstroms
C(44A)-C(45A)	1.34(2)
C(45A)-C(46A)	1.38(2)
C(51A)-C(52A)	1.37(1)
C(51A)-C(56A)	1.391(8)
C(52A)-C(53A)	1.39(1)
C(53A)-C(54A)	1.37(1)
C(54A)-C(55A)	1.34(1)
C(55A)-C(56A)	1.40(1)
C(61A)-C(62A)	1.39(1)
C(61A)-C(66A)	1.36(1)
C(62A)-C(63A)	1.38(1)
C(63A)-C(64A)	1.34(1)
C(64A)-C(65A)	1.36(1)
C(65A)-C(66A)	1.41(1)
Molecule B	
I(1B)-CU(1B)	2.6396(9)
I(2B)-CU(2B)	2.7604(9)
I(3B)-CU(3B)	2.8195(8)
I(4B)-CU(4B)	2.6565(9)
CU(1B)-S(1B)	2.388(2)
CU(1B)-S(4B)	2.309(2)

Table 12 Non-hydrogen interatomic distances of $[Cu_4(ptu)_6I_4]_2$ (cont).

Bond	Angstroms
CU(1B)-S(5B)	2.389(1)
CU(2B)-S(1B)	2.292(2)
CU(2B)-S(2B)	2.345(1)
CU(2B)-S(6B)	2.319(2)
CU(3B)-S(2B)	2.327(2)
CU(3B)-S(3B)	2.304(2)
CU(3B)-S(5B)	2.281(2)
CU(4B)-S(3B)	2.327(1)
CU(4B)-S(4B)	2.359(2)
CU(4B)-S(6B)	2.333(2)
S(1B)-C(1B)	1.720(8)
S(2B)-C(2B)	1.721(7)
S(3B)-C(3B)	1.715(7)
S(4B)-C(4B)	1.718(6)
S(5B)-C(5B)	1.723(7)
S(6B)-C(6B)	1.719(5)
N(11B)-C(1B)	1.334(9)
N(11B)-C(11B)	1.44(1)
N(12B)-C(1B)	1.31(1)
N(21B)-C(2B)	1.32(1)
N(21B)-C(21B)	1.41(1)

Table 12 Non-hydrogen interatomic distances of $[Cu_4(ptu)_6I_4]_2$ (cont).

Bond	Angstroms
N(22B)-C(2B)	1.309(9)
N(31B)-C(3B)	1.328(9)
N(31B)-C(31B)	1.44(1)
N(32B)-C(3B)	1.317(8)
N(41B)-C(4B)	1.31(1)
N(41B)-C(41B)	1.443(9)
S(2B)-C(2B)	1.721(7)
C(25B)-C(26B)	1.37(2)
C(31B)-C(32B)	1.38(2)
C(31B)-C(36B)	1.35(1)
C(32B)-C(33B)	1.40(2)
C(33B)-C(34B)	1.35(2)
C(34B)-C(35B)	1.39(3)
C(35B)-C(36B)	1.42(2)
C(41B)-C(42B)	1.37(1)
C(41B)-C(46B)	1.38(1)
C(42B)-C(43B)	1.40(1)
C(43B)-C(44B)	1.37(2)
C(44B)-C(45B)	1.34(2)
C(45B)-C(46B)	1.42(1)
C(51B)-C(52B)	1.37(1)

Table 12 Non-hydrogen interatomic distances of $[Cu_4(ptu)_6I_4]_2$ (cont).

Bond	Angstroms
C(51B)-C(56B)	1.371(9)
C(52B)-C(53B)	1.39(1)
C(53B)-C(54B)	1.37(1)
C(54B)-C(55B)	1.35(2)
C(55B)-C(56B)	1.37(1)
C(61B)-C(62B)	1.34(1)
C(61B)-C(66B)	1.38(2)
C(62B)-C(63B)	1.39(1)
C(63B)-C(64B)	1.33(2)
C(64B)-C(65B)	1.38(3)
C(65B)-C(66B)	1.41(2)

Table 13 Non-hydrogen interatomic angles of $[Cu_4(ptu)_6I_4]_2$.

Bond	Degrees
Molecule A	
I(1A)-CU(1A)-S(1A)	108.29(5)
I(1A)-CU(1A)-S(4A)	119.01(5)
I(1A)-CU(1A)-S(5A)	115.68(5)
I(2A)-CU(2A)-S(1A)	115.11(5)
I(2A)-CU(2A)-S(2A)	99.25(5)
I(2A)-CU(2A)-S(6A)	106.82(5)
I(3A)-CU(3A)-S(2A)	103.95(4)
I(3A)-CU(3A)-S(3A)	110.95(5)
I(3A)-CU(3A)-S(5A)	116.06(4)
I(4A)-CU(4A)-S(3A)	117.59(6)
I(4A)-CU(4A)-S(4A)	114.58(5)
I(4A)-CU(4A)-S(6A)	112.57(5)
CU(1A)-S(1A)-CU(2A)	109.41(7)
CU(1A)-S(1A)-C(1A)	107.5(2)
CU(2A)-S(1A)-C(1A)	107.6(2)
CU(2A)-S(2A)-CU(3A)	104.43(7)
CU(2A)-S(2A)-C(2A)	104.4(2)
CU(3A)-S(2A)-C(2A)	99.4(2)
CU(3A)-S(3A)-CU(4A)	116.03(8)
CU(3A)-S(3A)-C(3A)	110.7(2)

Table 13 Non-hydrogen interatomic angles of $[Cu_4(ptu)_6I_4]_2$ (cont).

Bond	Degrees
CU(4A)-S(3A)-C(3A)	109.4(2)
CU(1A)-S(4A)-CU(4A)	120.11(8)
CU(1A)-S(4A)-C(4A)	115.9(3)
CU(4A)-S(4A)-C(4A)	117.5(3)
CU(1A)-S(5A)-CU(3A)	115.45(6)
CU(1A)-S(5A)-C(5A)	111.4(2)
CU(3A)-S(5A)-C(5A)	108.9(2)
CU(2A)-S(6A)-CU(4A)	113.30(6)
CU(2A)-S(6A)-C(6A)	109.7(2)
CU(4A)-S(6A)-C(6A)	113.1(2)
S(1A)-CU(1A)-S(4A)	107.28(6)
S(1A)-CU(1A)-S(5A)	109.45(6)
S(4A)-CU(1A)-S(5A)	96.34(6)
S(1A)-CU(2A)-S(2A)	112.73(6)
S(1A)-CU(2A)-S(6A)	107.77(6)
S(2A)-CU(2A)-S(6A)	115.06(7)
S(2A)-CU(3A)-S(3A)	108.97(6)
S(2A)-CU(3A)-S(5A)	105.22(7)
S(3A)-CU(3A)-S(5A)	111.07(6)
S(3A)-CU(4A)-S(4A)	102.92(6)
S(3A)-CU(4A)-S(6A)	96.52(6)

Table 13 Non-hydrogen interatomic angles of $[Cu_4(ptu)_6I_4]_2$ (cont).

Bond	Degrees
S(4A)-CU(4A)-S(6A)	110.98(7)
C(1A)-N(11A)-H(1A)	115(5)
C(11A)-N(11A)-H(1A)	114(5)
C(2A)-N(21A)-C(21A)	129.2(6)
C(3A)-N(31A)-C(31A)	129.3(5)
C(4A)-N(41A)-C(41A)	128.8(6)
C(5A)-N(51A)-C(51A)	128.4(7)
C(6A)-N(61A)-C(61A)	125.8(6)
S(1A)-C(1A)-N(11A)	119.8(6)
S(1A)-C(1A)-N(12A)	119.4(6)
N(11A)-C(1A)-N(12A)	120.8(8)
N(11A)-C(11A)-C(12A)	123.0(6)
N(11A)-C(11A)-C(16A)	117.0(7)
C(12A)-C(11A)-C(16A)	119.9(7)
C(11A)-C(12A)-C(13A)	120.7(7)
C(12A)-C(13A)-C(14A)	119.6(8)
C(13A)-C(14A)-C(15A)	121(1)
C(14A)-C(15A)-C(16A)	119.8(8)
C(11A)-C(16A)-C(15A)	119.2(8)
S(2A)-C(2A)-N(21A)	122.0(5)
S(2A)-C(2A)-N(22A)	118.5(6)

Table 13 Non-hydrogen interatomic angles of $[Cu_4(ptu)_6I_4]_2$ (cont).

Bond	Degrees
N(21A)-C(2A)-N(22A)	119.5(7)
N(21A)-C(21A)-C(22A)	122.0(9)
N(21A)-C(21A)-C(26A)	118(1)
C(22A)-C(21A)-C(26A)	120(1)
C(21A)-C(22A)-C(23A)	119(1)
C(22A)-C(23A)-C(24A)	119(2)
C(23A)-C(24A)-C(25A)	117(2)
C(24A)-C(25A)-C(26A)	128(2)
C(21A)-C(26A)-C(25A)	117(1)
S(3A)-C(3A)-N(31A)	119.3(4)
S(3A)-C(3A)-N(32A)	121.3(6)
N(31A)-C(3A)-N(32A)	119.3(7)
N(31A)-C(31A)-C(32A)	118.5(7)
N(31A)-C(31A)-C(36A)	121.2(9)
C(32A)-C(31A)-C(36A)	120.2(9)
C(31A)-C(32A)-C(33A)	120.7(9)
C(32A)-C(33A)-C(34A)	118(1)
C(33A)-C(34A)-C(35A)	123(1)
C(34A)-C(35A)-C(36A)	118(1)
C(31A)-C(36A)-C(35A)	119(1)
S(4A)-C(4A)-N(41A)	120.4(5)

Table 13 Non-hydrogen interatomic angles of $[Cu_4(ptu)_6I_4]_2$ (cont).

Bond	Degrees
S(4A)-C(4A)-N(42A)	119.2(6)
N(41A)-C(4A)-N(42A)	120.4(6)
N(41A)-C(41A)-C(42A)	117.5(6)
N(41A)-C(41A)-C(46A)	120.4(6)
C(42A)-C(41A)-C(46A)	122.0(7)
C(41A)-C(42A)-C(43A)	117.6(9)
C(42A)-C(43A)-C(44A)	119(1)
C(43A)-C(44A)-C(45A)	122(1)
C(44A)-C(45A)-C(46A)	120(1)
C(41A)-C(46A)-C(45A)	119.4(8)
S(5A)-C(5A)-N(51A)	119.3(6)
S(5A)-C(5A)-N(52A)	119.9(5)
N(51A)-C(5A)-N(52A)	120.8(7)
N(51A)-C(51A)-C(52A)	122.2(5)
N(51A)-C(51A)-C(56A)	117.3(7)
C(52A)-C(51A)-C(56A)	120.3(7)
C(51A)-C(52A)-C(53A)	119.5(6)
C(52A)-C(53A)-C(54A)	120.1(9)
C(53A)-C(54A)-C(55A)	120.6(8)
C(54A)-C(55A)-C(56A)	120.7(7)
C(51A)-C(56A)-C(55A)	118.6(8)

Table 13 Non-hydrogen interatomic angles of $[Cu_4(ptu)_6I_4]_2$ (cont).

Bond	Degrees
S(6A)-C(6A)-N(61A)	120.8(5)
S(6A)-C(6A)-N(62A)	119.6(5)
N(61A)-C(6A)-N(62A)	119.6(5)
N(61A)-C(61A)-C(62A)	120.0(6)
N(61A)-C(61A)-C(66A)	119.8(6)
C(62A)-C(61A)-C(66A)	120.3(6)
C(61A)-C(62A)-C(63A)	118.7(8)
C(62A)-C(63A)-C(64A)	121.2(8)
C(63A)-C(64A)-C(65A)	120.9(8)
C(64A)-C(65A)-C(66A)	119.2(9)
C(61A)-C(66A)-C(65A)	119.7(7)
Molecule B	
I(1B)-CU(1B)-S(1B)	110.04(5)
I(1B)-CU(1B)-S(4B)	118.73(5)
I(1B)-CU(1B)-S(5B)	112.63(5)
S(1B)-CU(1B)-S(4B)	107.25(7)
S(1B)-CU(1B)-S(5B)	110.96(6)
S(4B)-CU(1B)-S(5B)	96.46(6)
I(2B)-CU(2B)-S(1B)	113.49(5)
I(2B)-CU(2B)-S(2B)	109.25(5)
I(2B)-CU(2B)-S(6B)	110.50(5)

Table 13 Non-hydrogen interatomic angles of $[Cu_4(ptu)_6I_4]_2$ (cont).

Bond	Degrees
S(1B)-CU(2B)-S(2B)	107.96(6)
S(1B)-CU(2B)-S(6B)	110.95(6)
S(2B)-CU(2B)-S(6B)	104.24(6)
I(3B)-CU(3B)-S(2B)	105.84(4)
I(3B)-CU(3B)-S(3B)	103.71(5)
I(3B)-CU(3B)-S(5B)	111.73(4)
S(2B)-CU(3B)-S(3B)	109.54(6)
S(2B)-CU(3B)-S(5B)	111.25(7)
S(3B)-CU(3B)-S(5B)	114.21(6)
I(4B)-CU(4B)-S(3B)	114.43(6)
I(4B)-CU(4B)-S(4B)	112.32(5)
I(4B)-CU(4B)-S(6B)	114.78(5)
S(3B)-CU(4B)-S(4B)	104.02(6)
S(3B)-CU(4B)-S(6B)	98.17(6)
S(4B)-CU(4B)-S(6B)	111.86(7)
CU(1B)-S(1B)-CU(2B)	114.27(7)
CU(1B)-S(1B)-C(1B)	110.1(2)
CU(2B)-S(1B)-C(1B)	108.9(2)
CU(2B)-S(2B)-CU(3B)	108.37(6)
CU(2B)-S(2B)-C(2B)	102.9(2)
CU(3B)-S(2B)-C(2B)	105.1(2)

Table 13 Non-hydrogen interatomic angles of $[Cu_4(ptu)_6I_4]_2$ (cont).

Bond	Degrees
CU(3B)-S(3B)-CU(4B)	109.57(7)
CU(3B)-S(3B)-C(3B)	112.6(2)
CU(4B)-S(3B)-C(3B)	110.0(2)
CU(1B)-S(4B)-CU(4B)	119.93(8)
CU(1B)-S(4B)-C(4B)	115.3(3)
CU(4B)-S(4B)-C(4B)	118.2(2)
CU(1B)-S(5B)-CU(3B)	109.78(6)
CU(1B)-S(5B)-C(5B)	110.7(2)
CU(3B)-S(5B)-C(5B)	107.7(2)
CU(2B)-S(6B)-CU(4B)	115.92(7)
CU(2B)-S(6B)-C(6B)	109.6(2)
CU(4B)-S(6B)-C(6B)	110.0(2)
C(1B)-N(11B)-C(11B)	125.8(6)
C(2B)-N(21B)-C(21B)	128.0(6)
C(3B)-N(31B)-C(31B)	128.5(6)
C(4B)-N(41B)-C(41B)	128.6(7)
C(5B)-N(51B)-C(51B)	127.9(7)
C(6B)-N(62B)-C(61B)	125.2(6)
S(1B)-C(1B)-N(11B)	119.5(5)
S(1B)-C(1B)-N(12B)	119.7(6)
N(11B)-C(1B)-N(12B)	120.8(8)

Table 13 Non-hydrogen interatomic angles of $[Cu_4(ptu)_6I_4]_2$ (cont).

Bond	Degrees
N(11B)-C(11B)-C(12B)	119.4(7)
N(11B)-C(11B)-C(16B)	120.1(8)
C(12B)-C(11B)-C(16B)	120.3(9)
C(11B)-C(12B)-C(13B)	118.3(8)
C(12B)-C(13B)-C(14B)	121(1)
C(13B)-C(14B)-C(15B)	120(1)
C(14B)-C(15B)-C(16B)	120(1)
C(11B)-C(16B)-C(15B)	120(1)
S(2B)-C(2B)-N(21B)	120.8(5)
S(2B)-C(2B)-N(22B)	121.0(6)
N(21B)-C(2B)-N(22B)	118.2(7)
N(21B)-C(21B)-C(22B)	120.1(7)
N(21B)-C(21B)-C(26B)	120.1(7)
C(22B)-C(21B)-C(26B)	119.7(8)
C(21B)-C(22B)-C(23B)	119.3(9)
C(22B)-C(23B)-C(24B)	120(1)
C(23B)-C(24B)-C(25B)	121(1)
C(24B)-C(25B)-C(26B)	121(1)
C(21B)-C(26B)-C(25B)	119.7(9)
S(3B)-C(3B)-N(31B)	119.5(4)
S(3B)-C(3B)-N(32B)	120.3(6)

Table 13 Non-hydrogen interatomic angles of $[Cu_4(ptu)_6I_4]_2$ (cont).

Bond	Degrees
N(31B)-C(3B)-N(32B)	120.1(7)
N(31B)-C(31B)-C(32B)	117.0(7)
N(31B)-C(31B)-C(36B)	121(1)
C(32B)-C(31B)-C(36B)	122(1)
C(31B)-C(32B)-C(33B)	122(1)
C(32B)-C(33B)-C(34B)	117(1)
C(33B)-C(34B)-C(35B)	122(2)
C(34B)-C(35B)-C(36B)	121(1)
C(31B)-C(36B)-C(35B)	116(1)
S(4B)-C(4B)-N(41B)	119.8(5)
S(4B)-C(4B)-N(42B)	120.0(6)
N(41B)-C(4B)-N(42B)	120.2(6)
N(41B)-C(41B)-C(42B)	120.0(6)
N(41B)-C(41B)-C(46B)	117.8(6)
C(42B)-C(41B)-C(46B)	122.2(7)
C(41B)-C(42B)-C(43B)	118.4(8)
C(42B)-C(43B)-C(44B)	120(1)
C(43B)-C(44B)-C(45B)	121(1)
C(44B)-C(45B)-C(46B)	120.9(9)
C(41B)-C(46B)-C(45B)	117.3(9)
S(5B)-C(5B)-N(51B)	118.8(6)

Table 13 Non-hydrogen interatomic angles of $[Cu_4(ptu)_6I_4]_2$ (cont).

Bond	Degrees
S(5B)-C(5B)-N(52B)	120.2(5)
N(51B)-C(5B)-N(52B)	120.9(7)
N(51B)-C(51B)-C(52B)	122.3(6)
N(51B)-C(51B)-C(56B)	118.3(8)
C(52B)-C(51B)-C(56B)	119.3(7)
C(51B)-C(52B)-C(53B)	119.2(7)
C(52B)-C(53B)-C(54B)	119.6(9)
C(53B)-C(54B)-C(55B)	121.3(9)
C(54B)-C(55B)-C(56B)	119.0(8)
C(51B)-C(56B)-C(55B)	121(1)
S(6B)-C(6B)-N(61B)	121.2(5)
S(6B)-C(6B)-N(62B)	120.3(5)
N(61B)-C(6B)-N(62B)	118.5(5)
N(62B)-C(61B)-C(62B)	121.8(8)
N(62B)-C(61B)-C(66B)	118.4(8)
C(62B)-C(61B)-C(66B)	119.9(8)
C(61B)-C(62B)-C(63B)	122(1)
C(63B)-C(64B)-C(65B)	124(1)
C(64B)-C(65B)-C(66B)	117(2)
C(61B)-C(66B)-C(65B)	120(1)

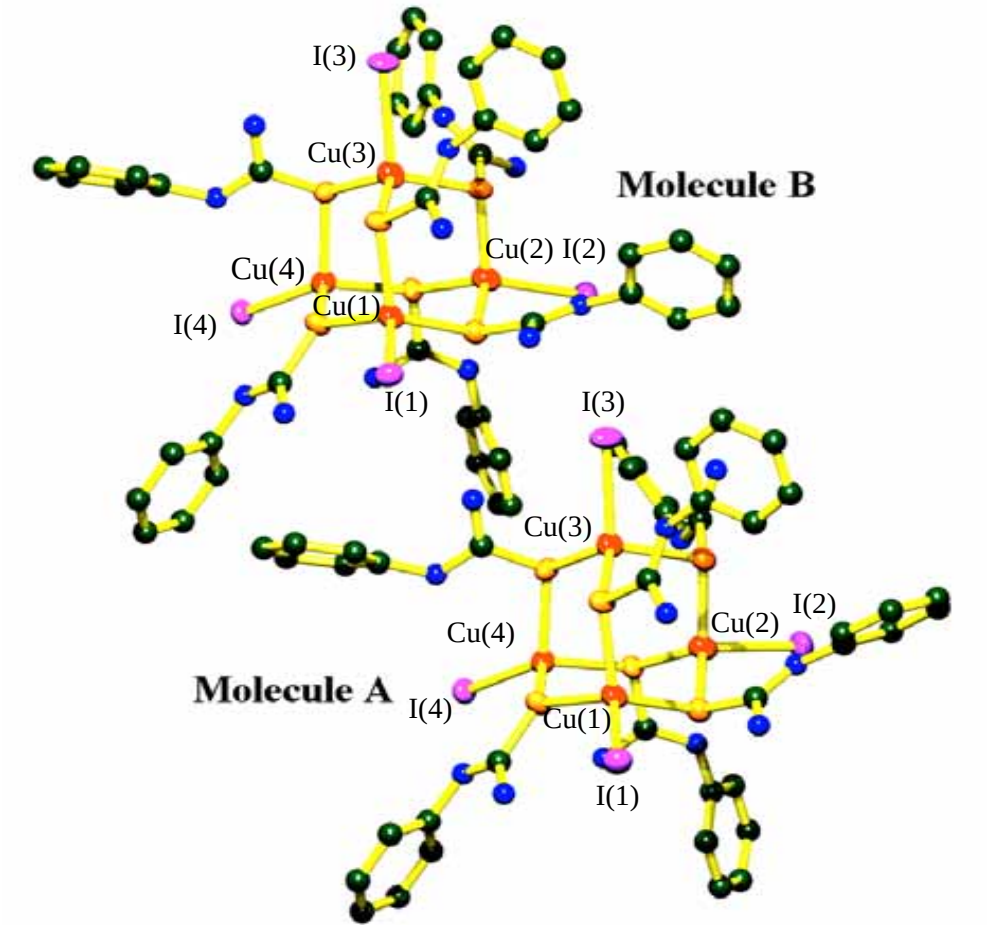

Figure 37 The structure of $[Cu_4(ptu)_6I_4]_2$ (H atoms omitted for clarity).

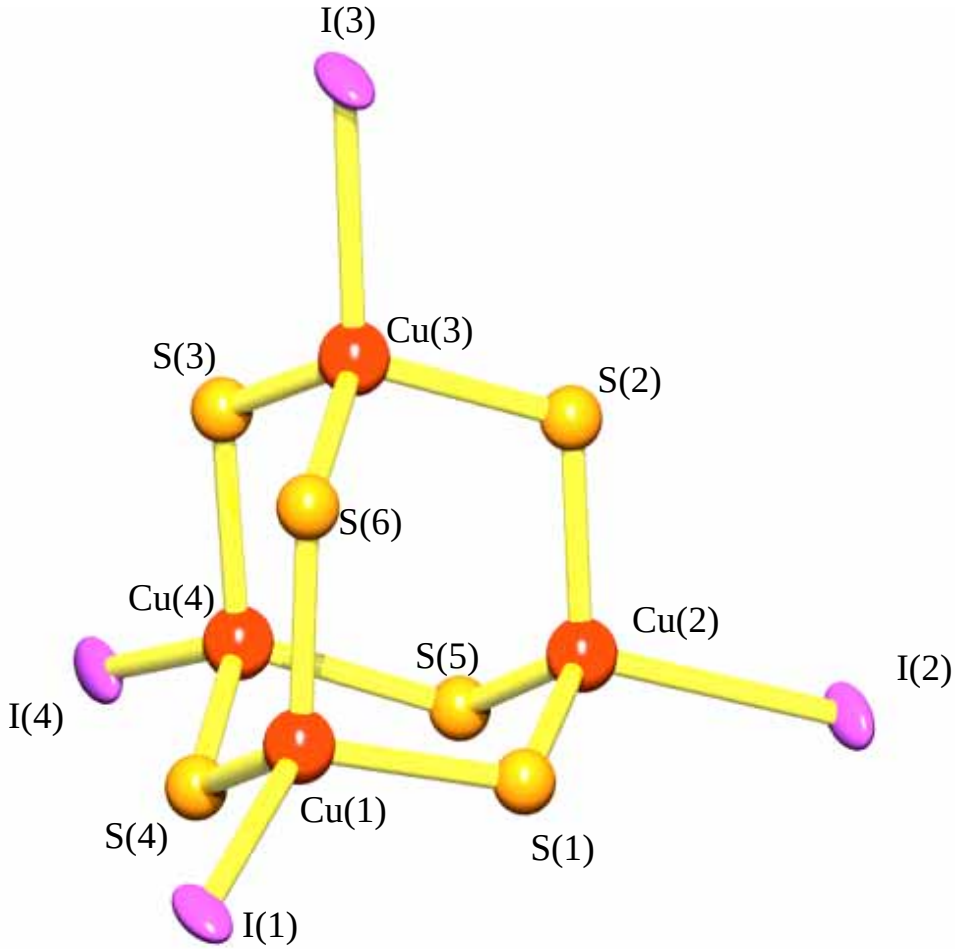

Figure 38 The core structure of $[Cu_4(ptu)_6I_4]$ (H, C and N atoms omitted for clarity).

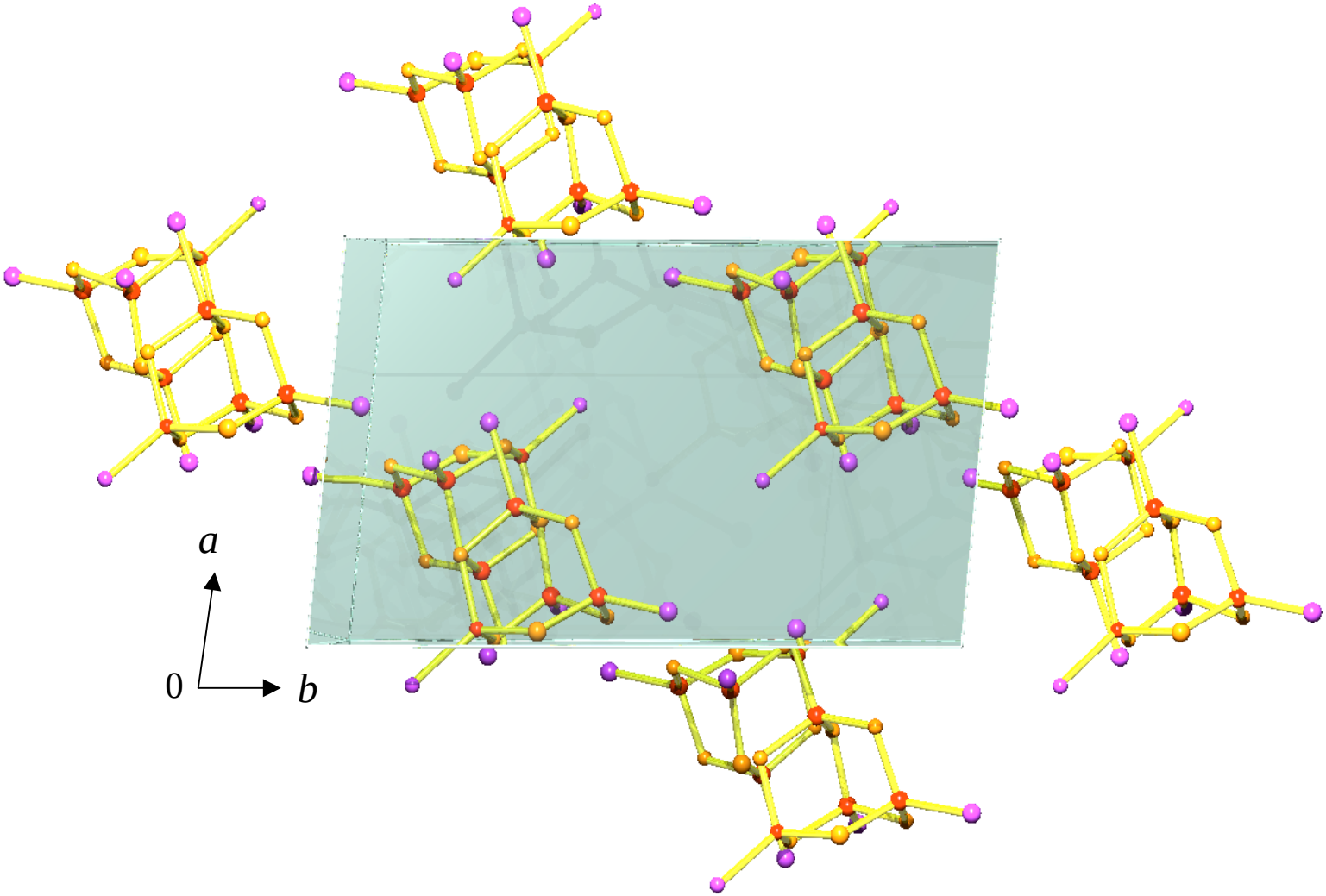

Figure 39 Unit cell contents of $[Cu_4(ptu)_6I_4]_2$ projected down *c*.

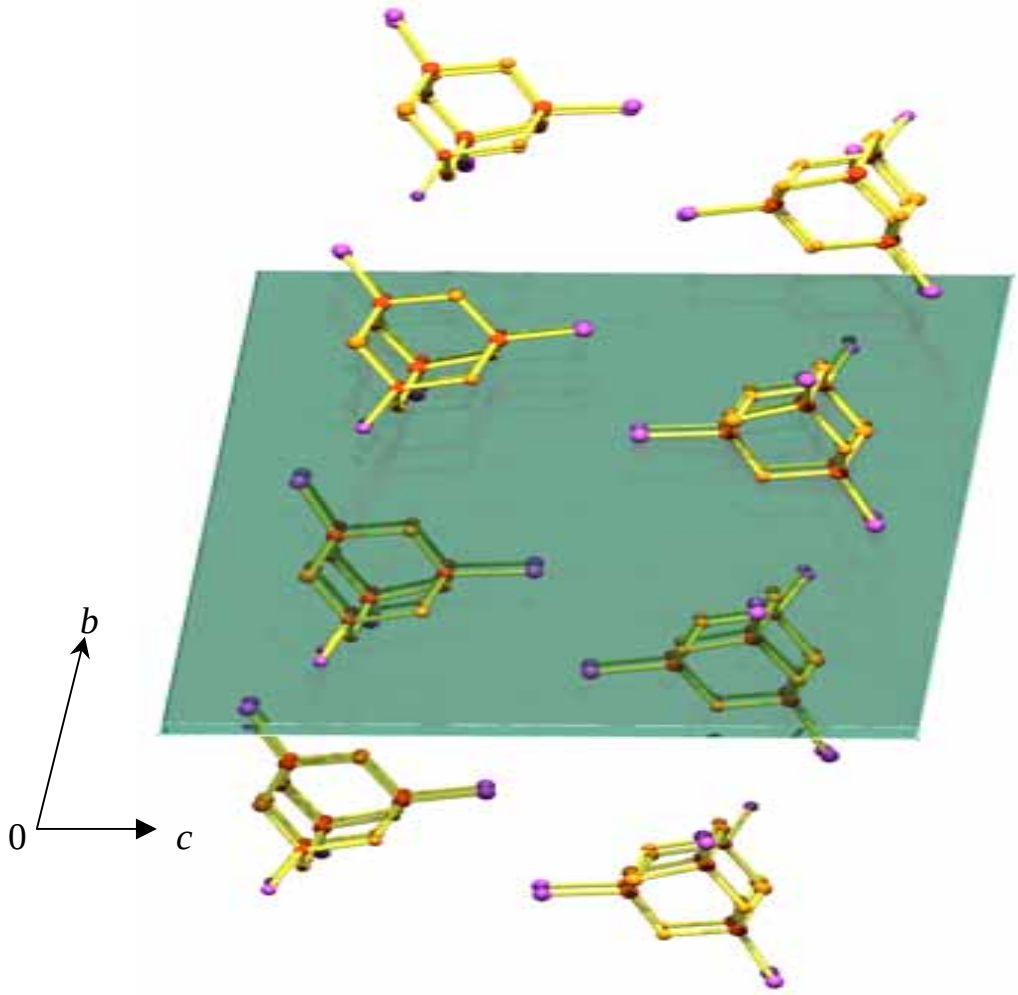

Figure 40 Unit cell contents of $[Cu_4(ptu)_6I_4]_2$ projected down *a*.