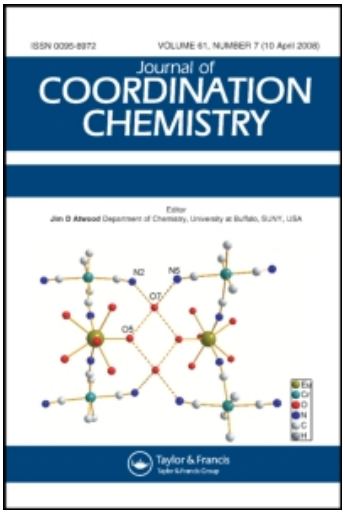

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COPPER (II) COORDINATION COMPOUNDS: CLASSIFICATION AND ANALYSIS OF CRYSTALLOGRAPHIC AND STRUCTURAL DATA

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COPPER (II) COORDINATION COMPOUNDS: CLASSIFICATION AND ANALYSIS OF CRYSTALLOGRAPHIC AND STRUCTURAL DATA

I. Mononuclear Tetra — and Pentacoordinate Compounds

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This review summarizes the data for over twelve hundred four - and five - coordinate copper(II) coordination compounds. The four-coordinate derivatives are mostly distorted square-planar. The five-coordinate derivatives are mostly square-pyramidal. The most common ligands are oxygen- and nitrogen- donors. There is a trend for the Cu-L distance to increase with covalent radius of the coordinated atom and also increasing coordination number. There are three types of isomerism - distortion, *cis*- and *trans*- and configuration. Several relationships are found and discussed.

Keywords: review; copper(II); crystallography; structures

CONTENTS

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0 ABBREVIATIONS

abapt	(2'–aminophenyl–2,6–diaza–6–methyl–9–amino–1 nonene
ac	acetate
ac–α–ala	N–acetyl–α–alaninate
acac	acetylacetonate, (2 ,4–pentanedionate)
acasp	N–acetyl–L–asparate
acaz	3, ll–diacetato–7–methyl–3 ,7,11, 17–tetraaza-bicyclo–[11.3.1]heptadeca–1(17) ,13,15–triene
acgln	N–acetyl–L–glutamine
acgly	N–acetylglycinate
acphim	N–n–decyl–o–hydroxyacetophenoniminate
acpn	3,3'dichloro–1,2'–(1,12–diphenyl–2, 6, 11–triaza-dodeca–1, 11–diene–l, 12–diyl)bisphenol
acpyr	4– (N–acetylamino)pyridine
acrp	monodeprotonated 4–hydroxy–6–methyl–3– [dimethyl-aminoacryloyl 3 –2H–pyran–2–one
ade	adenine
adeH	adeninium
adeNo	adenine–N^1–oxide, doubly deprotonated
ae	7–amino–4–methyl–5–aza–3–hepten–2–one
4 aepy	2–(2–aminoethyl) pyridine
ahmi	2–azohexamethylenimine
α –aib	α –aminoisobutyrate
3–alacac	3–allylacetylacetonate
β–alaH	β–alaninium
amen –qu	8,8' –bis(aminoethyl)–2,2' –biquinoline
amet	N, N' –bis (3–aminopropyl) –l, 2–ethanediamine
(amet) mfH_2	N–(2–aminoethyl) morpholinium
ampi	N–(2–ammoniumethyl)–piperazinium cation
2–ampy	2–aminomethylpyridine
amsal	N–{2[(2aminoethyl)amino]ethyl}salicylideneaminate
9–aneN_2S	1–thia–4, 7–diazacyclononane
9–aneN_3	1, 4, 7–triazacyclononane
12–aneN_4	1,4,7, 10–tetraazacyclodecane
12 –anebN_4	1, 4, 7, 10–tetrabenzyl–l, 4,7, 10–tetraazacyclodo-decane
12–aneS_4	1, 4, 7, 10–tetrathiacyclododecane
13–aneS_4	1, 4, 7, l0–tetrathiacyclotridecane

13 –aneN_3O	1–oxa–4, 7, 11–triazacyclotridecane
17–aneN_5	1, 4, 7, 11, 14–pentaazacycloheptadecane
anic	amidonikotinate
apip	(3S)–3–aminopiperidine
asaln	N–allylsalicylideneminate
L–asp	L–asparate
asp	asparaginate
ath	2–amino–l, 3–thiazoline
azaH	7–azaindole
azam	4, 7–diazadecanediamine
azaxa	1, 5,8,12–tetraaza–17–oxabicyclo[10.5. 2]nonadecane
azdec	(2S, 6R,(9S,13R)–2,6,9,13–tetraazatetradecane
azoc	4, 4' –methyl–4–aza–1, 7–heptadienyl–dinitriloK^{3}N)-bis(2–pentanonato–K^2 0)
bac	benzoylacetonate
bamp	bis–2,4–(2–amino–2–methylpropanamido) 2, 4–dimethylpentanone
bampy	2–benzothiazolin–2–ylideneaminoethylpyridine (picolinate)
bapur	6–benzylaminopurine
barb	Schiff base derived from barbituric acid
bbes	1, 5–bis (benzimidazol–2–yl) –3–thiapentane
bbdh	1, 6–bis (2–benzimidazolyl) –2, 5–dithiahexane
bbidh	1,6–bis(N–benzylimidazol–2–yl) –2, 5–dithiahexane
bbtt	1, 2–big (benzimidazol–2' –ylmethylthio) –benzene
bcp	2, 9–dimethyl–4, 7–diphenyl–1, 10–phenanthroline
bddh	1,6–bis(3,5–dimethyl–1–pyrazolyl) –2, 5–dithiahexane
bddn	1,9–bis(3,5–dimethyl–1–pyrazolyl) –3, 7–dithianonane
bddo	1,8–bis(3,5–dimethyl–1–pyrazolyl) –3, 6–dithiaoctane
bdma	bis[2–(3,5–dimethylpyrazolyl)ethyl] (2–methylthioethyl) amine
beeda	N, N' – (bis (2–benzimidazolylethyl)ethylenediamine
bedt–ttf	bis (ethylenedithio) tetrathiofulvalenium
behyacph	N–benzyl–o–hydroxyacetophenoneimine
benox	3,4:9,10–dibenzo–1,12–diaza–5,8–dioxo pentadecane
benz	N–3,4–benzosalicylidene–N'–methylenediamine

benzdm	N–3 ,4–benzosalicylidene–N,N'–dimethylethylene-diamine
bgH	N–benzenesulphonylglycinate
bgly	N–benzyloxycarbonyl–glycinate
bheg	N, N–bis (2–hydroxyethyl)glycinate
bhdhx	1,6–bis (4–imidazolyl) –2 ,5–dithiahexane
bimbph	2, 2' –bis (2–imidazolyl) biphenyl
bipyam	2, 2' –bipyridylamine
biu	biuretate
bmca	bis (methoxycarbimido) aminate
bmdhp	1,7–bis(N–methylbenzimidazol–2' –yl)– 2, 6–di-thiaheptane
bnzen	N, N' –dibenzylethylenediamine
bosf	bis (oxamido) trisulfane
bpac	N, N–bis(pyrazol–1–ylmethyl)aminoethane
bpdz	1, 7–bis (2–pyridyl) –2, 6–diazaheptane
bps	N, N' – (2, 2' –biphenyl) –bis (salicylaldiminate)
bpno	bis(1–pyrazolyl)methyl) (2, 2, 6, 6–tetramethyl–1–oxy–4–piperidinyl) amine
bpnp	2–[bis(2–pyridyl–methyl)aminomethyl] –4 –nitro-phenolate,
bppa	2–pyridyl–2–pyrimidylamine
bppn	N,N'–bis(2'–pyridinecarboxamido) –1, 3–propane
bpy	bipyridine
o–bpy	1, 2–bis(2, 2'–bipyridyl–6–yl)ethane
bpycp	1, 3–bis(6" –methyl–2,2" –bipyridyl)–2,2–bis(car-boxy) propane
bpydo	1, 9–bis–(2–pyridyl)–2, 5, 8–triazonane
bpym	2,2' –bipyrimidine
bpyO	2, 2' –bipyridine–N, N'–dioxide
bpz	monochlorid salt of the N–benzylpiperazinum(2+)
bquan	biquanide
bs–glyNO	N–benzenesulphonylglycinate (2–)
bta	benzotriazole
btma	tris (2–benzothiazolyl)amine
btos	benzoylhydrazinato–o–tosylamino–benzaldehyde
n–Bucbp	N–n–butyl–(5–chloro–α–phenyl–2–hydroxybenzili-dene) aminate
buox	3,3'(1,4–butanediyldiamino)bis(3–methyl–2–buta-none)dioxime

But–Megly	N–tert–butyl–N–methylglycinate
bz	benzoate
bzac	1–phenyl–1, 3–butanedionate
bzacac	ligand derived from benzoylhydrazone and acetylacetone
bzacen	Schiff base anion formed between ethane–1, 2–diamine and benzoylacetone
bz–D–prol	N–benzyl–D–prolinate
bz–L–prol	N–benzyl–L–prolinate
bz–L–val	N–benzyl–L–valinate
bzim	benzimidazole
bzimH	benzimidazolium
bzimp	2, 6–bis (2–benzimidazolyl) pyridine
bzph	2–aminobenzophenone
$bzpipH_2$	N–benzylpiperazinium
bzpyoxal	N–benzylpyridoxaldiminate
c	cubic
camph	3–nitrocamphorate
carboxam	bis (pyridine–2–carboxamide)
cbcx	N,N' –bis (β – carbamoylethyl) – trans –1, 2– cyclohexamine
cbp–phen–sal	Schiff base derived from 1, 2–diaminobenzene,5–chloro– 2–hydroxybenzophenone and substituted salicylaldehydes
cbp–phen OMesal	– " –
cbp–phen–Clsal	– " –
cbphex	2–carbamoylphenoxyacetate
cbps	N,N' bis {(5–chloro–2–hydroxyphenyl)phenylmethylene} –4–thiaheptane –l, 7–diamine
cdd	cyclotridecane–1, 3–dionate
chSpam	N–cyclohexylthiopicolinamidate
Cla	chloranilinate (2–)
$C_{l2}ac$	dichloracetate
Cl_3ac	trichloroacetate
Cl_3acH	trichloroacetic acid
2–Clbz	2–chlorobenzoate
5Cl–oha–shz	5–chloro–2–hydroxyacetophenone–salicylhydrazide
ClphS	p–chlorothiophenol
Clqo	4–chloro–1, 2–benzoquinone 2–oximate
2–cmpy	2–carbamoylpyrazine

cnd	dicyanoethenedithiolate
cnmet	tricyanomethanide
col	collidine
cpmp	1, 1–bis (6–carboxy–2–pyridyl) –1–methoxypropane
croc	croconate
18–crown–6	1, 4, 7, 10, 13, 16–hexaoxacyclooctadecane
csaldim	N–cyclohexylsalicylaldiminate
ctd	cytidine
ctdd	cyclotridecane–1, 3–dionate
cxphex	2–carboxyphenoxyacetate
cyclops	difluoro–3, 3'– (trimethylenedinitrilo) bis (2–butanone oximate)
cyclopsf	difluoro [3, 3'– (trimethylenedinitrilo) bis (2-butanone oximato)]borate
cyhis	cyclo–L–hystidyl
C_2H_3N	acetonitrile
$C_2H_5N_2O_2$	glycinehydroxamid acid
C_2H_8NOS	N–methylformothiohydroxamate
$C_3H_2N_3O_2$	6–azauracilate
$C_3H_2N_3O_3$	isocyanurate
$C_3H_2O_4$	malonate
$C_3H_4N_2Cl$	2–chloroimidazolium
C_3H_6O	acetone
$C_3H_6N_4S$	4–amino–1, 4–dihydro–3–methyl–1, 2, 4–triazoie–5–thione
$C_3H_7N_2S$	2–amino–2–thiazolium
$C_3H_8N_4$	malondiamidine
$(C_3H_8)_2N$	bis (isopropyl) ammonium
C_3Se_5	4, 5–di (hydroseleno) –1, 3–diselenole–2–selonate
$C_4H_4NO_2$	succinimidole
$C_4H_4O_5$	malate
$C_4H_6N_3O$	dicytosinium
$C_4H_7N_2S$	2–amino–4–methylthiazolium
$C_4H_7N_5O$	4–aminoimidazole–5–carboxamidoxime
$C_4H_8NO_3$	threonine
$C_4H_8N_3O$	2–imino–1–methyl–4–imidazolidinone (cretinine)
$C_4H_{10}N_4O$	1–amidino–O–ethylurea
$C_4H_{10}NO$	2–amino–2–methyl–1–propanolate
$C_4H_{10}NO_3$	2–amino–2–hydroxymethyl–1, 3–propanediolate
$C_4H_{16}N_3$	bis (2–ammonioethyl) ammonium

$C_4H_{16}N_3$	diethylenetriammonium
$C_4O_2S_2$	dithioquadrate
C_4O_4	3, 4–dihydroxycyclobutenedionate
$C_5HN_3O_6$	5–nitrooratate
$C_5H_3N_2O_2$	pyrazinecarboxylate
$C_5H_4N_5O_2$	3–methyl–8–azaxanthinate
$C_5H_5N_2$	H–pyrrole–2–aldimine
$C_5H_6N_2O$	2–imidazolidine
$C_5H_6C_{12}N_3$	2, 6–diamino–3, 5–dichloropyridinium
$C_5H_8N_2S$	1, 3–dimethyl–2 (3H) –imidazolethione
$C_5H_8NS_2$	pyrrolidonecarbodithioate
$C_5H_8N_2$	3–ammoniumpyridinium
$C_5H_{10}N_3O_3$	N– (1–oximino–1–methylbutyl–2) –nitroso–hydroxylamine
C_5O_5	croconate (2–)
$C_5H_{12}N$	piperidinium
$C_5H_{11}N_3OS$	salicylaldehyde–S–methylthiosemicarbazone
$C_6H_3O_3S$	(thienyl–2)–2–glyoxylate
C_6H_6NO	2–acetylpyrrole
$C_6H_6N_4O_2$	pyrazine–2, 3–dicarboxamide
$C_6H_8BrN_2$	2–amino–5–bromo–3–methypyridinium
C_6H_9NOS	5– (2–hydroxyethyl) –4–methyl–3–thiazole
$C_6H_9N_2$	2–amino–3–methylpyridinium
$C_6H_{10}NOS$	5– (2–hydroxyethyl) –4–methylthiazolium
$C_6H_{10}NO_2$	1–aminocyclopentanecarboxylate
$C_6H_{10}N_4OS$	acetamidoacetonthiosemicarbazonate
$C_6H_{10}NS_2$	piperidine–1–dithiocarbamate
$C_6H_{10}N_2O_2$	1, 2–cyclohexanedione dioxime
$C_6H_{10}N_3OS_2$	Schiff base derived from diacetylmonooxime and hydrazindithiocarbonic acid
$C_6H_{11}NH_2$	cyclohexylamine
$C_6H_{13}NS_2$	(4–N–methylpiperidinium) disulfide
$C_6H_{13}N_3$	4– (2–ammonioethyl) –1–methyl–3H$^+$–imidazolium
$C_7H_8N_4O_2$	3, 7–dihydro–1, 3–dimethyl–1H–purine–2, 6–dione
$C_7H_{11}N_3OS_2$	acetamidoacetonmethyldithio–carbohydrazonate
$C_7H_{12}NO_2$	1–aminocyclohexanecarboxylate
$C_7H_{12}NS_2$	hexamethylenedithiocarbamate
$C_7H_{14}NS_2$	N, N–diisopropyldithiocarbamate
$C_7H_{18}N_2$	N–isopropyl–2–methyl–1, 2–propanediamine
C_8H_8NO	o–hydroxyacetophenoneimine

$C_8H_8NO_2$	2–hydroxyacetophenoximate
$C_8H_9N_3OS$	Schiff base derived from S–methyldithiocarbazate with 2–pyridinecarboxaldehyde N–oxide
$C_8H_{10}N_4O_5$	glycylglycylglycylglycine
$C_8H_{10}O_2Cl$	bis (2–chloro–4–acetylhexen–1–on–5)
$C_8H_{11}N_2$	N– [1–(2–pyrrolyl) ethylidene] ethylaminate
$C_8H_{11}O_2$	2–acetylcyclohexanonate
$C_8H_{12}N_4O_5$	(1–D–ribofuranosyl–1, 2, 4–triazole–3–carboxamide, (ribavirin)
$C_8H_{16}N_4O_2$	N, N'–bis (β–carbamoylethyl) ethylenediamine
n–C_8H_{18}	n–octane
C_9H_6NO	8–hydroxyguinolinate
$C_9H_9N_3OS$	S–methyl–N^1–(salicyliden) izothiosemicarbazidate
$C_9H_{10}NO_2$	2–hydroxo–4–methoxy–acetophenone
$C_9H_{10}NO_2$	2–hydroxyethyliminosalicylaldehydate
$C_9H_{11}N_5O_2$	α, β–didehydroglycylglycylhistaminate
$C_9H_{23}N$	methyl (2–phenylethyl) ammonium
$C_9H_{13}N_2$	N–tert–butylpyrrole 2–carbaldimine
$C_9H_{18}N_3O$	4– [2– (2– (aminoethylamino) ethylimino] pentan–2–onate
$C_{10}H_9N_2O_2$	2–carboxylate–N–ethylbenzimidazole
$C_{10}H_{10}NO$	N–allylsalicylaldiminate
$C_{10}H_{10}NO_3$	4–phenyl–oxazolidine–4'–carboxylate
$C_{10}H_{11}N_2S$	cond. product of acetone and thiobenzoylhydrazine
$C_{10}H_{13}N_2O$	α–hydroxy–α–phenylbutyramidine
$C_{10}H_{13}N_5O_6$	tetraglycylglycinate
$C_{10}H_{13}N_2O_2F_3$	4–(2'–oxo–3', 3' ,3'–trifluorpropylidenyl)–2, 2, 5, 5–tetramethyl–3–imidazolin–1–oxyl
$C_{10}H_{15}NO_3$	β–diketonate
$C_{10}H_{16}N_4O_2$	3–(ethoxycarbonyl)–l, 5–diphenylformazane
$C_{10}H_{20}O_5$	15–crown–5–ether
$C_{10}H_{26}N_4$	spermine
$C_{11}H_2N_7$	1, 2, 6, 7–tetracyano–3, 5–diimino–3, 5–dihydropyrrolizinidate
$C_{11}H_7O_2S_2$	3–hydroxy–1, 3–bis (2–thienyl) prop–2–en–1–one
$C_{11}H_9N_3S_2$	Schiff base derived from α–aminobenzaldehyde and S–methyldithiocarbazone
$C_{11}H_{14}NO$	N–n–butylsalicylaldiminate
$C_{11}H_{15}N_4O$	Shiff base prepared from acetylacetone, ethyle–

	nediamine and 4–formylimidazole
$C_{11}H_{16}N_2$	(4S, 7R) –7, 8, 8–trimethyl–4, 5, 6, 7–tetrahydro–4, 7–methano–2H(2H)–indazole
$C_{11}H_{17}O_2$	2–formyl–3–methyl–6–izopropylcyclohexanonate
$C_{11}H_{19}O_2$	dipivaloylmethane 2, 2, 6, 6–tetramethyl–3, 5–heptadione
$C_{11}H_{25}N_3$	1, 5, 9–triazacyclotetradecane
$C_{12}H_{10}NO$	2–hydroxy–N–methyl–1–napthylmethyleneiminate
$C_{12}H_{10}NO$	N–methyl–2–hydroxy–1–naphthaldiminate
$C_{12}H_{11}N_3O$	N–[2– (4–imidazolyl) ethyl] salicylidineaminate
$C_{12}H_{12}N_5O_2$	1,3–dimethyl–5–diazophenyl–6–aminouracitate
$C_{12}H_{16}NO$	o–hydroxyacetophenone–isobutylimine
$C_{12}H_{16}N_4O_4$	N, N –ethylenebis (isonitrosoacetylacetoneimine)
t–$C_{12}H_{17}N_2O_2$	N–t–butyl–pyridoxylideneiminate
n–$C_{12}H_{17}N_2O_2$	N–n –butyl–pyridoxylideneiminate
$C_{12}H_{17}N_3O_3$	N–(1–methyl–3–oxo–butyliden)–N –(1–methyl–2–isonitroso–3–oxobutyliden) ethylenediamine
$C_{12}H_{17}N_4O$	Schiff base derived from acetylacetone, propane–1, 3–diamine and 4–formylimidazole
$C_{12}H_{18}N_2O_2$	N, N–ethylene–bis (acetylacetoneiminate)
$C_{12}H_{18}N_4OSCl$	thiamine hydrochloride
$C_{13}H_{10}NO$	2–picolyl–phenylketonate
$C_{13}H_{11}N_5O_4$	6–amino–i, 3–dimethyl–5((2–carboxyphenyl) –azo) uracil(2–)
$C_{13}H_{12}NO_2$	N–ethanol–2–oxy–1–napthylideneaminate
$C_{13}H_{18}N_2O$	1–(n–butyl)–2–(o–hydroxyphenyl)–delta^2–imidazole
$C_{13}H_{18}N_7OBr$	synthetic analogue of bleomycin
$C_{13}H_{19}N_2OS$	3–(2–diethylammoniummethoxy)–1, 2–benzisothiazole
$C_{14}H_{10}N_2OS$	2–oxybenzaldehyde thiobenzoylhydrazonate
p–$C_{14}H_{12}NO$	N–p–tolylsalicylaldiminate
$C_{14}H_{14}N_4S_4Cl_4$	2–aminobenzothiazolium
$C_{14}H_{15}N_4O$	(4–imidazolyl)methyliminopropylsalicylidenimínate
$C_{14}H_{16}N_3OS$	N–2[(5'–methylimidazol–4' –yl)methylthio]ethyl–salicylideneiminate (1–)
$C_{14}H_{16}N_4S_4$	thioether–pyridazine macrocycle
$C_{14}H_{17}N_7O_2Br$	derivate of bleomycin
$C_{14}H_{20}NO$	N–n–hexyl–7–methylsalicylaldiminate

$C_{14}H_{22}N_2O$	lignocaine
$C_{14}H_{32}N_4$	(1SR,4RS,8SR,11RS)1,4 ,8,11–tetramethyl 1,4 ,8, 11–tetraazacyclotetradecane
$C_{15}H_{11}N_2O_2$	5, 5–diphenylhydantoinate
$C_{15}H_{18}N_4O_5$	ligand containing μ–al1koxo backbones and amido–pyridyl or amido–phenol 'end' groups
$C_{15}H_{26}N_2$	(–)–β–isosparteine
$C_{16}H_{14}N_2O_2$	N, N –ethylenebis (salicylaldiminate)
$C_{16}H_{14}N_2O_4$	N, N' –ethylenebis (3–hydroxysalicylideneimine)
$C_{16}H_{15}N_2OS$	thioacylhydrazone of aldehyde
$C_{16}H_{17}N_2O_2$	N–[2–(2–pyridyl)ethyl)–3–ethoxysalicylideneaminate(–2)
$C_{16}H_{17}N_2O_2$	5–hydroxymethyl–2–methyl–4 (phenylethylimino–methyl) –3–pyridinolate
$C_{16}H_{18}N_3S$	3, 9–bis (dimethylamino) phenazothionium
$C_{16}H_{20}N_2OS$	condensation product of β–diketone and thiobenzoylhydrazine
$C_{16}H_{21}N_4O_2$	viridamien
$C_{16}H_{22}N_2O_3$	2,2,5, 5–tetramethyl–3–aminopyrrolidin–1–imino–xyl–o–vanilate
$C_{16}H_{22}N_2O_4$	6, 11–dimethyl–7 ,1O–diazahexadeca–5, il–diene–2,4,13, 15–tetraonate (2–)
$C_{16}H_{24}N_3O_2$	(lS, 9S)–S–cyano–1, 9–bis (1–hydroxy–1–methyl–ethyl) semicorrinate
$C_{16}H_{27}N_4O$	macrocyclic tetraamine bearing a phenolic group
$C_{16}H_{32}N_4$	5, 7, 7, 12, 14, 14–hexamethyl–l, 4 , 8 ,ll–tetra–aza–cyclotetradeca–4 , ll–diene
$C_{16}H_{34}N_2O_3$	N–[2 '–(2"–pyridyl) ethyl]–4, 6–dimethoxysalicyLideneiminate
$C_{16}H_{34}N_{10}O_7$	oxalyldihydrazid
$C_{16}H_{35}N_5$	penta–azamacrobicycloalkane–12, 17–dimethyl–1,5,9,12, 17–penta–azabicyclo [7.5.5)nonadecane
$C_{16}H_{36}N_4O_4$	1, 4, 7, 1O–tetraoxa–13, 16, 19, 22–tetraazacyclote–tetracosane
$C_{17}H_{12}NO$	N–phenyl 2–oxy–1–naphtaldiminate
$C_{17}H_{16}N_2O_2$	N, N –trimethylenedisalicylideneaminate
$C_{17}H_{16}N_2O_3$	N,N –(2–hydroxy–propane–l, 3–diyl) bis(salicylaldiminate)
$C_{17}H_{16}N_3O$	2–methyl–2–methylimino–1–benzoylglyoxal–1–phenyl–hydrazoniminate

$C_{17}H_{17}N_2$	4–phenylamino–2–phenyliminopent 3 –enate
$C_{17}H_{17}N_2O_2$	1–(2 –hydroxyphenyl)–3–methyl–6–(2–pyridyl)–4–azahex–2–en–1–onate
$C_{17}H_{18}N_4$	{1, 2–bis–[(2–aminobenzylidene)–amino]propanate(2–)
$C_{17}H_{20}ON_7$	analogue of bleomycin
$C_{17}H_{20}N_2SCl$	2–chloro–10–(3–dimethylammoniopropyl)phenothiazinium
$C_{17}H_{21}N_2S$	promaziniumyl
$C_{17}H_{24}N_2O_3$	2, 2, 6, 6–tetramethylpiperidine–1–iminoxyl–o–valinate
$C_{17}H_{24}N_2S_4$	N, N' –trimethylenbis (methyl–2–amino–1–cyclopentene dithiocarboxylate
$C_{18}H_{14}N_4$	2, 2' –bis (2–imidazolyl)biphenyl
$C_{18}H_{17}N_3O_2S$	condensation product of salicylaldehyde with S–propyl–thiosemicarbazonesalicylaldehyde
$C_{18}H_{18}N_3O_2$	pyridoxylidenetryptamine Schiff base
$C_{18}H_{20}N_6$	3,7,14,18,23,24–hexa–azatricyclo 18.2.1.1tetracosane–2, 7, 9, 11, 13, 18, 20, 22–octaene
$C_{19}H_{11}N_2O$	N–p–dimethylmethylaminophenyl–2–hydroxy–1–naphthaldiminate
$C_{19}H_{14}N_4O$	1–(2–hydroxyphenyl) –3, 5–diphenylformazanate
$C_{20}H_{24}N_4O_3$	3–11–dimethyl–1, 13–bis (pyrrol–2–yl)–7–oxa–4,10–, diaza–trideca 2, 11–diene–1, 13–dionate(2–)
$C_{19}H_{17}N_2O$	N–n–dimethylaminophenyl–2–oxy–1–naphthaldiminate
$C_{19}H_{24}N_2O$	cinchoninium
$C_{20}H_{14}N_2O_2$	N, N –o–phenylenebis (salicylaldidiminate)
$C_{20}H_{14}N_2O_2S_2$	N, N'–ethylene–bis(3–hydroxy–2–benzo[b]thenylidene)diaminate
$C_{20}H_{24}N_6$	N, N –bis (benzimidazol–2–ylethyl)ethane–1, 2–diamine
$C_{20}H_{25}N_2O_2$	2, 2, 6, 6–tetramethyl–4–aminopiperidine–1–imioxyl
$C_{16}H_{23}N_2O$	Schiff base derived from 2, 2, 6, 6– tetramethyl–4–aminopiperidine
$C_{21}H_{17}N_4OS$	4–phenylthiosemicarbazone salicylideneantranilaldehyde
$C_{21}H_{20}N_2O_4$	3, 3–(propane–1, 3–diyldi–imino)bis[1–(o–hydroxyphenyl) prop–2–enolate
$C_{21}H_{25}NO_2$	α– (N–3, 5–di–tert–butyl–4–oxy–cyclohexa–2, 5–

	dien–1–imino)–N–oxy–vinyl–orto–oxybenzilidene
$C_{20}H_{23}N_2O_4$	4–(n–heptyl–oxy)–N–(4' –nitrophenyl)benzaldimine–2–olate
$C_{21}H_{26}NO_3$	4–(n–heptyl–oxy)–N–(4' methylphenyl) benzaldimine–2–olate
$C_{21}H_{29}N_3O_2$	1, 12, 16–triaza–3, 4:9, 10–dibenzo–5, 8–dioxacyclo–octadecane
$C_{21}H_{32}N_6$	1–(2' ,2"–bipyridyl–5'–yl–methyl)–1, 4, 8, 11–tetra–azacyclotetradecane
$C_{22}H_{22}N_2O_2$	1, 1–diphenyl–3, 3 –(ethylenediimino) di–1–butanonate
$C_{22}H_{22}N_4$	5, 7, 12, 14–tetramethyldibenzo[b, i] [1, 4, 8, 11)–tetraazacyclotetradeca–2, 4, 7, 9, 11, 14–hexaene–diide
$C_{22}H_{28}NO_2$	1–methoxy–2, 6–di–tret–butylphenyl –4–N–salicyl–aldiminate
$C_{22}H_{34}N_6$	3, 6, 12, 15–tetramethyl–18{[N(2, 6)–pyridino, N–1.2.1]$_2$–coronand–6}
$C_{23}H_{21}N_3O_3$	4–methoxymethyl–6–methyl–2–(salicylideneamino)–3(salicylideneaminomethyl) pyridinate (2–)
$C_{23}H_{24}N_2O_2$	propylenebis (benzoylacetoneiminate)
$C_{23}H_{28}NO_3$	α–(N–3, 5–di–tert–butyl–4–oxacyclohexa–2, 5–diene–1–imino)–N–hydroxyvinyl–orto–hydroxybenzilidene
$C_{23}H_{31}N_5$	dibenzo[k, r] [1, 5, 9, 13, 17]–penta–azacyclo–eicosa [9, 20]diene
$C_{24}H_{20}NO_6P_2$	tetraphenyl–imidodiphosphate
$C_{24}H_{23}N_5$	{7–(2–pyridyl)–dibenzo[b, k][1, 5, 9, 13] tetraaza–cyclopentadeca [4, 9]–diene (2–)
$C_{24}H_{36}N_6O_5$	macrocyclic ligand derived from the Schiff base[2 + 2] condensation of 2, 5–diformylfuran with 3–oxa–pentane–1, 5–diamine
$C_{24}H_{36}N_6O_6$	5(R), 12(S)–dimethyl–7(R), 14(S)–dipenyl–1(S), 4(S), 8(R), 11(R)–tetra–aza–cyclotetradecane
$C_{24}H_{36}N_{10}O_6$	N–phenyloxalyldihydrazide
$C_{25}H_{20}N_2O_2$	N, N –propylenebis (2–hydroxy–1–napthyl)methaniminate
$C_{25}H_{28}N_6O_2$	N, N' –trimethylen–bis– (–methyl–1–acetylglyoxal–1–fenylhydrozoniminate
$C_{26}H_{28}N_2O_4$	3,3 –(cis–1,2–cyclohexanediyldi–imino)bis [1–

	(o–hydroxy–phenyl) but–2–enoate
$C_{26}H_{36}NO_3$	N–p– (n–hexyloxy) phenyl, p– (n–heptyloxy) salicyl–aldiminate
$C_{30}H_{34}NO_4$	4–((4–butoxybenzoyl)oxy)–N–(4–n–hexylphenyl)salicyl–aldiminate
$C_{30}H_{37}O_8P_2$	l–oxo–1 , 2–diphenyl–3, 3, 5–tricarbbutoxy–1, 2–diphosphacyclopentanonate–4
$C_{31}H_{30}N_4O_4$	Schiff base derived from l–(pyrrol–2–y1)butane–1, 3–dione and 1, 3–bis (2–aminophenoxy)propane
$C_{31}H_{43}O_4$	1, 3–di (p–n–octyloxyphenyl)propane–1 , 3–dionate
$C_{32}H_{26}(CH_2)_nN_6O_2$	N,N ethylenebis 2–methyl–1–benzoylglyoxal–
n=2	1–phenylhydrazoneiminate
n=3	N,N trimethylenebis(...as previos)
n=4	N,N tetramethylenebis(...as previos)
$C_{33}H_{49}N_2O_4Si_2$	bis{ (4S,5S)–4–{ [(tert–butyl)dimethylsilyloxy]–methyl } –4, 5–dihydro–5–phenyloxazole}methanide
$C_{34}H_{26}N_6S_2$	2,2' –bis (1–phenyl–3–methyl–5–t–butylthiopyrazol–4–ylmethyleneamino) biphenyl
$C_{42}H_{56}N_2O_2$	1–methyl–4–oxo–3 , 3–diphenylhexyldimethylammonium
$C_{45}H_{26}N_4O$	5, 10, 15–triphenyl {2^2–oxo–benzo[$2^3$$2^4$]cyclohexa [a, b]porphinate (2–)
$C_{55}H_{60}N_4O_5$	2, 3, 7, 8, 12, 13, 17, 18–octaethyl–5–formyl–10–[2, 2–bis (benzyloxycarbonyl)vinyl] porphinate
$C_{62}H_{86}O_4$	bis (1, 3–di(p–n–octylphenyl)–propane–1, 3–dionate
$C_{74}H_{66}N_{12}O_4$	α, α, 5, 15 bis[N–(2–methylbenzimidazolyl)acetamidophenyl]– α, α, 10, 20–bis (pivalamidophenyl)porphine
daco	1, 5–diazacyclooctane
daddn	2, 7–diacetyl–1, 8–dihydroxy–3, 6–dimethylnaphthalene
daf	diaminofurozan (diamino–1, 2, 5–oxadiazole)
damet	bis (dimethylaminoethyl) ether
dap	1, 4–di (3–aminopropyl)–1, 4, 7–triazacyclononane
dapd	2, 6–diacetylpyridine dioxime
daph	2, 6–diacetylpyridine dihydrazone
dbcal	3, 5–di–tert–butylcatecholate
dbenzd	2, 2'–bis {2– (5, 6–dimethylbenzimidazolyl) }diethylsulphide
dbipyam	bipyridylaminate
dbm	dibenzoylmethane

dbz	dibenzylamine
dbzdto	N, N –dibenzyldithiooxamide
dcmcroc	4– (dicyanomethylene) –1, 2–dimercaptocyclopent–1–ene–3, 5–dionate–S, S)
dco	N, N–dimethylacetamidocyanooximate
ddad	3, 6–dimethyl–1, 8– (3, 5–dimethyl–1–pyrazolyl)–3, 6–diazaoctane
ddd	monoanion of 3, 9–dimethyl–4, 8–diaza–undeca–3, 8–diene–2, 10–dione dioxime
den	bis (2–aminoethyl) amine
dgx	diphenylglyoximate
diaza	3, 13–dimethyl–3, 6, 9, 12, 18–penta–azabicyclo [12. 3.1]octadeca–1(18), 14, 16, –triene
diazepam	7–chloro–1, 3–dihydro–1–methyl–5–phenyl–3H–1, 4–benzodiazepin–2–one
dibyo	diaza–1 , 4–bicyclo[2. 2. 2]octane
diclo	6, 20–dimethyl–6, 11, 12, 13, 14, 15, 20, 21–octahydro–5H–tribenzo [b, f, m] [1, 4, 8, 12)tetraazacyclopenta–diene
dien	diethylenetriamine
cis–[18]–dieneN$_4$	[5S(R), 10R(S)–2, 4, 4, 11, 11, 13–hexamethyl–1, 5, 10, 14–tetraazacyclooctadeca–1, 13–diene
trans–[14]–dieneN$_4$	5, 7, 7, 12, 14, 14–hexamethyl–1, 4, 8, 11–tetraazacyc–lotetradeca–4, 11, diene
trans–[18]–dieneN$_4$	[5R(S) ,14R(S)–2, 4, 4, 11, 13, 13–hexamethyl–1, 5, 10, 14–tetraazacyclooctadeca–1, 10–diene
dik	di (N–methyl–2–imidazolyl) ketone
dipen	15–aza–6–oxa–3, 9–dithiabicyclo [9. 3. 1]pentadeca–1(15), 11, 13–triene
dmaep	2–(2–dimethylaminoethyl)pyridine
dmc	2, 5–dimethoxycinnamic acid
dmen	N, N –dimethyl–1, 2–ethanediamine
dmf	dimethylformamide
dmit	4, 5–dimercapto–1, 3–dithiole–2–thionate (2–)
dmpo	P– (N, N' –dimethylamino–methyl) –P, P–diphenyl phos–phine oxide
dmpz.NCO	1–carbamoyl–3, 5–dimethylpyrazolate
dmsO	dimethylsulphoxide
dnsglyNO	N–dansglycinate (–2)
doct	3, 6–diazaoctane–1, 8–diamine

doxc	dihydro–1H, 3H, 5H–oxazolo 3, 4–oxazole–7a–carbo–xylate
dpa	di–2–pyridylaminate
dpm	di–pyridylmethane
dpq	2, 3–di(2–pyridyl)quinoxaline
dpt	bis (3–aminopropyl) amine
dpta	dipropylenetriamine
dpthn	N, N', N" –tris(dihydroxyphosphorylmethyl)–1, 4, 7–triazacyclononane
dqa	bis (8–quinolinyl) amide
5' –dqmp	2' –deoxyquanosine–5' –monophosphate
dsf	desferrithiocin
dth	2, 5–dithiahexane
dthp	2, 6–bis (2, 6–dithiaheptyl) pyridine
dtic	5–(3, 3–dimethyl–1–triazenyl) imidazole–4–carbox–amide
dto	dithiooxalate
dts	dithiosquarate
dzbx	3, 10–dithia–16–azabicyclo [10. 3. 1]hexadeca–1(16), 12, 14–triene
ebsr	(R, S) –N, N' –ethylene–bis (serinate)
edip	dihydrooethylendiamindi – (isopropylphosphonate)
edms	ethylenediaminemonosuccinate
edp	N, N' –ethylene–di–2–pyridine carboxamide
edph	1–oxyethylidenephosphonate
en	ethylenediamine
$en(ba)_2$	Schif base derived from benzoylacetone and ethylenediamine
$en(tfpd)_2$	N, N –ethylenebis (1, 1, 1–trifluoro–2, 4–pentane–dione)iminate
$en(tpm)_2$	N, N' –ethylene–bis (trifluoroacetylpivalylmetha–ne)iminate
eoa	ethanolammonium
1–eph	1–ephedrine
Etac	ethylacetate
Etacet	ethylacetoacetate
Et_2ala	d, 1–N, N–diethyl–α–alaninate
Et_2en	N, N' –diethylenediamine
Et_4en	N, N, N', N' –tetraethylenediamine
Et_2bzthioacam	N, N–diethyl– 2–benzylthioacetamidate

Et_2bzthiour	1, l–diethyl–3–benzoylthioureate
Etcps	N, N –ethylenebis (methyl–2–amino–1–cyclopentene–dithiocarboxylate)
Et_4dien	1, 1, 7, 7–tetraethyldiethylenetriamine
Et_2dsc	diethyldiselenocarbamate
Et_2dtc	diethyldithiocarbamate
$Et_2(gud)_2$	ethylenebisguanidine
eth	ethyleneglycol
$Etox(ts)_2$	3–ethoxy–2–oxobutyraldehydebis (thiosemicarbazonate)
$Etpy_4$	N–ethylpyridinium
EtSacac	N, N –ethylenebis (monothioacetylacetone) iminate
Etsalaldim	N–ethylsalicylaldiminate
$Et(salnim)_2$	N, N –ethylenebis (salicylideneiminate)
Et_2SPhbz	N–(diethylaminothiocarbonyl)–N –phenylbenzamidinate
etspy	2, 6–bis (ethylthiomethyl)pyridine
Ettraz	1–ethyl–1, 2, 4–triazole
eryan	anhydro–erythrit
F_3acac	trifluoroacetylacetonate
F_6acac	hexafluoroacetylacetonate
faxy	2–furancarboxylate
fch	formylcyclohexanone
fH	fumaric acid
fla	flavonolate
fpsem	2–formylpyridine thiosemicarbazone
ftbd	4, 4, 4–trifluoro–1– (2–thienyl)butene–1, 3–dionate
ftzh	fenethazinium
fuc	5–fluorouracil
ghl	glycyl–L–histidyl–L–lysine
ggly	glycylglycinate
L–glu	L–glutamate
gly	glycinate
glyno	N–benzenesuphonylglycinate (2–)
gly–L–tryp	glycyl–L–tryptophanate
glytyr	glycyl–L–tyrosinate
hx	hexagonal
Hampym	2–aminopyridinium
hapt	bis(2–hydroxyacetophenone)–trimethylenediimine
haza	C–rac–5, 5, 7, 12, 12, 14–hexamethyl–1, 4, 8, 11–tetra–

	azacyclotetradecane
$HB(Butpz)_3$	tert–butyl–substituted pyrazole
$HB(3, 5–iPr_2pz)_3$	hydrotris (3,5–isodipropyl–1–pyrazolyl)borate
$HB(3, 5–Me_2pz)_3$	hydrotris (3, 5–dimethyl–1–pyrazolyl)borate
Hbz	benzoylhydrazide
H_2bim	2,2' –bisimidazole
hepor	hemiporphyrazine
hex	hexamethylenetetramine
hib	(E) – (α– (hydroxyimino)benzyl)phosphonate
Hin	isonicotinic acid hydrazide
hist	histidinate
H_2Me_2pipz	N,N' –dimethylpiperazinum
HOEten	N– (2–hydroxyethyl)ethylenediamine
HOMepyS	3–hydroxy–6–methylpyridine–2thione
hsal	N,N'–4–methyl–4–azaheptane–1, 7–diyl–bis (salicy–lideneiminate)
hyaza	6–hydroxy–l, 5, 8, 12–tetraaza–17–oxabicyclo–[10. 5.2]nonadec–5–ene
ibbim	isobutyl derivative on the amine nitrogen atom of N,N–bis (benzimidazol–2–y1–methyl) amine
ibo	2,2' –iminobis (acetamidoxime)
ida	iminodiacetate
ileu	L–isoleucinate
imaz	l–methyl–2–imidazole carbaldehydazine
im	imidazole
imep	2, 6–bis [1– (2–imidazol–4–ylethylimino) ethyl] –py–ridine
imiso	1, 3–bis (5–methyl–2–pyridyl) imino (isoindoline)
imith	1, 5–bis (benzimidazol–2–y1)–3–thiapentane
5'–imp	inosine–5' –monophosphate
imsuc	iminodisuccinate
ipnp	4, 4'– [iminobis (1, 3–propanediylnitrilo)]–di–2–pentanonate
i–Prcbp	N–isopropyl–2–hydroxybenzilideneaminate
iprnam	N–isoprophyl–2–oxy–1–naphthylideneaminate
iqa–dpt	condensation product of 3–formylisoquinoline with bis (3–aminopropyl) –methylamine
iqu	1, 2, 3, 4–tetrahydroisoquinoline
$3, 5–I_2tyr$	3, 5–diiodo–L–tyrosinate
karbaz	tiosemikarbazone–o–aminobenzaldehyde

K ($C_{12}H_{24}O_6$)	18–crown–6 potasium
lac	lactate
L–ala	L–alaninate
leu–L–tyr	L–leucyl–L–tyrosine
lm	lumazine
L–tyr	L–tyrosinate
m	monoclinic
ma	methylamine
mac	mercaptoacetate
mad	9–methyladenine
mazoc	7, 9–diacetyl–6, 20–dioxo–8, 13, 17–trimethyl–26, 30–dioxa–9, 13, 17–triazacyclo [23.5.1.1] dotria–conta–1, 3, 5 (31), 7, 8, 21, 23, 25 (32) –octaenate
mbn	o–mercapto–benzoate
mbp	N, N'–bis [(2–hydroxy–5–methylphenyl) phenylmethy–lene) –4–azaheptane–l, 7–diaminate
mcpa	4–chloro–2–methylphenoxyacid
3–Meacac	3–methylacetylacetonate
Me_2ampp	2–dimethylaminomethyl–4–phenylphenol
mecry	α–methacrylate
mecyclo	1, 4–dimethyl–8– [2– (2– (pyridyl) ethyl]–1, 4, 8, 11–tetraazacyclotetradecane
medec	4–methyl–4, 7–diazadecanediamine
mehep	2, 7, 12–trimethyl–3, 7, 11, 17–tetraaza– bicyclo–[11,3,1]heptadeca–1(17),2,11,13,15–pentaene
memacet	6–methoxy–α–methylnaphthalene–2–acetic acid
memia	4– (5–methyl–4–imidazolyl) –1–amino–3–thiabutane
methio	2, 6–bis (((2– (methoxycarbonyl) phenyl) thio) me–thyl) pyridine
mg	L–methionylglycinate
mmbp	N, N'–bis [(2–hydroxy–5–methylphenyl) (4–methyl–phenyl) methylene]–3–azahexane–l, 6–diamine
mnpala	(2S, 8S) –2, 5, 8–trimethyl–5–nitro–3, 7–diazano–nane dionate
mnpgly	5–methyl–5–nitro–3, 7–diazanonanedioate
mnt	maleonitriledithiolate
monsal	N–{2– [2– (2–ammonioethylamino) ethylamino] ethyl}–salicylideneaminate
mpa	3, 3'–dimethyl–2, 2'–dipyridylamine
mpab	N, N–bis (3, 5–dimethyl–1–ylmethyl) aminobenzene

mpid	1, 3–bis (2– (4–methylpyridyl) imino) isoindolate
mpyx	2, 2–bis (6–methyl–2–pyridyl)–1, 3–dioxolane
Mebhdhx	1, 6–bis (5–methyl–4–imidazolyl)–2, 5–dithiahexane
6–Mebpy	6–methylbipyridine
Meen	N–methylenediamine
Mehyacph	N–metyl–o–hydroxyacetophenoneimine
Meim	N–methylimidazole
Meimith	1,3–bis(5–methyl–4–imidazolyl) –2–thiapropane
Meimol	1, 3– (bis (N–methyiimidazolimine) –propan–2–ol
Me–α–manpH	methyl–α–D–mannopyranosid
Menit	2, 4, 4, 5, 5–pentamethyl–4, 5–dihydro–1H–imidazo–lyl–1–oxy–3–oxide
MeOHbpe	N, N' –bis (2–pyridyl–methylene) ethane–1, 2–diamine with MeOH
4–MeOphex	p–methoxyphenoxyacetate
$(MeO)_3PhNH_3$	3, 4, 5–trimethoxyphenethylammonium
MeOsal	1H–indole–3–ethylene–3'–methoxy–salicylaldimi–nate
Meoxazaoxam	N–(4–methyl–6–oxo–3–azahept–4–enyl) oxamate (3–)
MePhEtNH	N–methyl phenethylammonium
Mephimac	N–(orto–methyl)–phenyliminodiacetate
Me–1, 3–pn	N–methyl–1, 3–propanediamine
2–Mepy	2–methylpyridine
3–Mepy	3–methylpyridine
4–Mepy	4–methylpyridine
4–MepyH	4–methylpyridinium
4–MepyNO	4–methylpyridine 1–oxide
Mepzimid	4–methoxy–2– (5–methoxy) –3–methylpyrazol–1–yl–6–methylpyrimidine
Mequin	5–S–methyl–8–merkaptoquinolinate
4–Mequinox	4–methyl–1–quinone–2–oximate
Mesaldim	N–methylsalicylaldiminate
4–Methz	4–methylthiazole
Me–tsc	S–metylisothiosemicarbazide
Me_2bpyH	N, N–dimethyl–4, 4–bipyridium
Me_2enO	N, N–dimethyl–ethylenediamine N–oxide
$Me_2Etecys$	dimethyl–N, N'–ethylenebis (L–cysteinate) (2–)
Me_2gly	N, N'–dimethylglycinate
$Me_2H_2Me_2malox$	4, 4'–oxalyldinitrilo (pent–2–en–2–olate) (2–)
Me_2ileu	L–N, N–dimethylisoleucinate

1, 2–Me_2im	1, 2–dimethylimidazole
$Me_2N(H)C_2H_4P(O)Ph_2$	[2– (diphenylphosphinyl) ethyl] dimethylammonium
2, 7–Me_2nphyr	2, 7–dimethyl–1, 8–naphthyridine
Me_2Opur	1, 3–dimetyl–2, 6–dioxopurine
Me_2Ph_2bpd	3, 7–dimethyl–1, 5–diphenylbispidone–9
2, 9–Me_2phen	2, 9–dimethylphenanthroline
α–Me_2PhNH	(+)–N,α–dimethylphenethylammonium
Me_2Phpz	3, 5–dimethyl–1–phenylpyrazolate
2, 6–Me_2py	2, 6–dimethylpyridine
2, 3–Me_2py	2, 3–dimethylpyridine
3, 4–Me_2py	3, 4–dimethylpyridine
3, 5–Me_2py	3, 5–dimethylpyridine
1, 4–Me_2pyH	1, 4–dimethylpyridinium
2, 6–Me_2pyNO	dimethylpyridine N–oxide
Me_2pyzNO	dimethylpyridazine N–oxide
3, 5–Me_2pz	3, 5–dimethylpyrazole
Me_2Sdaz	[N (1), N (1) –dimethyl] thioformohydrazidate
2, 4–Me_2thz	2, 4–dimethylthiazole
Me_2tn	2, 2–dimethyl–l, 3–diaminopropane
Me_2val	L–N, N–dimethylvalinate
Me_3bzN	trimethylbenzylammonium
1, 4, 5–Me_3im	1, 4, 5–trimethylimidazole
Me_3pcx	N,N'–trimethylenedi–2–pyridine–carboxamide
Me_4Brsaldim	2,2,5,5–tetramethylpirrolidin–1–iminooxy–3–N–(2–oxy–5–brom) –salicylaldiminate
Me_4cpS	N, N'–tetramethylenebis (methyl–2–amino–1–cyclo–pentenedithiocarboxylate)
Me_4en	N, N, N', N'–tetramethyl–1, 2–diaminoethane
Me_4Phdiam	N, N, N', N–tetramethyl–o–phenylenediamine
Me_4pn	N, N, N', N'–tetramethyl–1, 3–diaminopropane
Me_4pyal	N, N'–tetramethylene–bis (2–pyridinaldimine)
Me_4rol	2,2,5,5,–tetramethylpyrrolidine–1–oxyl–3–N–2–oxy–5–bromosalycylideneiminate
Me_4tu	tetramethylthiourea
Me_5dien	1,1',4,7,7'–pentamethyl–diethylene–triamine
nac	nitroacetate
nal	nalidixate
naph	N, N'–ethylen bis (1–iminomethyl–2–naphtolate)
napox	1,2–naphtoquinone–2–oxime–4–sulphonate
nbbim	n–butyl derivative on the amine nitrogen atom

	of N, N–bis (benzimidazol–2–yl–methyl) amine
ncb	cyanotrihydroborate
ndap	N, N'–bis (2–pyridylmethylene) –1, 3–diamino–2–methyl–2–nitropropane
ndcm	dicyanonitrosomethanide
4–NH_2bz	p–aminobenzoate
niaza	7–methyl–7–nitro–1,5,9,13–tetraaza–bicyclo [11. 2.2] heptadecane
nicOH	nicotinic acid N–oxide
niphen	nitroacetatephenone
nitph	2–phenyl–4, 4, 5,5–tetramethyl–4, 5–dihydro–1H–imidazolyl–1–oxyl–oxide
nitphen	2–phenyl–4, 4, 5, 5–tetramethylimidazoline–1–oxyl–3–oxide
nmf	N–methylformamide
nmp	N–methylphenazinium
4–NO_2pyNO	4–nitropyridine N–oxide
2–npa	2–nitrophenoxyethanoate
npc	p–nitrophenaceturate
nphyr	2, 2'–bi (1,8) naphthyridine
($NPMe_2$)$_5H_2$	1,5–dihydrodecamethylcyclopentaphosphonitrilium
$N_4P_4Me_8H$	octamethylcyclotetraphosphonitrilium
nsnph	2–nitroso–1–naphtole
nsp	bis (2–methylthio) ethyl (2–pyridylmethyl) amine
nuqu	N,N' –bis (8–quinolyl)ethylenediamine
oadp	oxalamide–N, N' –di–3–propionic acid
oaoH	oxamidate
$oaoH_2$	oxamidoxim
oatpp	octaalkyltetraporphyrine
$OCHMeCH_2NMe$	volatile amino–alkoxide
ochyacph	N–octyl–o–hydroxyacetophenoneimine
oflp	2–flourophenoxycetate
OHEtsalaldim	N–2–hydroxyethylsalicylaldiminate
OHcpb	2– (O–hydroxybenzilidene) amine
or	orthorhombic
ox	oxalate
oxap	1,4,10–trioxa–7,13–diazacyclopentadecane
p–3a	biosyntetic intermediate of bleomycin
pad	pyridine–2–amidoxime
pal	lactone of 4–pyridoxic acid

pan	1–(2–pyridylazo)–2–naphtolate
paphy	pyridine–2–aldehyde–2'–pyridylhydrazone
pba	1, 3–propanediyl–bis (oxamate)
pc	phthalocyanine
pcam	bis (2–pyridylcarbonyl) amide
pcd	N–phenyl–2–carbamoyl–5, 5'–dimethylcyclohexane–1,3–dionate
pcno	7, 19–diacetyl–6, 20–dioxo–8, 13, 18–trimethyl–26, 33–dioxa 9, 13, 17,triazatricyclo [23.8.1.1]penta–triaconta–1, 3, 5 (34), 7,18, 21, 23, 25 (35)–octaenate
pcnoc	7, 19–diacetyl–6, 20–dioxo–9,13 , 17–triazatricyclo [23.8.1.1]pentatriaconta–1,3,5(34),7,18,21,23, 25,(35)–octaenate
pco	2–pyridinecarboxamide 1–oxide
pcp	pentacyanopropenide
pcpx	N–2–pyridinylcarbonyl–2–pyridine carboximidate
pcx	pyridine–2–carbooxamido oxime
pcxb	N, N'bis (2'–pyridine–carboxamido) –1, 2–benzene
pcxc	N, N'–bis (2'–pyridine–carboxamido) –cis–1, 2–cyclohexane
pcxt	N, N'–bis (2'–pyridine–carboxamido) –trans–1, 2–cyclohexane
pdta	1, 2–bis (diphenylphosphineoxido) ethane
pdto	1, 8–bis (2–pyridyl) –3, 6–dithiaoctane
pea	bis (2– (2–pyridyl) ethyl) amine
peas	thioether
penoc	2, 13–dimethyl–3, 6, 9, 12, 8–pentaazabicyclo [12, 3, 1] octadeca–1 (18), 14, 16 triene
peph	(+) –pseudoephedrine
Ph	phenyl
3–Phacac	3–phenylacetylacetonate
Ph $(bzS)_2$	2, 2'–orthophenylenebis (benzothiazole)
Ph–C $(NSiMe_3)_2$	N, N, N'–tris (trimethylsilyl) benzamidate
Pheph	L–phenylephrine
PhEthyacph	N–2–phenylethyl–o–hydroxyacetophenoneimine
$PhMe_2pz$	1–phenyl–3, 5–dimethylpyrazole
Phnit	2–phenyl–4, 4, 5, 5–tetramethyl–imidazoline–1–oxyl–3–oxide
$PhpipH_2$	N–phenylpiperazinium
Ph–sal	N–phenylsalicylideneaminate

Ph_2pn	1, 3–diphenyl–1, 3–propanedionate
3, 5–Ph_2pz	3, 5–diphenylpyrazole
Ph_3AsO	triphenylarsine oxide
Ph_3P	triphenylphosphine
Ph_3PO	triphenylphosphine oxide
Ph_4P	tetraphenylphosphine
phalan	L–phenylalaninate
phcyclo	1,4,8,11–tetraazacyclotetradecane–diethylphosphate
phen	1, 10–phenanthroline
o–phen (biu)$_2$	o–phenylenebis (biuretate)
phenbq	1, 10–phenanthrenediolate
phenet	1, 2–bis (9–methyl–1, 10–phenanthrolin–2–yl) ethane
phenquin	9, 10–phenanthrenequinone
phex	phenoxyacetate
phim	N, N'– (1, 2–phenylene) bis (pyridoxal)hydrochlorideiminate
phS	thiophenol
pic	picoline
picl	4–amino–3, 5, 6–trichloropyridine–2–carboxylate
piedien	1, 9–bis– (2–pyridyl) –2, 5, 8–triazanonane
pincer	Sα, 15α–bis [(N– (5, 6–dimethylbenzimidazolyl) acetamido)phenyl]–10α, 20α–bis (pivalamidophenyl) porphine(2–)
piraz	picryl azide
pipd	piperidine
pium	N, N–bis (2–pyridylmethyl) –1–aminoethylammonium
pma	2–pyridylmethyl bis (2–ethylthioethyl)amine
pmbp	1–phenyl–3–methyl–4–benzoyl–pyrazolone–5
pmd	N, N'–bis (2–pyridylmethylene) –tetramethylenediamine
pmdp	N^1 isopropyl–2–methylpropane–1, 2–diamine
pmed	N, N'–bis { (2– (Phenylmethylthio) phenyl)methylene } ethane–1, 2–diamine
pmk	cis, trans–bis (2–pyridylmethyl)ketazine
pms	bis (2–pyridyl–methyl) (2– (methylthioethyl) amine)
pmtp	1, 5–bis (2–pyridylmethyl–amino) –3–thiapentane
1, 3–pn	1, 3–diaminopropane
pnao	3, 3'– (1, 3–propanediamino) bis (3–methyl–2–butanone oximate)

pn–2–ol	propan–2–ol
1,3–pn–2–ol	1, 3–diamino–2–propanol
pnp	p–nitrophenolate
ppm	2–picolyl–(2–pyridyl–methanol) methylamine
ppzb	hydrobis (3,5–diisopropyl–1–pyrazolyl) borate
pql	2– (2–pyridyl) quinazolin–4 (3H) –onate
Pqp	p–quarterpyridine
psal	N–phenylsalicylaldiminate
pspz	3, 6–bis (2–pyridylthio) pyridazine
Pr (acac)$_2$	4, 4'– (R–propylene–diimanato) –di– (3–penten–2–one)
pr (biu)$_2$	propylenebis (biuretate)
Prbzsalim	N–izopropyl–5,6–benzosalicylideneaminate
PrMeOsalim	N–izopropyl–3–methoxysalicylidineaminate
PrN_2O_2	N–nitroso–N–isopropylhydroxylaminate
procyclo	1,4,8,11–tetraazacyclotetradecane–ethylpropionate
Prsaldim	N–isopropylsalicylaldiminate
pt	*pterin*
pth	o–phtalate
ptr	ligand derived from pterin
4–pxa	4–pyridoxic acid
py	pyridine
pya	*pyrazine–2–carboxamide*
pya–dpt	condensation product of bis (3–aminopropyl) –amine with pyridine–2–carboxaldehyde
pyala	D–β– (2–pyridyl) –α–alaninate
2–pyc	pyridine–2–carboxylate
pydca	pyridine–2, 6–dicarboxylate
pyh	N– (2–pyridylmethylene) histamine
pyhis	Schiff base derived from 2–pyridine carbaldehyde and histamine
pymep	N–[2'– (6–methyl)pyridyl]methylene–2–(2' –pyridyl) ethylamine
pyNO	pyridine N–oxide
pyox	2– (2–pyridinyl) –4 ,4–bis (hydroxymethyl) –2–oxazoline
pyoxts	pyridoxalthiosemicarbazonate
pypn	Schiff base derived from picolinealdehyde N–oxide and 1,2–propanediamine
pyram	tris [2– (1–pyrazolyl) ethyl]amine

pyrem	bis (1–pyrazolyl–methyl) amine
pys	(2–pyrimidinyl) sulfanilamide
pytzim	2– (2–pyridyl) benzimidazole
pyx	pyridoxine
pyz NO	pyridazine N–oxide
pz	pyrazole
pzmet	2, 6–bis (pyrazol–l–ylmethyl)pyridine
qcarb	2–quinolinecarboxylate
qdt	quinoxaline–2 , 3–dithiolate
qu	quinoline
quen	1, 2–bis (8–quinolylmethyleneimino) ethane
quep	1, 5–bis (8–quinolylmethyleneimino) –3–aza–pentane
quin	quinolinium
qxa	quinoxaline
rph	(+ –) norephedrine
sach	saccharin, (o–sulphobenzoimide)
sad–Meen	N–salicylidene–N' –methylethylenediamine
sad–Me_2en	N–salicylidene–N , N' dimethylethylenediamine
sal	salicylate
salaldim	salicylaldiminate
salalgly	N–salicylideneglycinate
salam	N–salicylidene–αaminoisobutyrate
salamEtO	2– (salicylideneamino) ethanolate
salampH	N–(2–pyridylmethyl) salicylamine
salbh	salicylaldehydebenzoylhydrazonate
sald	salicylaldehydate
salenEt_2	N–(2–diethylaminoethyl)salicylaldimine
salimp	N–(2–pyridylmethyl) salicylideneaminate
salMetsc	S–methylthiosemicarbazone salicylaldehyde
salphen	N,N'– (1,2 –phenylene)bis (salicylaldiminate(2–)
salPhEtim	salicylal–α–phenylethyliminate
salth	salicylaldehyde s–methylthiosemicarbazone
sal_2tmput	2, 5–bis (salicylaldimino) –2 ,5–dimethylhexane (2–)
(S)–bap–(S)–val	Schif base derived from (S)–o–[(N–benzylpropyl)–amino] acetophenone and (S)–valine
SC_6F_5	pentafluorothiolate
$SCPh_3$	phenylthiolate
semqu	S–methyl–thiosemicarbazone–8–quinolinealdehyde
sglyc	β–thioglycole
slth	N–salicylidene–L–thereoninate

Spican	α–thiopicolinanilidate
spp	3–sulfidopropionate
stpp	tetraphenyl–21–thia–porhyrin
sttp	21–thiatetra–p–tolylporphyrine
sucim	succinimidate
tach	cis, cis–1,3, 5–triaminocyclohexane
tan	1–(2–thiazolylazo)–2–naphtolate
tapp	N,N'–bis (3–(2–thenylamino)propyl)piperazine
taprop	L–(+)–threo–2–amino–1–phenyl–1,3–propanediolate
tbaz	thiabenzole
tbpo	tribenzylphosphine oxide
tbsal	3,3',5,5'–tetra–tret–butyl–4,4', di–oxo–dicyclo–hexa–2,2',5,5,–tetraen–1,1–N,N'–disalicyliden–iminate
tcaz	monoprotonated thiocarbonylhydrazide
tcne	tricyanoethenolate
tcnq	7,7',8,8'–tetracyanoquinodimethane
tcyc	1,4,7–trithiacyclononane
tc–n,n'	tropocoronands,(n,n'=3,3;4,4;5,5)
tdt	toluene–3,4–dithiolate
teaz	1H–thiocarbonohydrazidium
ted	1,4,7–triazacyclododecane
tepa	tris(2–(2–pyridyl)ethyl)amine
terpy	2,2':6',2"–terpyridine
tes	1,4,7–triazacyclononane–N,N',N"–tris–2–ethane–sulphonate
tet	2,2'–bis(6–(2,2'–bipyridyl)biphenyl)
teta	macrocyclic amine
tetb	rac–5,7,7,12,14,14–hexamethyl–1,4,8, 11–tetra–azacyclotetradecane
tetim	tetraimine macrocycle
texa	6–methyl–6–nitro–1,4,8,11–tetraazabicyclo[9,3, 2]hexadecane
tfac	2–thenoyltrifluoroacetonate
tg	tetragonal
thcbh	thiocarbonohydrazide
thdam	2–(2'–thiazolylazolylazo)–5–diethylaminophenol
thdec	2,10–diaza–6–thiaundecane
thene	3,3',5,5'tetramethyldipyrromethene–4,4'–dicar–boxylate

thf	tetrahydrofuran
thiapy	5,8,11–trioxa–2,14–dithia[15](2,6)–pyridino–phane
thiocarb	pyridine–2,6–dithiocarbomethylamide
thiox	2–thiooxamat(NH_2–C(S)–CO_2)
thma	tris(hydroxymethyl)aminomethane
thpen	N,N,N',N'–tetrakis(2–hydroxy–propyl)ethylenedia–mime
thpuan	thiosemicarbazoneanilidepyrotartarate
tht	15–thia–1,5,8,11–tetraazabicyclo [10.5.2]nonade–cane
thym	thyminate
thyr	thiamine pyrophosphate
tim	2,3,9,10–tetramethyl–l,4,8,11–tetraaza–1,3,8, 10–cyclotetradecatetraene
tioam	nitrozothiocarbamylcyanmetanide
tioim	1–methyl–2–(2–(methylthio)ethylimidazole)
tmbc	1,4,8,11–tetra–methyl–1,4,8,11–tetraazadibenzo–[b,i] cyclotetradecane
tmbi	N,N'–bis(4–imidazolylmethylidene)–1,3–trimethy–lenediamine
tmp	tetramesitylporphyrinate
tmpa	tris[(2–pyridyl)methyl)]amine
tmpo	2,2,6,6–tetramethylpiperidinyl–1–oxy
tnb	1,3,5–trinitrobenzene
tod	2,2,7–trimethyl–3, 5–octanedionate
tol	toluene
ton	N,N'–(1,3–trimethylene)bis(2–oxy–1–naphthaldi–minate
topa	3–(2,4,5–trihydroxyphenyl) –DL–alanine
toslopdi	N, N' –bistoluene–p–sulphonyl–o–phenylediiminate
toxa	tetraaza–17–oxa–bicyclo [10.5.2] nonadec–6–ene
tpea	tris (2–pyrazolylethyl) amine
tph	theophyllinate
tpl	tropolone
tplb	1, 3, 5–tris (pyrazol–1–ylmethyl)benzene
tpp	tetra–p–tolylporphyrinate
tppb	tris (3–phenylpyrazolyl)hydroborate
tprp	α, β, gama, δ–tetra–n–propylporphine
tr	triclinic

trea	tris (2–aminoethyl) amine
tren	2, 2',2"–triaminotriethyl amine
trenen	N, N–bis (2–aminoethyl) diethylenetriamine
trf	triflate, (F_3CSO_3)
trg	trigonal
tridec	2,12–di(2–pyridyl)–3,7, 11–triazadeca–2, 11–diene
trien	triethylenetetraamine
trt	tartrate
ts–β–ala	N–tosyl–β–alaninate
tsc	thiosemicarbazide
tse	N, N' diethylthioselenocarbamate
tsgly	N–tosyl–glycinate
tsleuNO	N–tosyl–L–leucinate (2–)
tsnO	N–tosyl–DL–asparaginate
ttda	bis– (N, N'–dimethylacetamido) thioether
tu	thiourea
5'–ump	uridine–5'–monophosphate
ura	monodeprotonated form of 4 –methyl–amino–1,3–di–methyl–5((2' –carboxyphenyl)azo) uracil
urac	pentaamine ligand derived from uracil
4–vipy	4–vinylpyridine
xan	xantine
xyhist	pyridoxylidenehistamine
p–xyl	p–xylene
yun	yunainate
zala	N–benzyloxycarbonyl–alaninate
zimid	2–hydrazinato–4–hydroxy–6–methylpyrimidine
zoct	N–methyl–1, 4–diazabicyclo[2.2.2]octonium

1 INTRODUCTION

The chemistry of copper compounds has been extensively investigated and the relationship between structure and reactivity, ranging from industrial catalysis to biochemical activity, is of major importance. The overwhelming majority of X-ray studies of transition metal compounds are of copper compounds. Although the +2 oxidation state of copper is the most common by far, other known oxidation states include +1, +3 and +4, with copper(I) the most common of these.

The structural chemistry of over one thousand copper(I) compounds was reviewed recently[1] and several relationship were found and discussed. Many structural studies of

copper(II) compounds have been carried out, but have only been sporadically summarized in four annual reports.[2] The stereochemistry of some copper(II) complexes and the plasticity of their coordination spheres have been reviewed.[3] Cooperative effects between the isomeric types of copper(II) have also been reviewed.[4] Some relationships between the structural data and magnetic interactions in oxo-bridged binuclear copper(II) compounds were found and discussed.[5] Copper(II) carboxylates have also been comprehensively reviewed.[6] An overall survey and classification of the structures of mixed Cu(I)-Cu(II) compounds has been reviewed recently.[7]

The systems discussed in this manuscript are four- and five- coordinate copper(II) compounds. Within each coordination number, the compounds are listed in order of increasing covalent radius of the principle coordinating ligand atom and increasing complexity of the coordination sphere.

2 TETRACOORDINATE COPPER(II) COMPOUNDS

Structural data for mononuclear copper(II) compounds of coordination number four are summarized in Table I. There are almost six hundred examples. Two limiting configurations are generally observed, square planar and tetrahedral, with square planar dominant. Both of the limiting geometries occur with various degrees of distortion.

From Table I, one can see examples of uni-, bi-, tri- and even tetradentate ligands, creating various amounts of distortion about the copper(II) atom. In the series of bi-, tri- and tetradentate chelating ligands, different sizes of metal containing rings are observed which causes variations in observed bonding angles.

The effect of both electronic and steric hindrance of the coordinated atoms can be seen in the opening of the L-Cu-L bond angles of the respective metallocycles. For the four-membered metallocyclic rings the L-Cu-L intra-ligand angles (mean values) are 64.3° for oxygen donor, 67.4° for nitrogen donor, 77.5° for sulfur donor and 79.3° for selenium donor ligands. This reflects the difference in covalent radii of O(0.73Å), N(0.75Å), S(1.02Å) and Se(1.16Å).

TABLE I Crystallographic and Structural Data for Copper (II) Compounds: Coordination Numbers Three and Four

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore*	*Cu-L*	*L-Cu-L*			*Ref.*
$Ba[Cu\{(CF_3)_2MeCO\}_3]$ (blue)	m C2/c 4	23.843(12) 18.324(8) 10.998(6)	116.97	CuO_3	O	1.781(7)[b] 1.878(7) 1.889(6)	O,O	88.4(3)[b] 130.9(3) 140.7(3)	8
$(ClF_6)[CuF_4]$	m $P2_1/a$ not given	7.225(5) 9.621(2) 5.347(3)	not given	CuF_4	F	not given	F,F	not given	9

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$(SiF_6)[Cu(H_2O)_4]$ (blue)	m $P2_1/a$ not given	7.22(1) 9.64(1) 5.36(1)	105.2(3)	CuO_4	O	not given	O,O	not given	10
$[Cu(pyNO)_4](ClO_4)_2$ (not given)	m $P2_1/c$ 2	9.65(2) 14.30(2) 10.85(2)	122.0(5)	CuO_4	O	1.925(9,5)[b]	O,O	90.0(4,8)[b]	11
$[Cu(pyNO)_4](BF_4)_2$ (dark green)	m $P2_1/c$ 2	9.59(2) 14.30(2) 10.69(2)	122.0(30)	CuO_4	O	1.92(1,1)	O,O	90.0(4,1.6)	12
$Na_2[Cu\{(CF_3)_2CHO\}_4]$ (not given)	m C2/c 4	15.965(6) 12.652(3) 11.837(5)		CuO_4	O	1.942(5,26)	O,O	91.2(2,2.85)	13
$(Ph_4P)_2[Cu\{(CF_3)_2CHO\}_4]$ (not given)	m $P2_1/c$ 2	10.947(2) 15.901(3) 17.773(3)	92.50(2)	CuO_4	O	1.933(6,0)	O,O	90.0(2,1)	14
$[Cu(Me_3NCH_2CO_2)_4]$ $(ClO_4)_2$ (not given)	tg I42m 2	11.711(-) 11.711(-) 11.695(-)		CuO_4^{c1} CuO_4^{c2}	O O	1.89(1) 2.09(2)	O,O O,O	not given not given	15
$Cu(4\text{–}NO_2pyNO)_2(NO_3)_2$ (green)	m $P2_1$ 2	10.670(2) 8.1249(9) 9.699(2)	104.71(2)	CuO_4	O_2NO O	1.951(3,12) 1.923(3,13)	O,O	90.0(1,7.2) 172.9(1,2.3)	16
$[Cu(sal)_2(H_2O)_2]\cdot 2H_2O$ (blue)	m $P2_1/c$ 2	3.741(2) 17.667(16) 12.278(14)	93.37(7)	CuO_4	O	1.926(1,12)	O,O	91.51(5)	17
$Cu(sal)_2(H_2O)_2]\cdot 2H_2O$ (dark blue)	m $P2_1/c$ 2	3.728(8) 17.70(3) 12.27(2)	93.3(–)	CuO_4	O H_2O	1.84(–) 1.92(–)	O,O	90(–, 4)	18
$[Cu(4\text{–}MeOphex)_2(H_2O)_2]\cdot$ $2H_2O$ (blue)	or $Ccm2_1$ 4	7.07(2) 44.4(1) 6.26(2)		CuO_4	O H_2O	1.96(1,0) 1.95(2,2)	O,O	90.2(4, 2.1)	19
$Cu(cbphex)_2(H_2O)$ (not given)	tr P–1 1	4.0976(4) 9.936(1) 13.020(2)	103.88(1) 107.00(1) 97.61(1)	CuO_4	O H_2O	1.933(2) 1.961(3)	O,O	90.0(1,1.8)	20
$Cu(cxphex)_2(H_2O)_2$ (dark blue)	tr P–1 1	4.086(5) 9.954(12) 12.469(12)	72.87(9) 88.63(9) 82.74(10)	CuO_4	O H_2O	1.912(10) 1.912(10)	O,O	90.0(–)	21
$Cu(Ph_2P)_2(H_2O)_2$ (greenish-blue)	m I2/c 4	24.126(6) 8.510(2) 12.333(3)	90.73(5)	CuO_4	O H_2O	1.962(3) 1.912(3)	O,O	90.0(3,1)	22
$Cu(npc)_2(H_2O)_2$ (not given)	m $P2_1/c$ 2	11.558(1) 11.405(1) 8.041(1)	93.47(1)	CuO_4	O H_2O	1.933(4) 1.959(4)	O,O	90.0(2,1)	23
$Cu(L\text{–}C_4H_8NO_3)_2(H_2O)$ (blue)	m $P2_1$ 2	11.02(2) 4.90(1) 11.16(2)	93.5(5)	CuO_4	O H_2O	not given not given	O,O	not given	24
$Cu(dl\text{–}C_4H_8NO_3)_2$ (blue)	m Cm 8	19.77(2) 11.01(2) 10.64(2)	93.5(2)	CuO_4	O	not given	O,O	not given	24
$Cu(acac)_2$ (not given)	m $P2_1/n$ 2	11.364(4) 4.71(1) 10.323(1)	91.8(3)	CuO_4	O	1.92(1,1)	O,O	95.0(4)[d]	25

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$Cu(acac)_2$ (not given)	m $P2_1/n$ 4	11.331(9) 4.697(3) 10.290(9)	91.84(7)	CuO_4	O	1.913(4,1)	O,O	93.2(2)[d]	26
$Cu(3\text{–}Meacac)_2$ (green gray) (at 180(+ – 10)K)	tr P–1 1	8.036(7) 4.81(1) 9.086(7)	88.2(–) 108.9(–) 73.6(–)	CuO_4	O	1.908(4,1)	O,O	92.6(2)[d] 87.4(2)	27
$Cu(3\text{–}Phacac)_2$ (green)	m $P2_1/c$ 2	10.250(–) 6.778(–) 13.763(–)	93.55(–)	CuO_4	O	1.907(8,5)	O,O	91.4(3)[d] 88.6(3)	28
$Cu(3\text{–}alacac)_2$ (green gray)	m $P2_1/n$ 2	13.544(5) 4.677(3) 13.861(7)	110.79(3)	CuO_4	O	1.905(3,1)	O,O	91.76(12)[d] 88.24(12)	29
$Cu(acacC_2N_2)_2$ (dark green)	tr P–1 1	11.460(7) 6.112(5) 5.611(4)	79.5(1) 91.5(1) 104.0(1)	CuO_4	O	1.912(4,2)	O,O	90.0(2)[d]	30
$Cu(F_6acac)(acac)$ (not given)	tr P–1 2	8.775(3) 12.052(4) 6.978(3)	99.87(3) 114.13(3) 90.70(3)	CuO_4	F_6acO acacO	1.946(4) 1.887(4,3)	O,O O,O	91.5(1)[d] 94.7(1)[d]	31
$Cu(F_6acac)(bac)$ (not given)	m $P2_1/c$ 4	12.289(–) 8.571(–) 16.645(–)	108.21(–)	CuO_4	F_6acO bacO	1.952(–, –) 1.895(–, –)	O,O	91.0[d] 93.9[d]	32
$Cu(tfac)_2$ (dark green)	tr P–1 1	4.573(2) 9.2673(3) 11.0765(3)	80.98(2) 76.95(2) 79.42(1)	CuO_4	O	1.908(2,3)	O,O	93.3(1)[d] 86.7(1)	33
$Cu(Etacet)_2$ (green)	m $P2_1/n$ 2	11.598(6) 4.527(2) 13.791(6)	104.5(4)	CuO_4	O	1.91(1)	O,O	90.4(5)[d] 89.6(5)	34
$Cu(PrN_2O_2)_2$ (not given)	m C2/c 4	22.789(2) 4.865(1) 11.400(1)	not given	CuO_4	O	1.906(4)	O,O	81.99(6)[e] 98.01(6)	35
$Cu(C_6H_3O_3S)_2$ (not given)	tr P–1 1	5.073(2) 8.199(1) 8.770(2)	61.89(2) 82.28(2) 81.36(2)	CuO_4	O	1.932(4,33)	O,O	83.8(4)[e] 96.2(1)	36
Cu $(bzac)_2$ (bluish gray)	m $P2_1/c$ 2	4.475(5) 10.640(5) 18.486(10)	97.67(8)	CuO_4	O	1.923(5,9)	O,O	93.0(2)[d] 87.0(2)	37
$Cu(tod)_2$ (blue)	m $P2_1/n$ 4	20.369(4) 10.371(2) 11.526(2)	90.04(1)	CuO_4	O	1.884(7,12)	O,O	92.8(3,1)	38
$Cu(C_{11}H_{19}O_2)_2$ (dark purple)	m $P2_1/n$ 2	12.273(6) 11.040(4) 10.838(3)	117.98(1)	CuO_4	O	1.890(9,14)	O,O	93.2(3)[d] 86.8(3)	39
$Cu(C_{24}H_{20}NO_6P_2)_2$ (blue)	or Pbca 4	21.606(3) 9.188(1) 22.693(3)		CuO_4	O	1.933(3,1)	O,O	93.1(1)[d] 86.9(1)	40
$Cu(C_{30}H_{37}O_8P_2)_2$ $(Me_2CO)_2(H_2O)_2$ (not given)	tr P1 1	11.177(1) 12.077(1) 15.890(1)	112.32(1) 91.55(1) 106.26(1)	CuO_4	O	not given	O,O	not given	41
Cu $(C_5H_{10}N_3O_3)_2$ (not given)	m $P2_1/b$ 4	7.874(3) 11.031(5) 18.619(7)	78.76(3)	CuO_4	O	1.908(–)	O,O	81.9(–)[e] 98.1(–)	42

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$Cu(C_{31}H_{43}O_4)_2$ (not given)	tr P1 2	11.300(9) 16.101(1) 17.089(2)	82.23(1) 74.88(4) 77.43(3)	CuO_4	O	not given	O,O	not given	43
$Cu(fch)_2$ (dark green)	m $P2_1/c$ 4	11.435(2) 5.270(3) 12.173(2)	108.55(2)	CuO_4	O	1.903(5,11)	O,O	93.2(2)[d]	44
$Cu(C_8H_{11}O_2)_2$ (not given)	or Pbca 4	15.273(7) 6.369(2) 15.687(6)		CuO_4	O	1.896(4)	O,O	91.9(1)[d] 88.1(1)	45
$Cu(pmbp)_2$ (not given)	m $P2_1/c$ 2	6.809(3) 23.722(8) 9.102(3)	108.94(4)	CuO_4	O	1.901(5)	O,O	not given	46
$Cu(pcd)_2$ (blue)	m $P2_1/n$ 2	9.697(6) 23.07(3) 6.325(3)	97.51(4)	CuO_4	O	1.894(7,29)	O,O	92.3(3)[d] 87.7(3)	47
$(Cu(fla)_2)\cdot 2CHCl_3$ (not given)	tr P1 1	7.273(1) 10.961(1) 11.229(1)	103.77(1) 105.76(1) 99.61(1)	CuO_4	O	1.948(3,4)	O,O	85.7(2) 94.3(2)	48
$Cu(C_{11}H_{17}O_2)_2$ (dark green)	m $P2_1/c$ 2	10.642(1) 11.005(1) 9.295(1)	92.53(1)	CuO_4	O	1.907(3,10)	O,O	92.2(1)[d] 87.8(1)	49
$Cu(sald)_2$ (not given)	m $P2_1/n$ 2	8.72(2) 6.19(2) 11.26(3)	104.8(–)	CuO_4	O	1.92(2,6)	O,O	94.8(–)[d] 85.2(–)	50
$Cu(sald)_2$ (not given)	m $P2_1/c$ 2	11.75(3) 4.00(2) 12.4(3)	90.3(–)	CuO_4	O	1.92(–,2)	O,O	95(–)[d] 85(–)	51
$Cu(Ph_2pn)_2$ (green)	m C2/c 4	26.18(–) 6.07(–) 16.64(–)	115.3(–)	CuO_4	O	1.91(–)	O,O	93.2(–)[d] 86.8(–)	52
$Cu(Ph_2C_3HO_2)_2$ (dark green)	m I2/c 4	16.46(2) 5.95(1) 24.13(4)	103.0(5)	CuO_4	O	1.908(–,1)	O,O	93.0(–)[d]	53
$Cu(C_{10}H_{15}NO_3)_2$ (not given)	m $P2_1/c$ 2	13.003(4) 7.918(2) 10.641(4)	79.84(2)	CuO_4	O	1.885(7,8)	O,O	91.6(3)[d]	54
$Cu(tpl)_2$ (not given)	m $P2_1/c$ 2	3.800(5) 13.82(2) 11.60(2)	93.4(2)	CuO_4	O	1.909(10,20)	O,O	84.7(5)[e] 95.3(5)	55
$Cu(cdd)_2$ (not given)	m $P2_1/n$ 2	4.9657(7) 14.977(2) 12.670(2)	95.84(1)	CuO_4	O	1.929(3,1)	O,O	91.5(–)[d] 88.59(–)	56
$Cu(ctdd)_2$ (not given)	m $P2_1/c$ 2	4.900(3) 28.206(7) 9.060(3)	102.21(3)	CuO_4	O	1.924(3,2)	O,O	93.0(–)[d] 87.0(–)	56a
$Cu(Et_2ala)_2$ (red)	tr P–1 1	9.684(6) 7.945(6) 8.101(7)	100.57(5) 106.85 124.01(4)	CuO_4	O	1.971(6,60)	O,O	84.1(2)[e]	56b
$Cu(C_8H_{10}O_2Cl)_2$ (dark green)	tr P–1 not given	10.557(3) 7.884(2) 13.889(5)	112.48(2) 109.52(2) 102.57(2)	CuO_4	O	1.900(5,7)	O,O	91.6(2,5)[d] 88.8(2,0)	56c

TABLE I *(Continued)*

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$Cu(pmbp)_2$ (not given)	m $P2_1/c$ 2	6.809(3) 23.727(8) 9.102(3)	108.94(4)	CuO_4	O	1.901(–,5)	O,O	90(–)[d] 90(–);180(–)	56d
$Cu(C_{11}H_7O_2S_2)_2$ (reddish brown)	m $P2_1/c$ 2	11.841(6) 7.850(6) 11.586(9)	96.03(2)	CuO_4	O	1.910(3,2)	O,O	93.4(1)[d] 86.7(1)	56e
$Li_2[Cu(eth)_2]\cdot 6H_2O$ (not given)	tr P–1 1	4.849(2) 7.907(4) 8.643(4)	92.02(3) 99.23(2) 103.35(2)	CuO_4	O	1.931(2,10)	O,O	87.21(6)[e]	56f
$Na_2[Cu(eryan)_2]\cdot 4H_2O$ (not given)	tr P–1 1	5.218(3) 8.395(5) 9.112(5)	108.77(4) 98.86(4) 106.56(4)	CuO_4	O	1.938(2,0)	O,O	86.98(10)[e] 93.02(10)	56f
$K_2[Cu(eryan)_2]\cdot 4H_2O$ (not given)	tr P–1 1	5.176(4) 9.451(7) 9.372(6)	110.53(5) 103.85(3) 103.35(2)	CuO_4	O	1.922(2,3)	O,O	87.14(10)[e] 92.86(10)	56f
$Li_3[Cu(Me–a–manpH_2)$ $(Me–a–(manpH)]\cdot 5H_2O$ (not given)	or $P2_12_12_1$ 4	8.222(1) 12.112(2) 22.855(3)		CuO_4	O	1.929(2,5)	O,O	87.33(7,15)[e]	56f
$(enH_2)[Cu(ox)_2]$ (blue)	tr P–1 1	5.188(1) 6.641(1) 8.224(2)	115.14(2) 107.48(2) 77.68(2)	CuO_4	O	1.933(5,16)	O,O	85.2(2)[e]	56g
$Cu(C_2H_4O_2)_2$ $Ba(C_2H_6O_2)_6$ (deep blue)	m Cc 4	12.103(6) 13.527(3) 17.091(8)	93.17(2)	CuO_4	O	1.922(4,12)	O,O	86.7(4,2)[e] 93.3(2,4)	57a
$Cu(C_{62}H_{86}O_4)$ (not given)	tr P–1 1	10.341(3) 11.621(2) 12.817(2)	103.99(1) 92.73(2) 109.55(2)	CuO_4	O	1.903(4,15)	O,O	92.3(2)[d]	57b
$Cu(NH_3)_4I_4$ (not given)	m C2/m 2	14.172(4) 8.926(2) 6.558(2)	128.65(2)	CuN_4	N	2.013(5,0)	N,N	90.00(20,4)	58
$Cu(1,4,5–Me_3im)_4(ClO_4)_2$ (orange-brown)	or Pccn 4	13.65(1) 13.90(1) 17.54(1)		CuN_4	N	1.995(7) 2.004(7)	N,N	90.0(3,5)	59
$K_2(Cu(sucim)_4)\cdot 6H_2O$ (pink)	tr Pl 1	8.51(3) 8.50(3) 9.28(2)	97.4(3) 100.4(2) 79.9(2)	CuN_4	N	2.08(–,15)	N,N	86(–,8)	60
$Li_2(Cu(sucim)_4)\cdot H_2O$ (blue)	m $P2_1/a$ 4	26.61(2) 9.65(3) 8.58(2)	94.4(2)	CuN_4	N	1.98(–,2)	N,N	94(–,7) 154(–,2)	60
$Cs_2(Cu(sucim)_4)\cdot 2H_2O$ (violet)	tr Cl 2	9.19(–) 15.32(–) 8.39(–)	88.7(–) 92.0(–) 93.8(–)	CuN_4	N	2.00(2,0)	N,N	89(1,0)	61
p-xyl$(Ph_3P)_2Cu(NCS)_4$ (red violet)	m $P2_1/n$ 4	15.875(6) 23.453(5) 12.56(10)	100.12(4)	CuN_4	N	1.907(9,19)	N,N	97.6(3,1.5) 137.3(3,2.3)	62
$Cu(C_6H_{11}NH_2)_4(NO_3)_2$ (not given)	or $P2_12_12_1$ 4	13.68(4) 16.21(2) 13.55(1)		CuN_4	N	2.03(1,6)	N,N	93.1(7,4) 152.1(4,7)	63

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$Cu(NH_3)_2(C_3H_2N_3O_3)_2$	tr	9.051(15)	91.36(18)	CuN_4	H_3N	1.90(1,0)	N,N	82.9(1,10)	64
(not given)	P1	13.006(19)	82.69(19)		N	2.06(1,0)		97.1(1,10)	
	2	5.018(8)	93.23(18)						
$Cu(NH_3)_2(C_4H_4NO_2)_2$	tr	6.34(2)	89.0(5)	CuN_4	N	2.03(1,5)	N,N	91(1,0)	65
(red)	P1	9.33(2)	189.2(5)						
	1	5.30(2)	102.7(5)						
$Cu(NH_3)_2(C_5H_4N_5O_2)_2.2H_2O$	tr	8.811(2)	99.62(1)	CuN_4	H_3N	1.996(7)	N,N	90.0(4,5)	66
(not given)	P1	7.985(2)	83.32(1)		N	2.024(7)			
	1	6.934(1)	115.01(1)						
$Cu(NH_3)_2(C_{15}H_{11}N_2O_2)_2$	m	31.308(16)		CuN_4	H_3N	2.032(–)	N,N	not given	67
(deep-red)	C2/c	8.559(11)	107.15(1)		N	2.074(–)			
	4	11.258(5)							
$Cu(NCS)_2(py)_2$	m	9.2211(2)		CuN_4	SCN	1.94(2,0)	N,N	89.0(5)	68
(green)	C2/m	14.519(7)	108.66(2)		pyN	1.98(2,0)			
	2	5.626(1)							
$Cu(NCS)_2$(t-pic)$_{1.75}$	tr	9.843(3)	104.07(3)	CuN_4	SCN	1.94(1)	N,N	91.0(5)	69
(β-pic)$_{0.25}$[g]	P1	10.174(5)	90.92(3)		N	2.06(1)			
(green)	4	18.348(7)	111.37(3)	CuN_4	SCN	1.96(1)	N,N	89.9(5)	
					N	2.02(1)			
				CuN_4	SCN	1.95(1,1)	N,N	91.2(6,7)	
					N	2.03(1,1)			
$Cu(NCS)_2$(4-Mepy)$_2$[f]	m	9.808(6)		CuN_4	SCN	1.948(8,12)	N,N	90.0(4,2.5)	70
(dark green)	$P2_1$	26.752(10)	107.89(4)		pyN	2.021(8,18)			
	6	9.927(4)		CuN_4	SCN	1.936(8,3)	N,N	90.0(4,8)	
					pyN	2.064(8,10)			
				CuN_4	SCN	1.963(9,11)	N,N	90.0(4,2)	
					pyN	2.023(8,1)			
$Cu(NCS)_2$(4-Mepy)$_2$[f]	m	9.63(1)		CuN_4	SCN	1.92(1,3)	N,N	not given	71
(dark green)	$P2_1$	26.53(2)	106.40(7)		pyN	2.01(1,2)			
at 180K	6	9.84(2)		CuN_4	SCN	1.94(2,1)			
					pyN	2.05(1,0)			
				CuN_4	SCN	1.93(1,3)			
					pyN	2.00(1,2)			
$Cu(py)_2$(toslopdi)	m	16.894(2)		CuN_4	pyN	1.998(3,0)	N,N	81.0(1)[e]	72
(not given)	C2/c	11.662(2)	100.62(2)		N	1.942(3,0)		98.7(1)	
	4	14.753(4)				120.1(1,2.8)			
$[Cu(en)_2](SCN)_2$	tr	7.352(8)	86.93(–)	CuN_4	N	2.00(1,1)	N,N	91.1(–,3)[e]	73
(not given)	P1	9.364(5)	113.38(–)					95.2(–)	
	1	6.585(16)	125.13(–)						
$[Cu(en)_2]I_2.0.33dmf$	or	21.501(4)		CuN_4	N	2.10(5,1)	N,N	81(2,0)[e]	74
(blue)	$Bm2_1b$	15.770(4)						108(2,0)	
	8	12.016(7)							
$[Cu(en)_2][Cu(C_4O_2S_2)_2]$	m	19.145(6)		CuN_4	N	2.005(4,10)	N,N	not given	75
(black)	C2/c	8.230(1)	133.23(1)	CuS_4	S	2.308(1,13)	S,S	94.1(1)[e]	
	4	16.695(5)						96.0(1)	
$[Cu(en)_2][PtCl_2(Cu)]$	or	13.645(1)		CuN_4	N	2.031(4,0)	N,N	91.2(1,0)[e]	76
$(ClO_4)_4$	Icma	10.787(1)							
(red)	2	9.645(1)							
$[Cu(en)_2][PtBr_2(en)_2]$	or	13.599(1)		CuN_4	N	2.043(3,0)	N,N	90.9(1,0)[e]	76
$(ClO_4)_4$	Icma	10.917(1)							
(not given)	2	9.657(1)							
$[Cu(en)_2][PtBr_2(en)_2]$	or	13.625(2)		CuN_4	N	2.043(6,0)	N,N	90.9(2,0)[e]	76
$(ClO_4)_4$	Icma	10.905(2)							
(not given)	2	9.651(1)							

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$[Cu(Me4en)_2](ClO_4)_2$ (not given)	m $P2_1/n$ 2	7.453(1) 18.860(5) 7.615(1)	94.54(1)	CuN_4	N	1.998(4,5)	N,N	83.8(1)[c] 96.2(2)	77
$[Cu(Et_2en)_2](ClO_4)_2$ (brick red)	tr P1 2	17.868(1) 8.104(1) 10.039(1)	90.40(1) 131.63(1) 90.45(2)	CuN_4	N	2.032(4,29)	N,N	84.4(2)[c]	78
$[Cu(Et_2en)_2](ClO_4)_2$ (red) at 298K	tr P1 1	8.131(8) 8.762(13) 9.786(12)	65.33(16) 65.98(11) 63.34(8)	CuN_4	N	2.035(3,34)	N,N	84.9(1)[c]	79
$[Cu(Et_2en)_2](ClO_4)_2$ (blue violet) at 333K	m 12 4	13.34(1) 8.414(5) 9.978(5)	97.43(5)	CuN_4	N	2.034(9,18)	N,N	82.1(5)[c]	79
$[Cu(Et_2en)_2](NO_3)_2$ (red)	m $P2_1/n$ 2	9.76(5) 12.81(5) 8.24(5)	105.87(8)	CuN_4	N	2.046(5,35)	N,N	84.9(2)[c]	80
$[Cu(bquam)_2](CO_3).4H_2O$ (pink red)	m $P2_1/n$ 4	13.185(7) 17.546(8) 6.87(3)	107.01(4)	CuN_4	N	1.951(7,7)	N,N	89.2(5,1)[d] 90.9(5,7)	81
$[Cu(bquam)_2]Cl_2.2H_2O$ (red)	tr P1 2	6.801(3) 9.582(1) 12.485(2)	68.65(1) 72.91(2) 78.74(2)	CuN_4	N	1.949(5,8)	N,N	89.0(2,0)[d] 91.0(2,3)	82
$[Cu(bquam)_2]$ $[Cu(acac)_2Cl]_2$ (blue green)	or Pbca 4	15.218(2) 15.986(3) 14.563(3)		CuN_4	N	1.936(3,3)	N,N	88.2(1)[d] 91.8(1)	83
$[Cu(C_{11}H_2N_7)_2].2thf$ (purple)	or Pbca 2	13.233(2) 10.754(2) 21.411(4)		CuN_4	N	1.990(5,6)	N,N	92.1(2)[d] 87.9(2)	84
$[Cu(tach)_2](NO_3)_2$ (not given)	m C2/m 2	18.496(4) 7.289(2) 7.201(2)	110.22(2)	CuN_4	N	2.169(6,5)	N,N	85.7(1)[d] 89.7(1)	85
$[Cu(C_4H_{10}N_4O)_2]Br_2$ (not given)	m $P2_1/c$ 2	5.221(2) 12.306(3) 12.703(3)	95.94(3)	CuN_4	N	1.949(4,23)	N,N	88.8(2)[d] 91.2(2)	86
$(Cu(aepy)_2]I_2$ (dark olive green)	m $P2_1/c$ 2	8.304(1) 14.311(2) 7.677(2)	108.07(1)	CuN_4	N	2.022(3,6)	N,N	86.8(1)[d] 93.2(1)	87
$[Cu(bppa)_2](ClO_4)_2$ (not given)	m C2/c 4	9.356(8) 12.752(2) 19.353(4)	101.56(3)	CuN_4	N	1.976(1,5)	N,N	93.42(5)[d]	88
$[Cu(cyhis)_2]$ $(ClO_4)_2.4H_2O$ (violet)	trg $P3_221$ 3	8.450(3) 8.450(3) 42.00(6)		CuN_4	N	1.98(1,1)	N,N	90(1,1)	89
$[Cu(daco)_2](NO_3)_2$ (orange)	m $P2_1/n$ 2	7.9040(7) 15.694(1) 7.0886(7)	95.36(1)	CuN_4	N	2.016(1,19)	N,N	85.98(5)[d]	90
$[Cu(C_7H_{18}N_2)_2]$ $(C_3H_2O_4).3H_2O$ (violet)	m $P2_1/c$ 4	10.136(6) 16.124(10) 16.433(7)	110.19(4)	CuN_4	N	2.005(4,34)	N,N	not given	91
$Cu(bmca)_2$ (violet red)	m $P2_1/n$ 2	9.973(3) 5.657(1) 11.578(3)	99.73(2)	CuN_4	N	1.930(3,2)	N,N	87.5(–,0)[d] 92.5(–,0)	92

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$[Cu(C_2H_5N_2O_2)_2]\cdot 2H_2O$ (violet)	or Pbca 4	5.052(3) 11.152(2) 17.876(2)		CuN_4	N	1.923(9) 2.015(9)	N,N	81.7(3,0)[e]	93
$[Cu(bimbph)_2](ClO_4)_2$ (yellow green)	or Pbcn 8	17.581(3) 21.706(2) 19.154(2)		CuN_4	N	1.958(9,19)	N,N	96.2(3,3.5) 141.9(5,1.3)	94
$[Cu(C_3H_8N_4)_2](ClO_4)_2$ (red)	m I2/m 2	10.727(4) 9.719(3) 7.739(2)	92.12(2)	CuN_4	N	1.956(1)	N,N	89.38(6)[d]	95
$[Cu(C_4H_7N_5O)_2]$ $(ClO_4)_2$ (dark brown)	m $P2_1/c$ not given	4.989(1) 10.883(2) 16.648(2)	94.24(1)	CuN_4	N	1.969(4,1)	N,N	80.9(2)[e] 99.1(2)	96
$Cu(C_5H_5N_2)_2$ (deep purple brown)	m $P2_1/c$ 2	9.845(2) 5.562(3) 9.604(3)	103.07(1)	CuN_4	N	1.961(9,11)	N,N	82.4(3)[e] 97.6(3)	97
α–$Cu(dmpz.NCO)_2$ (violet)	m $P2_1/c$ 8	13.697(7) 14.759(7) 7.463(7)	114.01(3)	CuN_4	N	1.917(8,9)	N,N	81.3(3,3)[e] 99.4(3,4)	98
$[Cu(C_{12}H_{12}N_5O_2)_2]\cdot$dmso (black)	m $P2_1/n$ 4	12.878(2) 14.791(1) 17.268(2)	109.79(1)	CuN_4	N	1.941(7,22)	N,N	89.0(3,1)[d] 97.5(3,9)	99
$[Cu(C_{16}H_{24}N_3O_2)_2]\cdot$ 0.5Etac (dark violet)	trg $P3_221$ 4	10.678(1) 10.673(1) 53.119(6)		CuN_4		not given	N,N	not given	100
$Cu(C_{17}H_{17}N_2)_2$[g] not given	m $P2_1/c$	15.792(9) 23.306(9) 8	90.72(6) 15.979(6)	CuN_4 CuN_4	N N	1.97(1,2) 1.96(1,1)	N,N N,N	96.2(5,3)[d] 117.4(5,14.9) 97.3(5,8)[d] 116.8(5,15.3)	101
$Cu(thene)_2$ (dark green)	m $P2_1/c$ 4	8.09(1) 30.16(4) 16.01(2)	91.7(1)	CuN_4	N	1.99(4,3)	N,N	97.3(1.8,3.2)[d] 116.7(1.9,16.2)	102
$[Cu(bpy)_2](PF_6)_2$ (dark green)	tg $I4_1/acd$ 8	16.228(3) 16.228(3) 18.954(3)		CuN_4	N	1.985(11)	N,N	83.0(7)[e] 103.6(8)	103
$[Cu(C_{18}H_{14}N_4)_2]$ $(C1O_4)_2$ (green)	or Pbcn 8	17.581(3) 21.706(2) 19.154(2)		CuN_4 CuN_4	N N	1.957(7,4) 1.965(8,16)	N,N N,N	96.3(3,3.3)[d] 141.4(4,1.1) 96.2(3,2.6)[d] 141.8(5,2)	104
$[Cu(bcp)_2]BF_4\cdot$MeOH (brick red)	m $P2_1/c$ 4	11.131(3) 21.454(4) 18.900(3)	102.34(2)	CuN_4	N	2.022(4,10)	N,N	81.9(2,1)[e] 123.6(2,57)	105
$Cu(bipyam)_2(C1O_4)_2$ (blue)	m not given not given	9.35(2) 12.88(1) 19.69(2)	102.8(3)	CuN_4	N	1.97(1,3)	N,N	95.6(4)[d] 139.7(6,2.4)	106
$(Cu(dbipyam)_2$ (black)	m C2/c 4	14.691(6) 12.256(9) 11.945(2)	124.24(3)	CuN_4	N	1.954(2,2)	N,N	93.63(8)[d] 101.1(1,4) 138.17(8)	107
$Cu(C_9H_{13}N_2)_2$ (light green)	tr P–1 2	7.49(1) 11.26(2) 11.73(2)	81.67(–) 89.63(–) 76.27(–)	CuN_4	N	1.936(11,14) 2.056(13,12)	N,N	84.7(7,1)[e] 109.2(6,5)	108

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$Cu(C_9H_{13}N_2)_2$	tg	9.89(2)		CuN_4	N	1.922(15)	N,N	85.4(6,0)[e]	108
(dark green)	$P4_12_12$	9.89(2)				2.044(16)		107.3(6,0)	
	4	19.08(2)							
$Cu(mpa)_2$	or	8.639(1)		CuN_4	N	1.951(2,12)	N,N	93.3(1,5)[d]	109
(purple)	$P2_12_12_1$	14.358(4)						119.9(1,22.1)	
	4	17.510(3)							
$[Cu(dpm)_2](ClO_4)_2$	tr	8.646(1)	96.41(1)	CuN_4	N	2.019(5,8)	N,N	not given	110
(red violet)	P–1	8.916(1)	115.75(1)						
	2	9.068(1)	105.16(1)						
$Cu(C_{10}H_{16}N_4O_2)_2$	m	11.007(1)		CuN_4	N	1.944(2)	N,N	91.3(1)[d]	111a
(not given)	C2/c	13.005(1)	102.73(1)					104.2(1)	
	4	22.988(2)							
$Cu(C_{17}H_{16}N_3O)_2$	tr	6.149(2)	68.54(2)	CuN_4	N	1.936(4,20)	N,N	92.9(1,3)	111b
(not given)	P–1	9.890(2)	101.15(2)					101.3(2,2.2)	
	1	10.738(3)	92.85(2)					138.8(2,2.0)	
Cu(en) (biu)[g]	tr	7.541(2)	99.29(4)	CuN_4	biuN	1.910(3,1)	N,N	84.4(1)[e]	112
(red violet)	P1	9.032(6)	101.32(3)		enN	2.025(3,1)		92.6(1)[d]	
	4	12.078(5)	86.98(4)					94.2(1,3)	
				CuN_4	biuN	1.917(3,5)	N,N	84.1(1)[e]	
					enN	2.020(3,8)		91.6(1)[d]	
								92.8(1,1)	
$[Cu(H_2bim)_2]Cl_2$	m	7.940(3)		CuN_4	N	2.01(1,2)	N,N	81.6(5)[e]	113
$[Cu(H_2bim)Cl_2]_2$	$P2_1/c$	31.468(6)	114.2(1)	CuN_2Cl_2	N	2.01(1,1)	N,N	80.6(4)[e]	
(not given)	2	7.229(4)			Cl	2.254(4)	N,Cl	93.4(3)	
					μCl	2.297(4)		173.9(3)	
						2.804(5)	N,μCl	91.0(4)	
								161.5(4)	
							Cl,μCl	94.4(1)	
							μCl,μCl	94.1(1)	
$[Cu(dpta)(NCS)](NO_3)$	m	9.571(2)		CuN_4	N	2.036(6,47)	N,N	94.2(2,3)[d]	114
(blue)	$P2_1/c$	10.453(2)	108.29(2)		SCN	2.005(6)		84.5(2,1.2)	
	4	13.620(3)							
[Cu(pc)]I	tg	13.888(12)		CuN_4	N	1.935(6,0)	N,N	90.00(–,0)	115
(green bronze)	P4/mmc	13.888(12)							
	2	6.390(8)							
Cu(tprp)	m	5.015(7)		CuN_4	N	2.000(–,6)	N,N	90.0(–,0)[d]	116a
(purple)	$P2_1/c$	11.55(9)	99.1(2)						
	2	22.50(9)							
$Cu(C_{25}H_{28}N_6O_2)$	m	11.248(4)		CuN_4	N	1.964(5,9)	N,N	90.8(2,1.3)[d]	116b
(not given)	$P2_1/n$	11.269(4)						97.7(2,2.9)	
	4	15.869(5)	92.20(3)					150.4(1,5.3)	
Cu(pc)	m	19.6(–)		CuN_4	not given			not given	117
(not given)	$P2_1/a$	4.79(–)	120.6(–)						
	2	14.6(–)							
β-Cu(pc)	m	19.407(–)		CuN_4	N	1.935(5,5)	N,N	88.7(–)[d]	118
(not given)	$P2_1/a$	4.790(–)	120.93(–)						
	2	14.628(–)							
Cu(tc–3,3)	m	9.933(1)		CuN_4	N	1.939(6)	N,N	98.5(1)[d]	119
(brown)	$P2_1/n$	5.798(1)	91.82(1)					81.5(1)[e]	
	2	14.520(2)							
Cu(tc–4,4)	m	11.178(2)		CuN_4	N	1.938(7)	N,N	103.3(1)[d]	119
(brown)	$P2_1/c$	8.636(1)	90.39(2)					81.6(7)[e]	
	4	20.188(8)							

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
Cu(tc–5,5) (dark brown)	h P6$_5$22 6	11.044(2) 11.044(2) 30.390(3)		CuN_4	N	1.96(1)	N,N	111.5(4)[d] 81.7(6)[e]	119
Cu($C_{45}H_{26}N_4O$) (black green)	m $P2_1/n$ 4	18.532(5) 7.325(5) 23.932(5)	93.26(2)	CuN_4	N	1.994(13,22)	N,N	90.0(6,1.5)[d]	120
Cu($C_{17}H_{18}N_4$) (not given)	or $P2_12_12_1$ 4	9.096(2) 24.551(9) 7.159(3)		CuN_4	N	1.914(13,34)	N,N	82.6(5)[e] 91.4(5,2)[d] 95.0(5)	121
Cu($C_{18}H_{20}N_6$) (red brown)	or Pbcn 4	11.701(9) 13.701(9) 10.660(6)		CuN_4	N	2.001(31,2)	N,N	82.0(9,2.2)[e] 90.7(9)[d] 112.3(10)	122
Cu($C_{22}H_{22}N_4$)[g] (dark green)	m $P2_1/c$ 8	14.318(2) 16.427(2) 16.229(2)	100.01(1)	CuN_4 CuN_4	N N	1.934(2,14) 1.926(2,4)	N,N N,N	84.3(1,1)[e] 95.5(1,5)[d] 84.4(1,4)[e] 95.5(1,2)[d]	123
α-Cu($C_{24}H_{36}N_6O_6$) (purple)	or Pbca 8	21.559(3) 15.265(3) 16.239(3)		CuN_4	N	2.06(–,2)	N,N	not given	124
Cu($C_{24}H_{23}N_5$) (red black)	m $P2_1/c$ 4	10.582(3) 25.951(3) 7.736(3)	106.37(5)	CuN_4	N	1.968(12,21)	N,N	85.8(5)[e] 92.4(5,5.1)[d]	125
Cu($C_{33}H_{49}N_2O_4Si_2$)$_2$ (violet)	m $P2_1$ 2	11.740(3) 24.698(5) 12.545(3)	91.37(2)	CuN_4	N	1.9(–)	N,N	not given	126
Cu(bzacen.2C_2N_2) (not given)	m $P2_1/n$ 4	19.863(9) 12.184(8) 9.736(6)	98.4(1)	CuN_4	N	1.936(6,18)	N,N	86.2(2)[e] 90.6(3)[d] 93.3(3)	127
Cu($C_{32}H_{26}(CH_2)_2N_6O_2$) (not given)	m $P2_1/b$ 4	11.420(2) 23.244(2) 11.484(2)	90.42(3)	CuN_4	N	1.932(3,13)	N,N	91.3(1,1.75)[d] 86.4(1)[e] 101.7(1)	128
Cu($C_{32}H_{26}(CH_2)_3N_6O_2$) (not given)	m I2/a 4	23.479(7) 15.856(5) 8.244(2)	95.49(2)	CuN_4	N	1.945(3,8)	N,N	89.9(1)[d] 103.8(2)[h] 103.6(1)	128
Cu($C_{32}H_{26}(CH_2)_4N_6O_2$) (not given)	m $P2_1/b$ 4	11.475(2) 25.279(6) 11.152(2)	90.42(3)	CuN_4	N	1.949(5,35)	N,N	93.5(2,1.15)[d] 104.5(2)[h] 101.7(1)	128
Cu($C_5H_8N_2S$) (not given)	or Bmmb 4	8.745(–) 6.826(–) 11.306(–)		CuN_4	N	not given	N,N	not given	129
Cu($C_{55}H_{60}N_4O_5$) (not given)	tr P-1 2	13.441(2) 14.246(8) 13.220(3)	90.0(–) 105.65(2) 90.0(–)	CuN_4	N	1.99(2,6)	N,N	90.0(5,24)[d]	130
[$Cu_{0.5}$($C_{16}H_{21}N_4O_2$)]· 0.33 H_2O (blue)	rh R32 6	15.44(1)	65.02(5)	CuN_4	N	1.98(3,2)	N,N	92(1) 122(1,17)	131
[Cu($C_9H_{11}N_5O_2$)]·2H_2O (red)	tr P–1 2	7.315(2) 10.110(3) 9.609(3)	71.59(3) 86.66(2) 110.74(2)	CuN_4	N	1.957(5,71)	N,N	94.6(1,0)[d] 83.1(1,0)[e] 99.4(1,0)	132
[Cu(gly-L-tryp)].3H_2O (deep blue)	or $P2_12_12_1$ 4	7.74(–) 13.78(–) 14.81(–)		CuN_4		1.98(–)	N,N	not given	133

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$[Cu(C_{74}H_{66}N_{12}O_4)]\cdot$ 1.5 Et_2O.1tol (purple)	m C2/c 8	31.240(4) 16.769(5) 35.199(4)	121.4(1)	CuN_4	N·	1.968(20,13)	N,N	90.2(7,5)[d]	134
[Cu(pincer)]· 3 $CHCl_3$ (not given)	m $P2_1/n$ 4	17.290(4) 22.649(5) 22.596(5)	111.92(2)	CuN_4	N	1.986(–)	N,N	not given	135
$[Cu(Et(gud)_2)]Cl_2.H_2O$ (not given)	m $P2_1/c$ 4	6.97(1) 11.88(2) 18.50(3)	103.5(–)	CuN_4	N	1.963(–,60)	N,N	92.67(–,53)[d] 83.77(–)[e] 90.7(–)	136
$[Cu(C_{20}H_{24}N_6)]Br_2.2H_2O$ (deep blue)	m C2/c 4	9.919(2) 16.626(3) 14.102(3)	94.39(2)	CuN_4	N	2.010(4,27)	N,N	82.9(2,0)[e] 93.4(1,0)[d] 99.6(1,0)	137
$[Cu(o\text{–}bpy)](ClO_4)_2$ (blue)	m C2/c 4	17.966(4) 10.702(4) 15.527(4)	128.36(2)	CuN_4	N	2.006(4,16)	N,N	81.6(1,0)[e] 109.5(2)[h] 96.4(2)	138
$[Cu_{0.07}H_{1.86}(teta)]$ $(ClO_4)_2.2dmso$ (pale pink)	m $P2_1/n$ 2	12.330(4) 15.12(1) 8.808(2)	104.07(2)	CuN_4	N	2.066(2,57)	N,N	87.78(7)[e] 92.22(70)[d]	139
$[Cu(C_{10}H_{26}N_4)](ClO_4)_2$ (lilac)	m $P2_1/n$ 4	16.033(3) 14.701(4) 7.849(1)	91.66(1)	CuN_4	N	2.035(–)	N,N	94.6(–)[d] 87.6(–)[h] 89.3(–)	140
$[Cu(tapp)](ClO_4)_2$ (blue)	or C2ca 4	11.302(5) 16.239(7) 13.948(6)		CuN_4	N	2.017(4,12)	N,N	74.2(2)[e] 97.2(2,6)[d]	141
$[Cu(C_{14}H_{16}N_4S_4)_2]$ $(ClO_4)_2.CH_3CN.CHCl_3$ (red brown)	tr P–1 2	12.888(4) 17.462(6) 10.906(1)	96.07(2) 104.18(2) 94.51(2)	CuN_4	N	1.992(9,19)	N,N	90.0(4,4.6)	142
$[Cu(ndap)](ClO_4)_2$ (dark blue purple)	or $P2_1cn$ 4	9.083(2) 15.198(3) 16.025(3)		CuN_4	N	1.976(17,44)	N,N	83.5(7)[e] 92.5(6)[d] 103.8(5)	143
[Cu(cis–[18]dieneN$_4$)] $(ClO_4)_2$ (purple)	m C2/c 8	29.081(4) 14.013(3) 14.862(2)	113.95(–)	CuN_4	N	2.002(5,22)	N,N	94.1(2,3.4)[d] 91.7(2,16)[h]	144 145
[Cu(trans–[18]dieneN$_4$)] $(ClO_4)_2$ (orange)	or $P2_12_12$ 2	14.720(2) 12.308(2) 7.982(1)		CuN_4	N	2.015(8,38)	N,N	95.4(3)[d] 85.0(3)[h]	144 146
[Cu(trans–[14]dieneN$_4$)] $(ClO_4)_2$ (red)	m $P2_1/c$ 4	10.487(9) 16.971(15) 13.855(13)	105.17(7)	CuN_4	N	1.98(3,2)	N,N	94.4(5,3)[d] 85.6(5,6)[e]	147
$[Cu(C_{16}H_{32}N_4)](ClO_4)_2$ (orange)	m $P2_1/c$ 2	10.331(5) 10.641(15) 11.050(6)	111.96(14)	CuN_4	N	2.001(7,28)	N,N	94.8(2,0)[d] 82.5(2,0)[e]	148
$[Cu(ddad)](BF_4)_2$[g] (green)	not given	not given		CuN_4	N	1.975(14,24)	N,N	87.2(6)[e] 98.5(5)[d] 97.7(6,6)[d]	149
				CuN_4	N	1.975(14,46)	N,N	86.9(6)[e] 100.3(5)[d] 96.7(6,1.8)[d]	
$[Cu(tim)](BPh_4)_2$ (gold orange)	m $P2_1/c$ 2	11.997(2) 13.042(4) 16.391(4)	102.10(1)	CuN_4	N	1.944(6,4)	N,N	81.8(2)[e] 98.2(2)[d]	150
$[Cu(C_{24}H_{36}N_6O_5)]$ $(Bph_4)_2$ (aquamarine)	m C2/c 4	20.12(1) 14.48(1) 22.37(2)	110.1(1)	CuN_4	N	2.007(17,43)	N,N	98.8(6)[i] 89.9(7) 83.6(7)	151a

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$[Cu(C_{12}H_{24}N_4)](ClO_4)_2$ (not given)	m C2/m 2	13.481(6) 9.312(2) 9.052(3)	116.99(2)	CuN_4	N	2.010(2)	N,N	not given	151b
$(Cu(C_{15}H_{18}N_4O_5)$ (violet)	m $P2_1/a$ 4	7.998(2) 22.696(6) 9.463(3)	109.94(2)	CuN_4	N	1.999(6,65)	N,N	not given	151c
$[Cu(C_{21}H_{32}N_6)](ClO_4)\cdot MeNO_2$	tr P-1 2	8.730(2) 12.434(4) 14.768(4)	98.04(2) 106.15(2) 101.78(2)	CuN_4	N	2.026(–,36)	N,N	not given	151d
$[Cu(oatpp)]\cdot 2CH_2Cl_2$ (red)	tr P-1 2	13.145(4) 13.911(5) 16.604(5)	104.35(2) 97.44(2) 107.75(2)	CuN_4	N	1.977(5)	N,N	90.3(2)[d]	151e
$[Cu(tmp)]SbCl_6$ (not given)	tg $P4_2/n$ 4	25.038(15) 25.038(15) 9.302(13)		CuN_4	N	2.008(3,11)	N,N	not given	152
$[Cu(tpp)][SbCl_6]$ (purple)	tr P1 2	13.484(2) 13.924(3) 12.886(2)	98.90(1) 111.08(2) 106.97(2)	CuN_4	N	1.988(8,5)	N,N	90.0(3,5)[d]	153
$Na_2[Cu(C_{10}H_{13}N_5O_6)]\cdot 4.5H_2O$ (pink)	tr P1 2	7.306(4) 10.902(3) 12.012(30)	91.73(2) 103.64(4) 96.14(4)	CuN_4	N	1.952(7,81)	N,N	83.7(3,9)[j] 109.1(3)[j]	154
$Na_2[Cu(C_8H_{10}N_4O_5)]\cdot 10H_2O$ (pink)	tr P1 2	7.665(6) 10.204(9) 14.872(10)	90.0(–) 107.65(5) 90.0(–)	CuN_4	N	1.952(5,76)	N,N	83.4(2,6)[j] 109.8(2)[j]	155
$Na_2[Cu(o\text{–}phen(biu)_2)]\cdot 4dmso$ (red)	tr P1 2	9.753(10) 16.513(8) 9.588(3)	106.98(5) 93.24(4) 86.21(4)	CuN_4	N	1.943(4,17)	N,N	84.0(1)[e] 92.3(2,1)[d] 91.7(2)	156
$Na_2[Cu(pr(biu)_2)]\cdot 3dmso$ (dark red)	m $P2_1/c$ 4	8.198(16) 13.718(17) 21.58(6)	98.63(10)	CuN_4	N	1.956(4,31)	N,N	92.8(2,4.9)[d] 89.3(2)	156
$[C_4H_8N_3O]_2[CuCl_4]$ (not given)	m $P2_1/c$ 2	8.080(3) 7.83(2) 13.922(2)	113.77(2)	$CuCl_4$	Cl	2.251(1,18)	Cl,Cl	90.00(4,9)	157a
$(\beta\text{–alaH})_2[CuCl_4]$ (not given)	m $P2_1/c$ 4+2	7.407(2) 7.734(1) 24.236(6)	91.82(1)	$CuCl_4$	Cl	2.290(1,17)	Cl,Cl	90.0(1,1.5)	157b
$(bzimH)_2[CuCl_4]\cdot H_2O$ (pale green)	m $P2_1/c$ 4	16.040(3) 4.243(1) 27.501(6)	104.78(4)	$CuCl_4$	Cl	2.285(2,10)	Cl,Cl	90.00(8,80)	158
$(C_4H_{16}N_3Cl)[CuCl_4]$ (yelow)	or Pnma 4	7.112(–) 23.78(–) 7.342(–)		$CuCl_4$	Cl	2.274(9,2)	Cl,Cl	90.5(2)	159
$(C_{14}H_{14}N_4S_4Cl_4)[CuCl_4]$ (green)	m $P2_1/c$ 2	7.053(2) 9.747(2) 14.029(2)	98.48(2)	$CuCl_4$	Cl	2.270(2,1)	Cl,Cl	90.4(4)	160
$(C_{42}H_{56}N_2O_2)[CuCl_4]$ (dark green)	m $P2_1/c$ 2	16.602(11) 9.739(2) 12.650(2)	93.08(2)	$CuCl_4$	Cl	2.237(1,17)	Cl,Cl	90.0(–,0.5)	161
$(MePhEtNH)_2[CuCl_4]$ (green) (at 25°C)	m $P2_1/c$ 2	6.4953(3) 22.678(1) 8.844(6)	116.08(1)	$CuCl_4$	Cl	2.265(1,17)	Cl,C	90.0(1,1)	162

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$(MePhEtNH)_2$ $[CuCl_4]$ (yelow) (at 80°C)	m C2/c 4	24.93(3) 8.180(7) 12.586(8)	115.21(7)	$CuCl_4$	Cl	2.219(4,29)	Cl,Cl	94.6(1,4.0) 143.53(5)	162
$[(C_3H_8)_2N]_2$ $[CuCl_4]^g$ (green) low temp. phase	tr P1 6	7.245(1) 14.588(1) 21.738(1)	78.08(1) 103.59(1) 104.73(1)	$CuCl_4$ $CuCl_4$	Cl Cl	2.288(11,35) 2.266(11,33)	Cl,Cl Cl,Cl	90.0(4,3) 109.5(4,7.6)	163
$(C_{13}H_{19}N_2OS)_2[CuCl_4]$ (yellow)	m C2/c 4	25.24(1) 9.38(2) 13.58(1)	91.6(3)	$CuCl_4$	Cl	2.240(3,20)	Cl,Cl	95.93(6,2.7) 95.9(1,2.7)	164
$(Et_2NH_2)_2[CuCl_4]$ (green)	m $P2_1/c$ 8	25.055(9) 10.531(5) 13.455(5)	100.63(3)	$CuCl_4$	Cl	2.218(10,52)	Cl,Cl	96.6(4,2.6)	165
$Cs_2[CuCl_4]$ (not given)	or Pnam 4	9.7599(12) 12.3967(12) 7.6091(9)		$CuCl_4$	Cl	2.230(4,13)	Cl,Cl	100.7(1,1.0) 129.2(2,2.1)	166
$(Me_2NH_2)_3Cl[CuCl_4]$ (yellow)	or Pnma 4	11.304(10) 15.638(12) 9.957(6)		$CuCl_4$	Cl	2.230(9,2)	Cl,Cl	98.2(1,5) 135.8(2,3)	167
$(Me_3NH)_3Cl[CuCl_4]$ (orange)	m $P2_1/a$ 4	14.41(1) 12.04(1) 12.17(1)	93(–)	$CuCl_4$		not given	Cl,C	not given	168
$(Et_3NH)_2[CuCl_4]$ (not given)	m $P2_1/c$ 4	12.878(3) 13.079(3) 12.227(3)	97.85(–)	$CuCl_4$	Cl	2.241(3)	Cl,Cl	98.5(1,1.9) 134.8(1,2.1)	169
$(Me_4N)_2[CuCl_4]$ (not given)	or Pnma 4	12.30(2) 9.03(1) 15.59(2)		$CuCl_4$	Cl	2.23(1,2)	Cl,Cl	101.0(3,2) 129.3(3,2.9)	170
$(Et_4N)_2[CuCl_4]$ (orange)	tg P4/n 4	14.05(–) 14.05(–) 12.45(–)		$CuCl_4$	Cl	not given	Cl,Cl	not given	168
$(Et_4N)_2[CuCl_4]^g$ (orange red) (at 120K)	tg P4/n 4	13.984(–) 13.984(–) 12.232(–)		$CuCl_4$ $CuCl_4$	Cl Cl	2.236(4) 2.24(2,3) 2.46(2)	Cl,Cl Cl,Cl	103.5(1) 122.3(1) 101.4(6,2.5) 127.2(5,1.0)	171
$(C_5H_{12}N)_2[CuCl_4]$ (yellow)	m $P2_1/c$ 4	8.2221(2) 16.918(1) 12.1725(3)	100.542(–)	$CuCl_4$	Cl	2.249(1,23)	Cl,Cl	98.9(1,4.5) 133.5(1,2.9)	172
$[(C_3H_8)_2N]_2[CuCl_4]$ (green)	or Pnma 4	16.007(4) 12.262(3) 7.784(2)		$CuCl_4$	Cl	2.213(7,9)	Cl,Cl	98.5(2,5) 134.8(3,5)	173
$(eoa)_2[CuCl_4]$ (not given)	m C2/c not given	7.431(–) 7.511(–) 21.624(–)	89.56(–)	$CuCl_4$	Cl	2.288(–)		not given	174
$(bpz)_2[CuCl_4]$ (not given)	m Pc not given	21.954(–) 7.089(–) 9.139(–)	97.05(–)	$CuCl_4$	Cl	2.284(–,50)		not given	174
$(i\text{-}Bu_2NH_2)[CuCl_4]^g$ (orange)	tg I4bar 4	16.731(5) 16.731(5) 9.095(4)		$CuCl_4$	Cl	2.255(2)	Cl,Cl Cl,Cl	97.18(6) 138.6(1)	175
				$CuCl_4$	Cl	2.242(2)	Cl,Cl	97.98(6) 136.3(1)	
$(\alpha\text{-}Me_2PhNH)_2[CuCl_4]^g$ (bright yellow)	tr P1 2	12.115(3) 12.968(2) 8.741(2)	106.64(4) 100.25(2) 98.881(2)	$CuCl_4$ $CuCl_4$	Cl Cl	2.236(7,32) 2.241(76)	Cl,Cl Cl,Cl	97.0(1,1.6) 139.2(1,1) 97.6(1,7) 137.3(2,2.3)	176

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$\{(MeO)_3PhNH_3\}_2[CuCl_4]$ H_2O (orange)	tr P–1 2	8.698(10) 23.145(3) 7.427(1)	93.99(1) 99.22(1) 99.20(1)	$CuCl_4$	Cl	2.236(1,35)	Cl,Cl	99.7(1,3.4) 132.5(1,1.3)	177
$(Me_3bzN)_2[CuCl_4]$ (orange)	m $P2_1/n$ 4	9.584(10) 9.104(5) 28.434(10)	92.83(–)	$CuCl_4$	Cl	2.256(3,27)	Cl,Cl	99.4(1,1.1) 132.5(1,4)	178
$(C_6H_{13}N_3)[CuCl_4]$ (not given)	m $P2_1/c$ 4	10.849(4) 15.339(4) 7.876(2)	108.76(3)	$CuCl_4$	Cl	2.242(1,30)	Cl,Cl	100.5(1,2.7) 129.0(1,5.3)	179
$(C_5H_6Cl_2N_3)_2[CuCl_4]$ (yellow)	m $P2_1/c$ 4	8.931(4) 13.584(7) 16.054(5)	92.77(3)	$CuCl_4$	Cl	2.263(2,29)	Cl,Cl	92.6(1,2.5) 156.6(1,6)	180
$(C_6H_9N_2)_2[CuCl_4]$ (yellow)	m C2/c 4	13.377(–) 8.344(–) 15.941(–)	93.38(–)	$CuCl_4$	Cl	2.240(3,7)	Cl,Cl	96.7(1,7) 139.9(1,3.9)	181
$(MebpyH)_2[CuCl_4]$ (orange yellow)	or Pbcn 4	12.63(1) 16.18(1) 7.52(1)		$CuCl_4$	Cl	2.247(1,3)	Cl,Cl	100.6(1,1.4)	182
$\{(amet)mfH_2\}[CuCl_4]$ (yellow)	m $P2_1/a$ 4	15.909(3) 12.420(3) 6.355(1)	98.77(5)	$CuCl_4$	Cl	2.250(1,9)	Cl,Cl	98.8(1,2) 133.8(1,2)	183
$\{(amet)mfH_2\}[CuCl_4]$ (green)	m I2/a 8	15.934(3) 13.023(1) 14.069(3)	118.89(3)	$CuCl_4$	Cl	2.272(1,42)	Cl,Cl	94.0(1,4.2) 146.24(8)	183
$(C_5H_8N_2)[CuCl_4]$ (green)	m $P2_1/c$ 4	6.941(2) 8.384(2) 16.848(7)	94.63(3)	$CuCl_4$	Cl	2.280(1,1.3)	Cl,Cl	90.4(1,2.0)	184
$(C_4H_{10}NO)_2[CuCl_4]$ (not given)	or Pnma 4	7.703(2) 20.939(4) 9.274(2)		$CuCl_4$	Cl	2.280(2,27)	Cl,Cl	90.0(1,1.1)	184
$(PhpipH_2)[CuCl_4]$ (yellow green)	or $P2_12_12_1$ 4	17.698(2) 8.615(1) 9.841(1)		$CuCl_4$	Cl	2.250(3,21)	Cl,Cl	96.1(1,1.7) 142.1(3,1.0)	185
$(bzpipH_2)_2[CuCl4]$ (green)	m Pc 2	21.954(2) 7.0889(5) 9.1391(9)		$CuCl_4$	Cl Cl	2.245(4,11) 2.334(4)	Cl,Cl	90.0(2,1.8)	186
(bzpipzn)$[CuCl_4]^k$ (green)	m $P2_1$ 8	12.0757(3) 28.480(1) 9.9258(9)	109.54(1)	$CuCl_4$	Cl	2.249(9,29)	Cl,Cl	97.4(3,3.5) 137.9(3,2)	187
				$CuCl_4$	Cl	2.228(19,34)	Cl,Cl	93.3(7,4.4) 151.8(4,6)	
				$CuCl_4$	Cl	2.247(10,35)	Cl,Cl	98.3(4,2.9) 135.3(4,7)	
				$CuCl_4$	Cl	2.230(18,65)	Cl,Cl	93.5(6,6.1)	
(bzpipzn)$[CuCl_4]..5H_2O^g$ (yellow)	m $P2_1/a$ 8	17.015(1) 16.977(2) 11.377(2)	97.156(4)	$CuCl_4$ $CuCl_4$	Cl Cl Cl	2.227(2,18) 2.321(2) 2.251(2,33)	Cl,Cl Cl,Cl	99.3(1,3.1) 132.3(1,3.4) 98.8(1,1.4) 133.8(1,4.1)	187
$(C_4H_6N_3O)_2[CuCl_4]$ (brown)	tr P1 2	13.689(2) 9.537(1) 6.936(1)	102.93(2) 105.59(2) 112.24(2)	$CuCl_4$	Cl	2.235(3,31)	Cl,Cl	97.0(1,1.2) 139.2(1,6)	188
$(C_{19}H_{24}N_2O)[CuCl_4]_2.3H_2O$ (green yellow)	or $P2_12_12_1$ 4	15.414(3) 36.719(6) 7.974(2)		$CuCl_4$	Cl	2.249(5,28)		111.8(2,36.7)	189

TABLE I *(Continued)*

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$(PPh_4)_2[CuCl_4]\cdot H_2O$	m	20.131(2)		$CuCl_4$	Cl	2.243(2,17)	Cl,Cl	100.8(1,4.5)	190
(orange)	$P2_1/n$	13.568(2)	109.09(1)					128.7(1,1.3)	
	4	17.018(2)							
$(tbpo)_2[CuCl_4]$	tg	19.585(2)		$CuCl_4$		not given		not given	191
(yellow)	$P4_2/n$	19.585(2)							
	2	9.883(1)							
$(tbpo)_2[CuCl_4]$	tr	13.471(4)	82.31(2)	$CuCl_4$		not given		not given	192
(not given)	P1	14.685(5)	78.03(2)						
	2	19.875(4)	86.56(2)						
$(tbpo)_2[CuCl_4]$	tr	13.398(6)	82.08(3)	$CuCl_4$	Cl	2.256(3)		not given	192
(not given)	P1	14.522(4)	78.52(3)						
(at 143K)	2	19.676(1)	87.56(3)						
$[(NPMe_2)_5H_2][CuCl_4].H_2O$	tr	9.034(6)	91.66(7)	$CuCl_4$	Cl	2.255(3,37)	Cl,Cl	99.0(1,2.2)	193
(orange)	P1	14.390(8)	96.52(9)					133.5(1,3)	
	2	10.924(8)	109.77(5)						
$(Me_3S)_2[CuCl_4]^g$	m	15.752(4)		$CuCl_4$	Cl	2.244(2,15)	Cl,Cl	100.8(1,8)	194
(yellow)	$P2_1/n$	12.231(2)	114.60(1)					128.7(1,8)	
	8	17.462(3)							
				$CuCl_4$	Cl	2.249(2,14)	Cl,Cl	98.4(1,1.4)	
								135.1(1,1.1)	
$(C_3H_7N_2S)_2[CuCl_4]$	m	27.728(7)		$CuCl_4$	Cl	2.246(1,26)	Cl,Cl	97.8(1,2.4)	195
(not given)	C2/c	7.800(3)	112.04(3)					136.5(1,4.5)	
thermochrom	8	15.600(8)							
$(C_4H_7N_2S)_2[CuCl_4]$	tr	7.804(1)	103.50(1)	$CuCl_4$	Cl	2.248(1,17)	Cl,Cl	98.8(1,3.2)	195
(not given)	P1	8.534(1)	99.39(1)					133.9(1,3.3)	
thermochrom	2	13.814(1)	104.17(1)						
$(C_6H_{13}NS_2)_2[CuCl_4]$	or	12.583(12)		$CuCl_4$	Cl	2.25(1,4)	Cl,Cl	98.4(9,9)	196
(yellow)	Ib2	26.550(18)						135(1,1)	
	8	12.437(12)							
$(C_{17}H_{21}N_2S)[CuCl_4]$	m	7.548(6)		$CuCl_4$	Cl	2.248(2,53)	Cl,Cl	99.1(1,3.5)	197
(not given)	$P2_1/c$	14.613(23)	91.69(–)					133.1(1,0)	
	4	18.271(23)							
$(ath)_2[CuCl_4]$	m	27.772(13)		$CuCl_4$	Cl	2.246(1,25)	Cl,Cl	97.8(1,2.3)	198
(yellow)	C2/c	7.811(4)	112.09(–)					136.5(1,4.6)	
	8	15.609(7)							
$(bedt\text{-}ttf)_3[CuCl_4]\cdot H_2O$	tr	16.634(–)	90.72(–)	$CuCl_4$	Cl	2.25(–,–)	Cl,Cl	not given	199
(not given)	P1	16.225(–)	93.24(–)						
	2	8.980(–)	96.76(–)						
$(ftzh)[CuCl_4]^g$	tr	20.433(5)	91.31(3)	$CuCl_4$	Cl	2.251(2,68)	Cl,Cl	97.6(1,1.7)	200
(black)	P1	12.721(4)	94.56(3)					137.2(1,2.2)	
	4	7.526(2)	99.69(2)	$CuCl_4$	Cl	2.251(2,33)	Cl,Cl	98.3(1.4.1)	
								135.3(1,1.4)	
$(C_{17}H_{20}N_2SCl)_2[CuCl_4]_2^g$	or	23.745(4)		$CuCl_4$	Cl	2.252(4,44)	Cl,Cl	109.5(1,12.2)	201
(not given)	Pnma	13.897(3)		$CuCl_4$	Cl	2.254(3,43)	Cl,Cl	96.9(1,2.5)	
	4	12.580(2)						138.3(1,9.5)	
$CuCl_2(C_{12}H_{18}N_4OSCl)$	m	9.488(5)		$CuCl_4$	Cl	2.243(4,40)	Cl,Cl	98.8(1,1.5)	202a
(yellow orange)	$P2_1/c$	16.871(7)	117.2(2)					133.8(1,2.4)	
	4	12.940(5)							
$(4\text{-}MepyH)_2[CuCl_4]$	m	7.192(1)		$CuCl_4$	Cl	2.246(2,38)	Cl,Cl	97.18(5,1.66)	202b
(pale yellow)	Cc	20.598(4)	107.27(1)						
	4	11.928(1)							

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$(1,4\text{-}Me_2pyH)_2[CuCl_4]$ (yellow)	m C2/c 4	13.117(3) 7.896(3) 17.767(4)	94.87(2)	$CuCl_4$	Cl	2.242(2,5)	Cl,Cl	98.76(4,74) 134.03(4,1.77)	202c
$(C_{14}H_{22}N_2O)_2[CuCl_4]$ (orange)	m $P2_1/n$ 4	10.392(1) 24.455(1) 13.665(1)	98.08(1)	$CuCl_4$	Cl	not given	Cl,Cl	not given	202d
$[Cu(bpydo)_3][CuCl_4]\cdot 0.5H_2O$ (yellow)	m $P2_1/c$ 4	15.283(2) 14.166(1) 17.335(1)	91.11(1)	$CuCl_4$ CuO_6	Cl O	not given not given	Cl,Cl O,O	not given not given	202e
[Cu(piedien)][$CuCl_4$] (blue)	m $P2_1/n$ 4	11.822(2) 13.845(3) 13.619(3)	93.17(2)	$CuCl_4$ CuN_5	Cl N	2.270(1,23) see Table 2	Cl,Cl	109.4(1,4.9)	203
[$CuCl_4$] $[Cu(C_{22}H_{34}N_6)]\cdot 2H_2O$ (green)	m $P2_1/c$ 4	15.467(4) 11.287(9) 17.459(5)	106.45(2)	$CuCl_4$ CuN_6	Cl N	2.240(2,14) see Table 4		not given	204
$(Me_3NH)_3$ $[CuCl_4][CuCl_3]$ (orange)	m Cc 4	14.30(3) 24.67(4) 6.30(2)	92.52(–)	$CuCl_4$	Cl	2.24(1,6)	Cl,Cl	109.5(4,1.7)	205
$Cu(C_5H_8NS_2)_2$ (not given)	tr P1 1	7.477(3) 8.057(2) 6.373(1)	104.77(1) 94.06(2) 76.60(2)	CuS_4	S	2.296(1,16)	S,S	77.58(5)[1] 102.42(5)	206
$[Cu(C_6H_{10}NS_2)_2]$ (black)	m $P2_1/c$ 2	6.159(1) 8.567(1) 15.264(2)	95.52(1)	CuS_4	S	2.296(2,8)	S,S	77.6(1)[1]	207
$[Cu(C_6H_{10}NS_2)_2]$ (black brown)	m $P2_1/c$ 2	6.170(6) 8.600(6) 15.220(11)	95.31(5)	CuS_4	S	2.295(3,9)	S,S	77.7(1)[1] 102.3(1)	208
$Cu(C_7H_{12}NS_2)_2$ (not given)	m $P2_1/c$ 2	6.64(–) 9.18(–) 14.56(–)	99.42(–)	CuS_4	S	2.297(1)	S,S	77.8(–)[1]	209
$Cu(C_7H_{14}NS_2)_2$[g] (deep red)	tr P1 2	11.573(4) 11.706(4) 7.626(5)	96.25(4) 96.30(4) 88.72(3)	CuS_4 CuS_4	S S	2.285(2,2) 2.285(2,6)	S,S S,S	76.66(8)[1] 103.34(8) 77.30(8)[e] 102.7(8)	210
$Cu(Et_2dtc)_2$ (not given)	m $P2_1/c$ 4	10.4(–) 10.7(–) 16.8(–)	113(–)	CuS_4	S	2.315(2,17)		not given	211
$(Me_4N)_2[Cu(mnt)_2]$ (not given)	m $P2_1/c$ 4	13.230(3) 11.518(9) 16.269(6)	95.07(2)	CuS_4	S	2.259(4,9)	S,S	92.5(1,0)[e] 96.1(2,8) 148.3(2,13)	212
$(n\text{-}Bu_4N)_2[Cu(mnt)_2]$ (dark brown)	tr P1 1	11.149(5) 13.201(8) 9.403(6)	105.44(5) 114.92(5) 72.09(9)	CuS_4	S	2.276(1,11)	S,S	90.7(1)[e] 89.3(1)	213
$(n\text{-}Bu_4N)[Cu(tdt)_2]$ (emerald green)	m C2/c 8	42.510(8) 8.586(2) 18.716(7)	105.49(2)	CuS_4	S	2.164(12,26)	S,S	91.6(4,2)[e] 88.4(4,1.6) 177.1(5,1.0)	214
$(n\text{-}Bu_4N)_2[Cu(dcmcroc)_2]$ (blue black)	or Pbca 8	18.087(7) 32.325(9) 18.236(7)		CuS_4	S	2.280(2,4)	S,S	92.9(1,5)[e] 154.1(1,3)	215

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$(Etpy_4)_2[Cu(dmit)_2]$ (dark brown)	m C2/m 4	20.04(2) 14.56(2) 10.19(1)	109.2(1)	CuS_4	S	2.272(3,2)	S,S	94.0(1)[e] 99.5(1) 135.8(2,4.9)	216
$(nmp)_2[Cu(cnd)_2]$ (black)	m $P2_1/n$ 2	11.417(2) 8.126(2) 17.674(7)	92.11(2)	CuS_4	S	2.276(2)	S,S	91.1(3)[e] 88.9(3)	217
$(guin)_2[Cu(mnt)_2]$ (reddish brown)	tr P1 1	7.404(3) 7.452(3) 13.090(5)	106.71(2) 109.99(3) 91.19(3)	CuS_4		not given		not given	218
$(Ph_4P)_2[Cu(qdt)_2]$ (not given)	m $P2_1/c$ 2	9.9320(4) 23.822(1) 11.9178(5)	95.08(1)	CuS_4	S	2.260(1,16)	S,S	90.5(1)[e]	219
$(Ph_4P)_2[Cu(dts)_2]$ (violet)	m $P2_1/n$ 4	11.018(3) 15.404(5) 14.575(4)	94.57(1)	CuS_4	S	2.326(4,4)	S,S	93.14(–)[e] 86.86(–)	220
$(C_{16}H_{18}N_3S)_2[Cu(mnt)_2]\cdot$ (C_3H_6O) (green)	tr P–1 2	10.346(3) 14.522(3) 15.524(5)	93.69(3) 90.69(2) 105.87(3)	CuS_4	S	2.520(2,11)	S,S	92.9(2,3)[e] 96.8(2,1.3)	221
$[(Cu(dbzdto)_2](ClO_4)_2$ (not given)	m $P2_1/a$ 2	16.435(3) 11.126(2) 10.297(2)	102.94(2)	CuS_4	S	2.289(4,8)	S,S	91.2(1)[e]	222
$[Cu(C_{14}H_{28}S_4)](ClO_4)_2$ (not given)	m $P2_1/c$ 6	11.733(2) 18.558(6) 16.465(3)	109.10(2)	CuS_4 CuS_4O	S S O	2.30(–,2) 2.30(–,1) 2.35(–,2)	S,S S,S S,O	not given not given not given	223
$[K(C_{12}H_{24}O_6)]_2[Cu(dto)_2]$ dmf (green)	m $P2_1/c$ 2	11.488(2) 8.543(2) 23.526(7)	93.71(2)	CuS_4	S	2.261(2,8)	S,S	91.1(1)[e] 88.9(1)	224
$(Me_4N)_2[CuBr_4]$ (not given)	or Pnma 4	12.600(4) 9.326(2) 15.825(6)		$CuBr_4$	Br	2.426(5)	Br,Br	102.3(1,3) 125.0(2,1.6)	225
$(C_5H_8N_2)[CuBr_4]$ (violet)	m $P2_1/c$ 4	7.179(1) 8.766(2) 17.218(3)	95.29(1)	$CuBr_4$	Br	2.428(4,20)	Br,Br	90.0(1,3)	184
$(C_6H_9N_2)_2[CuBr_4]$ (dark brown)	m C2/c 4	13.715(2) 8.7162(2) 16.013(4)	93.79(2)	$CuBr_4$	Br	2.377(2,8)	Br,Br	97.6(1,9) 137.2(1,3.8)	181
$(ipa)_2[CuBr_4]$ (black)	m $P2_1/n$ 4	10.8127(3) 14.623(1) 14.2048(5)	106.918(2)	$CuBr_4$	Br	2.384(1,21)	Br,Br	98.4(1,1.9) 135.1(5,1.5)	172
$(C_{11}H_{18}N_2)[CuBr_4]\cdot H_2O$ (black)	m $P2_1/c$ 4	7.413(2) 16.46(1) 14.961(8)	104.78(4)	$CuBr_4$	Br	2.382(2,61)	Br,Br	106.2(1,6.1) 125.6(1)	226
$(C_9H_{23}N)_2[CuBr_4]$ (brown - red)	m C2/c 4	25.98(2) 9.045(5) 10.986(5)	111.08(4)	$CuBr_4$	Br	2.380(3)	Br,Br	96.1(1,1.8) 142.1(1)	226
$(n\text{–}Bu_4N)_2[CuBr_4]$ (dark purple)	tr not given 8	15.5(1) 6.56(5) 43.24(5)	80.7(–) 94(–) 91.8(–)	$CuBr_4$	Br	not given	Br,Br	not given	227

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
(enH.HBr)$_2$[CuBr$_4$]	m	6.78(1)		CuBr$_4$	Br	2.404(10,64)	Br,Br	105.9(3,12.2)	228
(dark red)	$P2_1/m$	20.15(1)	94.92(10)					141.1(3)	
	2	6.33(1)							
(Ph$_3$AsO)$_2$[CuBr$_4$]	m	17.569(3)		CuBr$_4$	Br	2.389(1,49)	Br,Br	99.7(1,1)	229
(purple)	C2/c	13.090(2)	105.64(2)					130.8(1,8.4)	
	4	16.933(2)							
(C$_6$H$_8$BrN$_2$)(C$_6$H$_9$N$_2$)	m	15.913(5)		CuBr$_4$	Br	2.376(3,37)	Br,Br	99.7(1,3.3)	230
[CuBr$_4$][g]	$P2_1/a$	7.764(3)	97.33(2)					131.4(1,2)	
(brown black)	4	16.297(5)		CuBr$_4$	Br	2.395(3,37)	Br,Br	101.7(1,6.4)	
								126.8(1,4.4)	
(T118–crown–6)$_4$[CuBr$_4$]	c			CuBr$_4$	Br	2.311(2)	Br,Br	not given	231
[TlBr$_4$]$_2$	F23	20.897(2)							
(black)	2								
[Cu(17–aneN$_5$)][CuBr$_4$]	m	9.088(2)		CuBr$_4$	Br	not given	Br,Br	not given	232
(dark blue)	Pn	11.692(1)	90.28(3)						
	2	9.832(5)		CuN$_5$	N	see Table 2			
(Me$_4$N)$_2$[Cu(C$_3$Se$_5$)]·	or	10.289(3)		CuSe$_4$	Se	2.366(3)	Se,Se	95.6(1)[e]	233
2MeCN	Ibam	23.367(6)							
(black)	4	15.519(7)							
Cu(Et$_2$dsc)$_2$	m	9.88(1)		CuSe$_4$	Se	2.905(3)	Se,Se	79.3(1,2)[f]	234
(black)	$P2_1/c$	10.86(1)	113.2(3)					99.4(1,3)	
	4	17.17(1)						165.8(1,6.5)	
[Cu(acasp)(2–cmpy)]	m	14.127(1)		CuO$_3$N	acO	1.899(9,3)	O,O	96.5(3)[d]	235
(ClO$_4$)·H$_2$O	$P2_1/a$	7.442(1)	93.36(1)		pyO	2.009(8)		92.2(3)	
(green)	4	13.584(2)			pyN	1.992(9)	N,O	81.0(4)[e]	
								90.1(4)	
[Cu(5Cl–oha–shz)]·dmf	tr	8.012(2)	88.80(1)	CuO$_3$N	O	1.904(3)	O,O	92.1(2,7)	236
(dark green)	P–1	8.359(1)	88.48(1)		N	1.933(4)	N,O	83.0(2)[e]	
	2	13.906(1)	82.01(1)		dmfO	1.971(3)	N,O	92.9(2)[d]	
[Cu(NH$_3$)$_2$(C$_5$HN$_3$O$_6$)]·H$_2$O	m	10.417(2)		CuN$_3$O	N	2.019(3)	N,N	92.9(1)	237
(light blue)	$P2_1/c$	7.212(1)	94.30(2)		O	1.978(2)		98.8(1)	
	4	14.378(3)			H$_3$N	1.987(3,4)	N,O	81.2(1)[e]	
								87.6(1)	
(Cu(C$_8$H$_{11}$N$_2$)(C$_6$H$_6$NO)]	or	7.146(1)		CuN$_3$O	N	1.961(3,19)	N,N	82.6(1)[e]	238
(black)	Pbca	19.762(3)			N	1.935(3)	N,O	82.1(1)[e]	
	8	19.443(4)			O	2.022(2)	N,N	103.8(1)	
							N,O	91.5(1)	
[Cu(dpa)(Ph–sal)](ClO$_4$)	tr	10.631(3)	104.16(2)	CuN$_3$O	N	1.974(2,13)	N,N	92.32(9)[d]	239
(yellow)	P–1	11.010(2)	113.98(3)		N	1.964(2)	N,O	94.96(8)[d]	
	2	11.347(4)	96.50(2)		O	1.874(2)	N,N	97.93(9)	
							N,O	96.08(9)	
[Cu(C$_{21}$H$_{29}$N$_3$O$_2$)H$_2$O]	m	16.856(7)		CuN$_3$O	N	2.02(3,5)	N,N	85(1)[e]	240
(ClO$_4$)$_2$.(H$_2$O)	$P2_1/c$	10.717(4)	110.59(5)		H$_2$O	1.96(2)	N,N	90(1)[d]	
(deep blue)	4	16.738(18)					N,O	92(1)	
[Cu[HB(Butpz)$_3$](CF$_3$SO$_3$)]·	m	10.367(6)		CuN$_3$O	N	1.941(8)	N,N	94.2(3,3)	241
C$_7$H$_8$	$P2_1/n$	20.555(7)	90.80(5)			2.034(8,8)		98.5(3)	
(not given)	4	15.39(1)			O	1.947(7)	N,O	121.2(3,5.8)	
[Cu(NH$_3$)(C$_{19}$H$_{14}$N$_4$O)]	m	24.231(4)		CuN$_3$O	N	1.929(5,1)	N,N	89.4(2)[d]	242
(not given)	P2/n	6.522(1)	90.30(3)		O	1.933(4)	N,O	84.4(2)[e]	
	4	11.449(2)			H$_3$N	1.998(5)	N,N	102.0(2)	
							N,O	87.5(2)	
[Cu(C$_{13}$H$_{11}$N$_5$O$_4$)py]$_2$·	m	9.740(4)		CuN$_3$O	N	1.930(6,15)	N,N	91.9(2)[d]	243
0.5H$_2$O	$P2_1/c$	19.259(7)	108.58(3)		O	1.909(4)	N,O	93.6(2)[d]	
(black)	2	10.361(3)			pyN	2.026(6)	N,N	93.5(2);156.4(3)	
							N,O	92.4(2);151.8(3)	

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$Cu(C_9H_9N_3OS)(im)$ (dark brown)	m $P2_1/n$ 4	11.963(3) 15.047(3) 7.899(3)	91.61(2)	CuN_3O	N O imN	1.946(4,10) 1.906(3) 1.986(4)	N,N N,O N,N N,O	80.2(2)[e] 92.0(2)[d] 97.6(2) 90.5(2)	244
[Cu(ae)(5-Meim)] (ClO_4) (not given)	tr P-1 2	9.184(1) 12.828(2) 7.627(1)	94.64(1) 105.84(1) 106.75(1)	CuN_3O	N O imN	1.973(4,40) 1.906(3) 1.978(3)	N,N N,N N,O N,O	85.0(1)[e] 94.3(1);175.5(1) 92.8(1)[d] 88.2(1);175.4(1)	245
[Cu(sad-Meen)(tph)]·H_2O (violet red)	or $P2_12_12_1$ 4	23.080(16) 10.480(6) 7.627(1)		CuN_3O	N O tphN	1.997(1,23) 1.902(1) 1.986(1)	N,N N,O N,N N,O	84.30(6)[e] 92.00(6)[d] 96.10(6) 89.00(6)	246
[Cu(sad-Me_2en)(tph)]· $3.5H_2O$ (not given)	or Pnna 8	12.570(4) 14.983(5) 23.249(8)		CuN_3O	N O tphN	2.013(8,69) 1.910(6) 1.969(7)	N,N N,O N,N N,O	84.3(3)[e] 92.6(3)[d] 92.8(3) 90.6(3)	247
$Cu(C_{12}H_{15}N_3O)$ (violet)	m $P2_1/c$ 4	7.180(3) 11.888(7) 14.769(9)	103.03(4)	CuN_3O	N O	1.944(5,20) 1.899(4)	N,N N,O N,O	83.1(2,9)[e] 92.62(19) 97.17(19);177.50(20)	248
Cu{(S) -bap-(S) -val} (not given)	or $P2_12_12_1$ 4	12.846(2) 19.427(3) 9.464(2)		CuN_3O	N O	1.936(7,77) 1.925(4)	N,N N,O	not given not given	249
[Cu($C_9H_{18}N_3O$)](ClO_4)·H_2O (dark violet)	tr P-1 2	8.603(2) 9.666(2) 9.993(3)	77.41(2) 67.59(2) 80.94(2)	CuN_3O	N O	1.988(2,56) 1.919(2)	N,N N,O	84.8(1,4)[e] 95.2(1)[d]	250
[Cu($C_{11}H_{15}N_4O$)](ClO_4) (dark red)	m $P2_1/n$ 4	22.146(2) 9.659(1) 7.126(1)	98.35(1)	CuN_3O	N O	1.963(3,41) 1.881(3)	N,N N,O N,O	82.8(1,1.0)[e] 97.1(1)[d] 98.2(1)	251
[Cu($C_{12}H_{17}N_4O$)](ClO_4) (not given)	tr P-1 2	10.551(4) 11.602(3) 7.307(1)	98.95(1) 96.99(2) 113.04(2)	CuN_3O	N O	1.981(6,41) 1.901(5)	N,N N,O	79.5(2)[e] 97.4(2)[d] 87.7(2) 95.1(2)	251
[Cu($C_{14}H_{15}N_4O$)](Bph_4) (black)	m $P2_1/n$ 4	20.822(4) 14.132(3) 10.698(2)	98.63(2)	CuN_3O	N O	1.994(6,44) 1.910(5)	N,N N,O	95.2(2)[d] 80.2(2)[e] 95.5(2)[d] 89.1(2)	252
[Cu[Ph-C($SiMe_3$)$_2$] [Ph-C($NSiMe_3$)($NHSiMe_3$)] CuCl} (dark green)	tr P-1 2	11.885(4) 13.037(3) 13.326(4)	67.02(3) 74.10(3) 70.33(3)	CuN_3Cl	N N Cl	2.007(4,23) 1.999(4) 2.251(1)	N,N N,Cl	67.4(2)[1] 127.8(2,24.6) 125.4(1,24.3) 103.2(2)	253
Cu(bpy)(tcne)Cl (dark green)	tr P-1 2	9.963(3) 9.922(4) 8.505(3)	101.58(3) 99.73(3) 67.08(3)	CuN_3Cl	N tcneN Cl	2.003(4,7) 1.907(5) 2.261(1)	N,N N,N N,Cl	81.42(2)[e] 92.9(2) 92.3(1,3.1)	254
Cu(dqa)Cl (dark)	m $P2_1/n$ 4	12.683(3) 15.050(4) 7.542(2)	91.15(2)	CuN_3Cl	N Cl	1.967(2,32) 2.235(7)	N,N N,Cl N,Cl	82.8(1,2)[e] 97.2(1,8) 97.2(1,8)	255
[Cu(bamp)Cl]·thf (pale blue)	or $Pna2_1$ 4	15.953(3) 13.711(2) 10.229(2)		CuN_3Cl	N Cl	1.982(4,98) 2.236(2)	N,N N,Cl	82.2(2,1.2)[e] 97.6(1,8.0)	256
Cu(SC_6F_5)[HB(3,5-iPr_2 $pz)_3$].0.5(n-C_8H_{18}) (not given)	m $P2_1/a$ 4	25.364(7) 16.166(3) 9.924(3)	90.52(3)	CuN_3S	N S	1.930(9) 2.078(9,41) 2.176(4)	N,N N,S	91.7(4,2.2)[d] 123.3(3,11.3)	257
Cu($SCPh_3$)[HB(3,5-iPr_2 $pz)_3$]	not given	not given		CuN_3S	N S	not given 2.12(2)		not given	257

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$Cu(C_{11}H_9N_3S_2)(NH_3)$	or	17.074(4)		CuN_3S	N	1.93(–,2)	N,N	87(–)[e]	258a
(not given)	$Pna2_1$	5.733(2)			H_3N	2.04(–)		91(–)[d];89(–)	
	8	25.167(3)			S	2.29(–)	N,S	79(–)	
$[Cu(C_{11}H_{25}N_3)Br](ClO_4)$	or	14.365(4)		CuN_3Br	N	2.023(16,7)	N,N	96.2(3,8)	258b
(blue green)	Pnma	10.194(3)			Br	2.383(3)		147.9(6)	
at 148K	4	11.491(6)					N,Br	134.6(5)	
$Cu(Ph_3P)$ $[HB(3,5\text{–}Me_2pz)_3]$	m	26.951(4)		CuN_3P	N	2.098(14,12)	N,N	90.6(5,1.1)[d]	259a
(not given)	C2/c	18.003(2)	124.53(1)		P	2.166(6)	N,P	124.8(4,3.4)	
	8	18.363(3)							
$[Cu(ahmi)Cl_3]_2$	m	10.757(2)		$CuCl_3O$	Cl	2.239(2,3)	Cl,Cl	99.2(1,3)	259b
$[Cu(ahmi)_6]$	$P2_1/c$	19.787(3)	101.26(1)		O	1.954(4)		137.55(7)	
(not given)	2	14.528(2)					Cl,O	95.6(1,1.5)	
								138.3(1)	
				CuO_6	O	1.951(4,0)	O,O	90.0(2,3.8)	
						1.962(4,0)			
						2.514(4,0)			
$(C_3H_4N_2Cl)[CuCl_3(H_2O)]$	m	9.023(1)		$CuCl_3O$	Cl	2.277(5,19)	Cl,Cl	93.5(1,5)	260
(yellow)	$P2_1/c$	13.881(2)	97.8(2)		H_2O	2.041(6)	Cl,O	86.3(2,1.7)	
	4	7.341(1)							
$[Me_2N(H)C_2H_4P(O)Ph_2]$	m	12.713(1)		$CuCl_3O$	Cl	2.218(10,18)	Cl,Cl	111.6(4,18.4)	261
$[CuCl_3]$[g]	Cc	12.633(1)	91.05(1)		O	2.01(2)	Cl,O	109.1(6,26.7)	
(orange)	8	24.474(2)		$CuCl_3O$	Cl	2.224(9,40)	Cl,Cl	111.4(4,18.0)	
					O	1.99(2)	Cl,O	109.0(6,22.8)	
(Hampym)$[CuCl_3(H_2O)]$	m	3.9025(6)		$CuCl_3O$	Cl	2.280(1,15)	Cl,Cl	92.8(1,1)	262
(green)	Cc	13.788(3)	93.99(1)		H_2O	1.982(2)	Cl,O	87.1(1,1)	
	4	16.826(3)							
$(H_2Me_2pipz)[CuCl_3(H_2O)]_2$	m	6.714(2)		$CuCl_30$	Cl	2.273(3,23)	Cl,Cl	92.4(2,1.2)	262
(green)	$P2_1/n$	6.215(2)	95.2(6)		H_2O	2.010(4)	Cl,O	87.7(2,1.6)	
	2	19.545(6)							
(quin)$[CuCl_3(qu)]$	tr	9.310(6)	92.59(3)	$CuCl_3N$	Cl	2.238(2,33)	Cl,Cl	8.80(6,21.67)	263a
(orange)	P–1	12.012(4)	109.10(5)		N	2.008(4)	Cl,N	108.8(1,10.9)	
	2	8.410 (4)	97.98(4)						
$Cu(N_4P_4Me_8H)Cl_3$	or	15.70(1)		$CuCl_3N$	N	2.042(–)	Cl,Cl	97.6(–);143(–)	263b
(yellow)	Pbca	17.72(8)			Cl	2.232(–,30)	Cl,N	96.6(–,2);133.9(–)	
	8	14.52(6)							
$(C_6H_{10}NOS)[CuBr_3$	m	8.016(4)		$CuBr_3O$	Br	2.383(3,22)	Br,Br	111.5(1,16.5)	264
(C_6H_9NOS)	$P2_11$	17.190(8)	103.34(6)		N	1.96(1)	Br,N	108.7(5,22.5)	
(dark red)	2	7.322(4)							
$[Cu(daf)_2(H_2O)_2](NO_3)_2$	m	6.382(1)		CuO_2N_2	H_2O	1.963(2)	O,N	90.0(1,1.8)	265
(bright green)	$P2_1/c$	16.294(4)	109.32(2)		N	1.989(2)			
	2	7.232(2)							
$Cu(C_3H_2N_3O_2)_2(H_2O)_2$	tr	6.774(2)	92.75(2)	CuO_2N_2	H_2O	1.964(4)	O,N	90.4(1)	266
(violet)	P–1	8.348(2)	102.16(3)		N	1.972(2)	O,O	180.0(1)	
	1	4.878(2)	74.94(2)				N,N	180.0(1)	
$Cu(Me_2PhPz)_2(NO_3)_2$	or	10.613(2)		CuO_2N_2	O	2.028(5,12)		not given	267
(blue)	$P2_12_12_1$	13.188(3)			N	1.989(6,18)			
	4	17.715(3)							
$Cu(2,6\text{–}Me_2py)_2(HCO_2)_2$	tr	7.247(6)	65.10(1)	CuO_2N_2	O	1.948(2)	O,N	90.0(6,1.0)	268
(violet)	P–1	7.703(2)	76.21(1)		N	2.033(1)			
	1	8.520(1)	73.87(1)						
$[Cu(py)_2(ac)_2]\cdot py$	m	17.22(2)		CuO_2N_2	O	2.008(–,5)		not given	269
(not given)	Cc	5.92(2)	116.6(5)		N	2.015(–,9)			
	4	22.14(2)							

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$Cu(ac)_2(col)_2$ (purple)	m $P2_1/c$ 2	7.819(4) 16.319(7) 8.304(2)	101.82(2)	CuO_2N_2	acO N	1.952(3,0) 2.034(4,0)	O,O O,N	180.0(3) 90.0(1,3)	270
$Cu(ac)_2(2\text{–}Meim)_2$ (light blue)	or $P2_12_12_1$ 4	7.538(1) 7.710(1) 26.310(5)		CuO_2N_2	acO N	2.000(5,22) 1.976(5,2)	O,O N,N O,N	88.9(2) 94.8(2) 91.2(2,1.6)	271
$Cu(ac)_2(1,2\text{–}Me_2im)_2$[g] (light blue)	m $P2_1/c$ 4	15.574(2) 7.952(1) 14.752(1)		CuO_2N_2	acO N	1.984(4) 1.995(5)	O,O O,N N,N	90.7(2) 90.3(2) 93.9(3)	271
				CuO_2N_2	acO N	1.995(5) 2.002(6)	O,O O,N N,N	88.5(3) 92.2(2) 94.8(3)	
$Cu(dbz)_2(Etac)_2$ (deep violet)	m A2/a 4	19.235(8) 11.944(2) 17.137(5)	111.13(3)	CuO_2N_2	O N	1.916(5) 2.026(6)	O,N	94.6(2)	272
$[Cu(acgln)_2(Meim)_2]\cdot 2H_2O$ (light blue)	m C2 2	15.602(7) 7.353(2) 13.951(2)	110.69(3)	CuO_2N_2	O MeimN	1.987(3) 1.976(2)	O,O O,N N,N	174.4(1) 89.8(1,1) 172.5(2)	273
$[Cu(ac\text{–}\alpha\text{–}ala)_2(Meim)_2]\cdot 2H_2O$	tr P–1 1	7.666(1) 8.430(1) 9.955(1)	106.33(1) 86.27(1) 109.34(1)	CuO_2N_2	O N	1.942(3) 1.959(5)	O,N	90.3(2)	274
$[Cu(zala)(Meim)_2]\cdot EtOH$ (blue violet)	m $P2_1/c$ 2	11.112(1) 18.840(1) 8.965(1)	105.380(2)	CuO_2N_2	O MeimN	1.970(4) 1.977(6)	O,N	90.3(2) 89.7(2)	275
$Cu(ts\text{–}\beta\text{–}ala)_2(pipd)_2$ (violet)	tr P–1 1	9.305(1) 9.637(2) 12.727(2)	61.50(2) 63.26(1) 71.68(1)	CuO_2N_2	O N	1.970(2) 2.028(2)	O,O O,N N,N	180.0(1) 90.0(1,10) 180.0(2)	276
$[Cu(acac)(phen)](NO_3)\cdot 3H_2O$	tr P–1 2	10.212(8) 10.144(3) 10.890(6)	110.80(1) 102.49(2) 101.37(2)	CuO_2N_2	O N	1.899(3,7) 2.000(4,4)	O,O N,N O,N	94.6(2)[d] 81.5(2)[e] 91.2(2,4) 168.2(1,1.1)	277
$[Cu(bpy)(H_2O)(C_4O_4)]\cdot H_2O$ (brown)	or Pbca 8	17.182(3) 13.094(3) 12.321(2)		CuO_2N_2	H_2O oxO N	1.967(3) 1.933(3) 2.000(4,5)	O,O N,N O,N	96.0(1) 80.9(1)[e] 91.6(1,29) 172.3(1,2.7)	278
$Cu(bpy)(ONO)_2$ (blue)	m $P2_1/c$ 4	8.39(1) 10.08(1) 15.14(2)	110.04(10)	CuO_2N_2	ONO N	1.987(10,1) 1.982(9,2)	O,O O,N N,N	90.2(4) 94.7(4,3) 81.3(4)[e]	279
$[Cu(4\text{–}NH_2bz)_2(bpy)]\cdot O.5H_2O$ (blue)	m C2/c 8	25.244(4) 11.924(2) 22.453(4)	138.09(2)	CuO_2N_2	O N	1.963(2,31) 1.999(2,17)	O,O O,N N,N	92.5(1) 94.6(1,9) 165.0(1,3.1) 81.2(1)[e]	280
$Cu(phen)(acgly)_2$ (dark blue)	m C2/c 4	8.85(1) 16.45(1) 14.74(3)	102.3(1)	CuO_2N_2	O N	1.928(3) 2.007(3)	O,O O,N N,N	93.9(1) 92.6(1) 82.1(1)[e]	281
$Cu(dmen)(NO_3)_2$ (blue)	tg $P4_12_12$ 4	8.797(2) 8.797(2) 12.957(3)		CuO_2N_2	NO_3 N	1.993(3) 2.000(3)	O,O O,N N,N	86.1(1) 95.5(1) 165.5(1) 86.6(1)[e]	282
$[Cu(daddn)(en)]\cdot MeOH$ (blue black)	or Pbca 8	14.515(2) 16.596(3) 16.406(3)		CuO_2N_2	O enN	1.900(7,4) 2.006(8,3)	O,O O,N N,N	94.2(3,0) 90.3(4,5) 84.9(4,0)	283
$[Cu(bpy)(dbcal)]\cdot 1.5CH_2Cl_2.0.5H_2O$ (purple)	m I2/a 8	29.019(4) 9.982(2) 18.620(3)	92.70(1)	CuO_2N_2	O N	1.886(5,15) 1.996(6,3)	O,O N,N O,N	88.7(2)[e] 81.3(2)[e] 95.2(2,20)	284

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
[Cu(bpy)(ox)]	m	22.740(5)		CuO_2N_2	O	1.917(2,0)	O,O	85.5(1)[e]	285
$[Cu_2(bpy)_2(ox)(H_2O)_2]$	C2/c	10.508(1)	92.31(1)		N	1.968(2,0)	N,N	82.9(1)[e]	
$(BF_4)_2$[m]	4	16.129(2)					O,N	96.96(9)	
(dark blue)				CuO_3N_2		see Table 2			
[Cu(bpy)(ox)]	m	21.739(2)		CuO_2N_2	O	1.912(2,0)	O,O	86.3(1)[e]	285
$[Cu_2(bpy)_2(ox)(H_2O)_2]$	C2/c	10.458(1)	95.69(1)		N	1.956(2,0)	N,N	86.6(1)[e]	
$(NO_3)_2$[m]	4	16.023(2)					O,N	95.21(7)	
(dark blue)				CuO_3N_2		see Table 2			
[Cu(bpy)(ox)]	m	22.819(3)		CuO_2N_2	O	1.921(2,0)	O,N	85.5(1)[e]	285
$[Cu_2(bpy)_2(ox)(H_2O)_2]$	C2/c	10.583(2)	91.52(2)		N	1.984(2,0)	N,N	82.3(1)	
$(ClO_4)_2$[m]	4	16.389(2)					O,N	96.24(9)	
(dark blue)				CuO_3N_2		see Table 2			
$Cu(\alpha\text{–aib})_2$	m	10.470(3)		CuO_2N_2	O	1.946(2)	O,N	84.0(1)	286
(deep blue)	$P2_1/c$	5.335(1)	115.6(2)		N	1.981(3)	O,N	96.0(1)	
	2	10.201(3)					N,N	180.0(1)	
							O,O	180.0(1)	
							N,N	180.0(1)	
							O,N	84.0(1)[e];96.0(1)	
$[Cu(C_4H_{10}NO)_2]\cdot H_2O$	m	19.531(7)		CuO_2N_2	O	1.916(3)	O,N	84.9(1)[e]	287
(violet)	C2/c	5.966(1)	92.55(3)		N	1.994(4)			
	4	10.328(4)							
$[Cu(C_4H_{10}NO)_2].2bz$	m	5.654(2)		CuO_2N_2	O	1.933(5)	O,N	84.7(2)[e]	288
(violet)	$P2_1/c$	22.97(1)	101.66(3)		N	1.972(5)			
	2	9.166(4)							
$Na_2[Cu(adeNO)_2]\cdot 8H_2O$	tr	5.418(1)	106.41(1)	CuO_2N_2	O	1.948(2)	O,N	83.6(2)[e]	289
(green)	P–1	10.246(1)	96.71(1)		N	1.898(2)	O,N	96.4(1)	
	1	10.600(1)	99.71(1)						
$[Cu(C_6H_6N_4O_2)_2](C1O_4)_2$	tr	12.21(8)	84.75(4)	CuO_2N_2	O	1.86(1)	O,N	80.8(5)[e]	290
(blue)	C–1	7.65(6)	101.5(5)		N	1.99(1)	O,N	99.2(5)	
	2	11.06(8)	196.9(5)				O,O	180.0(5)	
							N,N	180.0(5)	
$[Cu(C_9H_6NO)_2](tcnq)$	tr	12.00(1)	112.5(5)	CuO_2N_2	O	1.926(3)	O,N	84.3(3)[e]	291
(blue)	P–1	7.54(1)	88.75(50)		N	1.946(3)	O,N	95.7(3)	
	1	7.12(1)	96.75(50)				O,O	180.0(3)	
							N,N	180.0(3)	
$Cu(Etsalaldim)_2$	m	9.824(12)		CuO_2N_2	O	1.890(6,5)	O,N	92.6(4,8)[d]	292
(black)	$P2_1/c$	8.43(1)	101.0(2)		N	1.956(10,8)	O,N	92.1(4,1.0)	
	4	20.989(26)					N,N	156.6(7)	
							O,N	151.7(6)	
$Cu(salamEtO)_2$[g]	m	18.323(4)		CuO_2N_2	O	1.877(2)	N,O	92.0(1)[d]	293
(dark green)	$P2_1/c$	4.813(1)	98.84(1)		N	2.010(2)	N,O	88.0(1)	
	4	19.770(4)					N,N	180.0(1)	
							O,O	180.0(1)	
				CuO_2N_2	O	1.822(2)	O,N	91.2(1)[d]	
					N	1.998(2)	O,N	88.8(1)	
							N,N	180.0(1)	
$Cu(C_9H_{10}NO_2)_2$	m	6.154(3)		CuO_2N_2	O	1.924(6)	O,N	88.2(3)[d]	294
(red purple)	$P2_1/c$	18.092(8)	100.39(4)		N	1.915(8)	O,N	91.8(3)	
	2	7.540(3)					O,O	180.0(3)	
$[Cu(C_{10}H_{10}NO)_2]\cdot$	m	28.16(–)		CuO_2N_2		not given		not given	295
H_2O	$P2_1/c$	7.62(–)	127(–)						
(bright green)	4	11.10(–)							
$Cu(C_{10}H_{10}NO_3)_2$	m	11.939(4)		CuO_2N_2	O	1.855(5)	O,N	77.6(8)[e]	296
(deep blue)	$P2_1/c$	8.887(2)	95.61(3)		N	2.173(5)	O,N	102.4(8)	
	2	8.611(3)					O,O	180.0(8)	
							N,N	180.0(8)	

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*		*L-Cu-L*		*Ref.*
$Cu(C_{10}H_{13}N_2O_2F_3)_2$	or	10.556(3)		CuO_2N_2	O	1.903(6)	O,N	93.2(2)[d]	297
(green brown)	$P2_1/c$	20.598(5)			N	1.966(6)	O,N	95.9(2)	
	2	5.787(2)					O,O	143.4(2)	
							N,N	47.0(2)	
$Cu(C_{10}H_9N_2O_2)_2$	rh	32.673(5)	90(–)	CuO_2N_2	O	1.968(6)	O,N	84.0(2)[e]	298
(purple)	R3bar	32.673(5)	90(–)		N	1.944(5)	O,N	96.0(3)	
	9	4.698(1)	120(–)				O,O	180.0(3)	
							N,N	180.0(3)	
$Cu(Prbzsalim)_2$	m	12.295(2)		CuO_2N_2	O	1.892(5,6)	O,N	91.8(2,6)[d]	299
(brown)	$P2_1/c$	18.937(17)	94.51(2)		N	1.980(5,5)	O,N	94.6(2,1)	
	4	10.442(1)					O,O	151.8(2)	
							N,N	153.8(2)	
$Cu(C_{16}H_{17}N_2O_2)_2$	m	11.340(6)		CuO_2N_2	O	1.909(1)	O,N	90.4(1)[d]	300
(green brown)	$P2_1/c$	8.916(2)	90.600(6)		N	2.017(2)	O,N	89.6(1)	
	2	14.283(1)					N,N	180.0(1)	
							O,O	180.0(1)	
$Cu(C_{17}H_{12}NO)_2$	m	24.260(8)		CuO_2N_2	O	1.881(3)	O,N	90.3(2)[d]	301
(dark red)	$P2_1/c$	5.897(1)	120.50(2)		N	2.013(4)	O,N	89.7(2)	
	2	10.509(2)							
$Cu(MeOsal)_2 \cdot H_2O$	m	18.657(12)		CuO_2N_2	O	1.918(2)	O,N	90.4(1)[d]	302
(not given)	C2/c	7.194(1)	91.92(2)		N	2.006(2)	O,N	89.6(1)	
	4	23.932(1)							
$Cu(C_{19}H_{11}N_2O)_2$[g]	m	25.087(8)		CuO_2N_2	O	1.875(6)	O,N	96.29(4)[d]	303
(dark red)	B2	15.243(6)			N	2.037(7)	O,N	96.9(4)	
	4	8.099(3)	98.67(3)				O,O	134.2(3)	
							N,N	145.0(3)	
				CuO_2N_2	O	1.926(6)	O,N	94.3(4)[d]	
					N	1.942(7)	O,N	96.4(4)	
							O,O	149.2(3)	
							N,N	143.2(3)	
$Cu(C_{38}H_{30}N_2O_4)$[g]	m	9.824(3)		CuO_2N_2	O	1.857(4,6)	O,N	91.4(3,10)[d]	304
(not given)	$P2_1/a$	35.530(9)	98.97(2)		N	1.992(5,13)	O,N	88.6(3,11)	
	8	17.552(6)					O,O	179.5(3)	
							N,N	176.3(3)	
				CuO_2N_2	O	1.876(4,6)	O,N	90.3(3,9)[d]	
					N	2.023(5,5)	O,N	89.1(3,14)	
							O,N	178.6(3)	
							N,N	177.7(3)	
$Cu(C_{19}H_{17}N_2O)_2$	m	25.087(8)		CuO_2N_2	O	1.901(5,26)	O,N	35.0(3,1.0)[d]	305
(dark red)	B2	15.243(6)			N	1.990(7,48)	O,N	96.5(3,5)	
	4	8.099(3)	98.67(3)						
$Cu(C_{20}H_{23}N_2O_4)_2$	m	22.223(9)		CuO_2N_2	O	1.889(4,6)	O,N	91.8(2,1)[d]	306
(not given)	$P2_1/n$	9.285(3)	92.77(4)		N	2.004(6,7)	O,N	88.2(2,10)	
	4	18.489(9)					O,O	173.2(2)	
							N,N	174.6(3)	
$Cu(C_{21}H_{26}NO_3)_2$	m	40.50(7)		CuO_2N_2	O	1.902(4,11)	O,N	92.0(1,1.4)[d]	307
(not given)	C2/c	11.263(4)	106.15(2)		N	2.023(4,1)	O,N	88.8(2,3.8)	
(at 173K)	8	17.175(3)					O,O	102.7(1)	
							N,N	170.4(1)	
$Cu(C_{21}H_{26}NO_3)_2$[g]	m	43.662(7)		CuO_2N_2	O	1.888(3)	O,N	91.7(1)[d]	308
(not given)	C2/c	10.267(2)	107.29(2)		N	2.025(3)	O,N	88.3(1)	
(at 223K)	8	18.506(4)					N,N	180.0(1)	
				CuO_2N_2	O	1.880(3)	O,N	95.6(1)[d]	
					N	1.977(3)	O,N	100.3(1)	
							N,N	136.6(1)	
							O,O	136.2(1)	
$Cu(C_{22}H_{28}NO_2)_2$	tr	9.338(9)	78.77(7)	CuO_2N_2	O	1.90(–)	O,N	88.7(–)[d]	309
(green)	P–1	9.184(5)	104.76(7)		N	2.049(–)	O,N	91.3(–)	
	1	12.814(13)	101.70(6)				O,O	180(–)	
							N,N	180(–)	

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$Cu(C_{26}H_{36}NO_3)_2$	tr	11.280(5)	97.85(1)	CuO_2N_2	O	1.908(10)	O,N	91.3(4)[d]	310
(not given)	P–1	13.598(1)	96.76(3)		N	2.007(10)	O,N	88.7(9)	
	3	25.650(2)	100.37(3)	CuO_2N_2	O	1.884(10,8)	O,N	91.4(4,5)[d]	
					N	2.032(9,8)	O,N	92.9(5,9)	
$Cu(Et_2ala)_2$	tr	9.684(6)	100.57(5)	CuO_2N_2	O	1.911(5)	N,O	84.1(2)[e]	311
(red)	P–1	7.495(6)	106.85(4)		N	2.031(6)	N,O	95.9(2)	
	1	8.101(7)	124.01(4)				N,N	180.0(2)	
							O,O	180.0(2)	
$Cu(bzpyoxal)_2$	m	9.561(9)		CuO_2N_2	O	1.900(3,0)	O,N	92.4(1,5)[d]	312
(dark green)	$P2_1/a$	16.605(8)	104.14(1)		N	1.966(3,2)	O,N	93.2(1,5)	
	4	17.561(2)					O,O	154.5(1)	
							N,N	154.9(1)	
β–Cu[(bzacen)(C_2N_2)]$_2$	tr	11.460(7)	79.5(1)	CuO_2N_2	O	1.904(5)		not given	127
(not given)	P–1	6.112(5)	91.5(1)		N	1.909(5)			
	1	5.611(4)	104.0(1)						
$Cu(Prsaldim)_2$	or	12.87(4)		CuO_2N_2	O	1.879(7,9)	O,N	94.7(4,3)[d]	313
(not given)	Pbca	20.68(3)			N	1.985(10,6)	O,N	100.5(4,2)	
	8	14.58(3)					N,N	137.7(4)	
							O,O	137.1(4)	
$[Cu(pya)_2](ClO_4)_2$	m	10.36(1)		CuO_2N_2	O	1.963(4)	O,N	82.4(2)[e]	314
(blue)	$P2_1/a$	9.89(1)	110.7(1)		N	1.999(2)	O,N	127.2(3)	
	2	8.77(1)							
[Cu(2–pyc)$_2$]KSCN	or	8.433(17)		CuO_2N_2	O	1.942(5)	O,N	83.5(2)[e]	315
(royal blue)	Pnam	14.274(26)			N	1.961(6)	O,N	96.5(2)	
	4	12.842(20)							
$Cu(salPhEtim)_2$	or	16.355(9)		CuO_2N_2	O	1.93(–)	O,N	90.0(–)[d]	316
(dark violet)	$P2_12_12_1$	8.874(5)			N	1.99(–)			
	4	17.992(5)							
$Cu(salPhEtim)_2$	m	11.154(5)		CuO_2N_2	O	not given	O,N	not given	317
racemat	$P2_1/c$	19.91(2)	114.2(2)						
(not given)	4	12.490(5)							
$Cu(csaldim)_2$	tr	12.035(5)	104.86(1)	CuO_2N_2	O	1.896(2)	O,N	90.2(1)[d]	318
(brown)	P–1	7.810(3)	102.06(1)		N	2.034(2)	O,N	89.8(1)	
	1	6.475(3)	97.67(1)						
$Cu(iprnam)_2$	m	12.295(4)		CuO_2N_2	O	1.892(3,1)	O,N	91.7(1,6)[d]	319
(dark brown)	$P2_1/c$	18.843(5)	85.23(3)		N	1.966(4,4)	O,N	94.7(1,2)	
	4	10.427(3)							
[Cu(iprnam)$_2$]·2tcnq	tr	11.118(3)	92.97(1)	CuO_2N_2	O	1.898(3)	O,O	88.7(1)[d]	319
(black)	P–1	14.178(1)	101.54(2)		N	2.001(3)	O,N	91.2(1)	
	1	7.141(1)	103.88(2)						
$Cu(C_{12}H_{10}NO)_2$	m	10.40(2)		CuO_2N_2	O	1.87(1)	O,N	91.3(3)[d]	320
δ modification	$P2_1/c$	5.88(1)	95.2(1)		N	1.98(1)	O,N	88.7(3)	
(green)	2	15.61(2)							
$Cu(C_8H_8NO)_2$[g]	tr	11.436(1)	103.95(1)	CuO_2N_2	O	1.876(2)	O,N	91.3(1)[d]	321
(brown)	P–1	12.370(1)	111.168(8)		N	1.922(3)	O,N	88.7(1)	
	3	9.446(1)	102.729(5)				O,O	180.0(1)	
							N,N	180.0(1)	
				CuO_2N_2	O	1.896(2,2)	O,N	90.8(1,6)[d]	
					N	1.922(3,5)	O,N	89.5(1,5)	
							O,O	173.4(1)	
							N,N	175.6(1)	

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$Cu(C_{13}H_{12}NO_2)_2$	m	5.5406(4)		CuO_2N_2	O	1.894(3,1)	O,N	91.0(1,3)[d]	322
(yellow)	$P2_1$	17.0461(9)	93.99(1)		N	2.000(3,2)	O,N	89.3(1,5)	
	2	11.3726(6)					O,O	175.8(1)	
							N,N	175.2(1)	
$Cu(C_{13}H_{26}NOF_6)_2$	or	16.225(5)		CuO_2N_2	O	1.920(8,14)	O,O	167.3(4)	323
(deep purple)	$P2_12_12_1$	18.021(5)			N	2.060(11,15)	O,N	93.5(4,4)[d]	
	4	13.248(5)					O,N	87.4(4,3)	
							N,N	173.7(4)	
$Cu(Me_2ampp)_2$	m	11.051(2)		CuO_2N_2	O	1.891(3,7)	O,N	92.90(11,13)[d]	324
(dark brown)	$P2_1/n$	9.577(4)	101.29(3)		N	2.074(3,5)	O,N	87.69(11,19)	
	4	12.436(12)					O,O	172.28(7)	
							N,N	171.14(7)	
$Cu(C_5H_3N_2O_2)_2$	m	5.0340(4)		CuO_2N_2	O	1.93(1)	O,N	84.5(2)[e]	325
(dark blue)	$P2_1/c$	15.332(1)	106.63(1)		N	1.98(1)	O,N	95.5(2)	
	2	7.071(1)					O,O	180.0(2)	
							N,N	180.0(2)	
$Cu(PhEthyacph)_2$	m	25.455(4)		CuO_2N_2	O	1.865(2)	O,N	91.54(8)[d]	326
(tan)	I2/a	8.420(3)	94.02(3)		N	1.977(2)	O,N	92.16(8)	
	4	12.469(6)							
$Cu(behyacph)_2$[g]	m	17.645(6)		CuO_2N_2	O	1.886(2)	O,N	91.65(9)[d]	326
(green)	$P2_1/n$	8.465(3)	97.17(1)		N	1.977(2)	O,N	92.04(9)	
	4	16.509(3)		CuO_2N_2	O	1.884(2)	O,N	90.53(9)[d]	
					N	1.990(2)	O.N	91.88(9)	
$Cu(ochyacph)_2$	tr	8.078(2)	100.76(3)	CuO_2N_2	O	1.906(2)	O,N	88.40(7)[d]	326
(red brown)	P-1	15.787(4)	114.38(3)		N	1.982(2)	O,N	92.60(7)	
	1	6.778(1)	78.40(5)						
$Cu(Mehyacph)_2$	m	14.6999(9)		CuO_2N_2	O	1.873(2)	O,N	88.70(9)[d]	326
(brown)	$P2_1/a$	7.8478(4)	93.282(6)		N	1.990(2)	O,N	91.30(3)	
	2	6.899(1)							
$[Cu(Mesaldim)_2]\cdot 2tnb$	m	11.726(4)		CuO_2N_2	O	1.881(4)	O,N	91.2(2)[d]	327
(dark brown)	$P2_1/c$	9.327(2)	93.55(5)		N	1.983(5)	O,N	88.8(2)	
	2	14.10(1)							
$Cu(C_8H_8NO_2)_2$	m	7.898(1)		CuO_2N_2	O	1.881(3,4)	O,N	90.7(2,4)[d]	328
(not given)	$P2_1/c$	9.989(1)	94.41(1)		N	1.963(4,5)	O,N	89.3(2,10)	
	4	19.035(3)					O,O	178.9(2)	
							N,N	171.8(2)	
$Cu(Me_2val)_2$	or	6.698(4)		CuO_2N_2	O	1.899(2,3)	O,N	84.4(1,1)[e]	329
(red)	$P2_12_12_1$	21.631(10)			N	2.024(3,2)	O,N	96.3(1,9)	
	4	12.011(9)					N,N	161.5(1)	
							O,O	175.7(1)	
$Cu(Et_2ala)_2$	tr	7.454(3)	118.69(4)	CuO_2N_2	O	1.0910(2)	O,N	84.1(1)[e]	330
(blue)	P-1	8.092(3)	93.78(3)		N	2.033(2)	O,N	95.9(1)	
	1	8.210(2)	100.46(3)						
$Cu(C_{14}H_{20}NO)_2$	m	7.760(2)		CuO_2N_2	O	1.893(11)	O,N	89.7(5)[d]	331
(reddish brown)	$P2_1/c$	15.909(5)	100.8(3)		N	2.012(12)			
	2	10.605(7)							
$Cu(acphim)_2$	tr	7.931(8)	80.1(6)	CuO_2N_2	O	1.975(5)	O,N	88.1(2)[d]	332
(not given)	P-I	17.96(1)	110.9(4)		N	2.047(5)			
	1	6.69(1)	100.0(6)						
$Cu(C_{18}H_{18}N_3O_2)_2$	m	23.088(8)		CuO_2N_2	O	1.93(2,1)	O,N	92(1,1)[d]	333
(dark green)	C2/c	6.987(1)	99.25(3)		N	1.99(2,2)	O,O	156(1)	
	4	23.641(8)					N,N	172(1)	

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*		*L-Cu-L*		*Ref.*
$Cu(C_9H\ NO_2)_2$[g]	m	18.41(2)		CuO_2N_2	O	1.872(7)	O,N	91.7(3)[d]	334
(yellow brown)	$P2_1/c$	4.83(1)	99.1(5)		N	2.011(8)	N,O	88.3(3)	
	4	19.86(2)		CuO_2N_2	O	1.869(8)	O,N	91.2(4)[d]	
					N	2.015(9)	N,O	88.8(4)	
$Cu(C_{30}H_{34}NO_4)_2$	m	21.995(8)		CuO_2N_2	O	1.895(8,5)	O,N	88.7(4,2)	335
(brown)	$P2_1/c$	18.016(3)	107.94(3)		N	2.03(1,1)	O,N	93.1(5,12)[d]	
	4	14.957(4)							
$Cu(C_4H_{10}NO_3)_2]NaClO_4 \cdot$	m	14.2872(6)		CuO_2N_2	O	1.908(–,2)	N,O	94.1(–,1)[d]	336
H_2O	C2/c	10.9454(4)	96.290(3)		N	1.999(–,2)	N,O	85.9(–,1)	
(violet)	4	11.1921(5)					N,N	180(–)	
							O,O	180(–)	
α–$Cu(C_9H_6NO)_2$	m	7.40(3)		CuO_2N_2	O	1.939(–)	O,N	85.2(–)[e]	337
(brown)	$P2_1/c$	3.84(2)	98.1(2)		N	1.984(–)	O,N	94.8(–)	
	2	24.37(9)					O,O	180(–)	
							N,N	180(–)	
$[Cu(C_{10}H_{13}N_2O)_2] \cdot 2H_2O$	m	12.46(1)		CuO_2N_2	O	1.948(–,29)	O,N	96.9(–,7)[e]	338
(blue)	$P2_1$	8.50(1)	120.0(1)		N	1.949(–,4)	O,N	83.1(–,2)	
	2	11.47(1)							
$Cu(C_{13}H_{10}NO)_2$	m	9.55(1)		CuO_2N_2	O	1.917(7)	O,N	91.5(1,1.8)[d]	339
(brown)	$P2_1/n$	22.40(2)	97.8(2)		N	2.006(9)			
	4	10.01(1)							
$Cu(C_{11}H_{14}NO)_2$	m	10.99(2)		CuO_2N_2	O	1.901(–)	O,N	89.05(–)[d]	340
(brown)	$P2_1/c$	7.36(2)	120.00(4)		N	2.019(–)	O,N	90.95(–)	
	2	14.81(3)					N,N	180(–)	
							O,O	180(–)	
$[Cu(C_{17}H_{24}N_2O_3)_2] \cdot$	tr	14.549(–)	106.33(–)	CuO_2N_2	O	1.905(–,22)	O,N	92.1(–,1.3)[d]	341
C_3H_6O	P–1	13.357(–)	83.63(–)		N	2.005(–,26)	O,N	91.4(–,5)	
(not given)	2	10.219(–)	102.80(–)				O,O	160.2(–)	
							N,N	159.4(–)	
$Cu(C_{16}H_{22}N_2O_3)_2$	tr	13.846(11)	110.84(5)	CuO_2N_2	O	1.877(10,17)	O,N	92.0(9,2.0)[d]	342
(dark brown)	P–1	13.355(11)	87.48(5)		N	1.973(20,8)	O,N	92.0(9,2.0)	
	2	10.254(5)	76.36(6)				O,O	158.0(9)	
							N,N	159.0(9)	
$Cu(C_{12}H_{16}NO)_2$	m	11.286(3)		CuO_2N_2	O	1.891(2)	O,N	88.3(2)[d]	343
(red brown)	$P2_1/a$	15.241(4)	103.75(2)		N	2.003(2)	O,N	91.6(3)	
	2	6.804(4)							
$Cu(C_{12}H_{10}NO)_2$	m	3.805(3)		CuO_2N_2	O	1.922(3)	O,N	89.7(1)[d]	344
(brown)	$P2_1/n$	19.371(5)	95.98(4)		N	1.974(3)	O,N	90.4(1)	
	2	12.518(1)							
$Cu(Etsalaldim)_2$[g]	or	11.04(4)		CuO_2N_2	O	1.887(9,0)	O,N	87.5(3)	345
(dark green)	$Pbc2_1$	16.57(2)			N	2.003(9,3)	O,N	92.4(3,3)[d]	
	8	18.48(2)					O,O	171.0(3)	
							N,N	177.0(3)	
				CuO_2N_2	O	1.873(9,13)	O,N	88.0(3)	
					N	1.995(9,8)	O,N	92.2(3,2)[d]	
							O,O	168.4(3)	
							N,N	174.2(3)	
$Cu(Etsalaldim)_2$	m	9.80(2)		CuO_2N_2	O	1.891(–,20)	O,N	93.8(–,7)[d]	346
(dark green)	$P2_1/c$	8.42(2)	101.3(3)		N	1.942(–,24)	O,N	91.9(–,7)	
	4	21.12(2)					O,O	152.4(–)	
							N,N	155.9(–)	
$Cu(C_{11}H_{14}NO)_2$	or	9.109(7)		CuO_2N_2	O	1.898(6,5)	O,N	94.7(3,1.4)[d]	347
(not given)	$P2_12_12_1$	11.166(5)			N	1.985(6,25)	O,N	97.7(3,2.4)	
	4	21.349(7)					O,O	137.4(3)	
							N,N	145.3(3)	

TABLE I *(Continued)*

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$Cu(p\text{-}C_{14}H_{12}NO)_2$	m	13.584(7)		CuO_2N_2	O	1.899(7)	O,N	92.0(4)[d]	348
(not given)	$P2_1/a$	7.55(1)	110.8(8)		N	2.010(10)	O,N	not given	
	2	12.221(9)							
$Cu(OHEtsalaldim)_2$	m	18.66(4)		CuO_2N_2	O	1.92(–)	O,N	91.8(–)[d]	349
(dark green)	$P2_1/c$	4.71(1)	97.8(1)		N	1.98(–)	O,N	88.2(–)	
	2	19.99(4)							
$Cu(asaln)_2$	m	10.871(8)		CuO_2N_2	O	1.876(3,8)	O,N	90.4(2,4)[d]	350
(dark tan)	$P2_1/c$	7.58(1)	127.0(8)		N	2.026(6,23)	O,N	89.8(2,7)	
	4	27.579(7)							
$Cu(salaldim)_2$	m	12.99(2)		CuO_2N_2	O	1.91(–)	O,N	92.6(–)[d]	351
(not given)	$P2_1/c$	5.85(1)	94.5(1)		N	1.904(–)	O,N	87.4(–)	
	2	8.08(2)							
$Cu(PrMeOsalim)_2$	or	14.996(1)		CuO_2N_2	O	1.889(7,8)	O,N	95.3(3,6)[e]	352
(green)	Pbca	16.552(1)			N	1.977(8,1)	O,N	95.8(3,33)	
	8	17.088(1)					O,O	145.0(3)	
							N,N	146.1(3)	
$Cu(n\text{-}C_{12}H_{17}N_2O_2)_2$	m	21.992(11)		CuO_2N_2	O	1.900(4)	O,N	90.7(2)[d]	353
(green)	C2/c	7.788(3)	128.05(3)		N	1.981(6)	O,N	90.4(2)	
	4	17.604(12)					O,O	167.2(2)	
							N,N	170.5(2)	
$Cu(t\text{-}C_{12}H_{17}N_2O_2)_2$	m	11.19(1)		CuO_2N_2	O	1.894(5,5)	O,N	94.8(3,1)[d]	354
(deep green)	C2/c	20.06(2)	99.7(1)		N	1.973(6,1)	O,N	97.1(3,2)	
	8	23.99(2)					O,O	136.7(4)	
							N,N	147.5(4)	
$[Cu(t\text{-}C_{12}H_{17}N_2O_2)_2]\cdot$	trg	16.82(3)		CuO_2N_2	O	1.87(2)	O,N	93.3(7)[d]	354
0.3MeOH	R3barc	16.82(3)			N	2.01(2)	O,N	96.4(8)	
(deep green)	18	48.59(5)					O,O	146.2(7)	
							N,N	146.3(7)	
$Cu(C_6H_{10}NO_2)_2$	m	10.824(12)		CuO_2N_2	O	1.91(1)	O,N	84.5(–)[e]	355
(blue)	$P2_1/a$	5.496(6)	94.28(12)		N	1.98(1)	O,N	95.5(–)	
	2	10.798(14)							
$Cu(C_{13}H_{18}N_2O)_2$	m	12.77(–)		CuO_2N_2	O	1.88(1)	O,N	88.9(3)[d]	356
(yellow brownish)	$P2_1/c$	6.97(–)	112.0(–)		N	1.95(1)	O,N	not given	
	not given	15.1(–)							
$Cu(OCHMeCH_2NMe)_2$	m	5.643(3)		CuO_2N_2	O	1.856(3)		not given	357
(purple)	$P2_1/c$	10.357(4)	92.49(5)		N	2.052(3)			
	2	11.723(5)							
$Cu(C_{16}H_{23}N_2O)_2$	tg	10.017(3)		CuO_2N_2	O	1.99(–)	O,N	94(–)[d]	358
(not given)	$P4_1(4_3)2_12$	10.017(3)			N	2.17(–)	O,N	85(–)	
	4	30.924(5)							
$Cu(C_7H_{12}NO_2)_2\cdot H_2O$[n]	m	10.750(3)		CuO_2N_2	O	1.940(4,10)	O,N	85.1(2,2)[e]	359
(blue)	$P2_1/c$	13.643(4)	100.51(2)		N	1.981(4,2)		175.2(2,2.2)	
	8	22.819(5)					N,N	95.2(3)	
				CuO_3N_2	O	1.962(4,5)	O,N	84.4(3,1)[e]	
					N	2.002(4,4)		94.7(2,1.4)	
					H_2O	2.383(5)	N,N	175.7(2)	
$[Cu(C_9H_6NO)_2]$picraz	m	16.14(4)		CuO_2N_2	O	1.95(1)	O,N	85.5(–)[e]	360
(magentared)	A2/a	30.93(8)	105.6(2)		N	1.96(1)	O,N	94.5(–)	
	4	6.90(2)							
Cu(i-Bucbp)$_2$	tr	10.964(5)	99.52(5)	CuO_2N_2	O	1.880(4,1)	O,N	90.3(2,3)[d]	361
(green)	P–1	11.490(5)	97.07(5)		N	1.992(5,4)	O,N	90.6(2,2)	
	2	12.861(7)	97.59(6)				O,O	167.6(2)	
							N,N	172.2(2)	

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$Cu(i\text{–}Bucbp)_2$	tr	8.900(2)	102.54(4)	CuO_2N_2	O	1.899(4,26)	O,N	89.0(2,2.0)	361
(red)	P–1	9.991(2)	94.61(4)		N	2.011(5,50)	O,N	91.1(2,5)	
	2	17.998(3)	92.49(2)				O,O	177.5(2)	
							N,N	178.5(3)	
				CuO_2N_2	O	1.883(4,2)	O,N	88.8(2,2)[d]	
					N	2.029(5,27)	O,N	91.2(2,1.0)	
							O,O	177.8(3)	
							N,N	176.9(2)	
$Cu(n\text{–}Bucbp)_2$	m	9.026(4)		CuO_2N_2	O	1.885(4,3)	O,N	91.8(2,6)[d]	361
(dark green)	$P2_1/c$	19.52(3)	94.46(7)		N	1.994(5,2)	O,N	92.5(2,3)	
	4	17.88(2)					O,O	158.9(2)	
							N,N	156.6(2)	
$Cu(n\text{–}Prcbs)_2$	or	12.830(4)		CuO_2N_2	O	1.881(4,7)	O,N	94.9(2,5)[d]	362
(green black)	Pbca	14.596(9)			N	1.979(5,5)	O,O	137.2(2)	
	8	20.714(4)					N,N	137.9(2)	
							O,N	100.3(2,7)	
$Cu(bs\text{–}glyNO)_2$	or	23.333(8)		CuO_2N_2	O	1.923(3,7)	O,N	84.2(1,0)	363a
(deep blue)	Pbca	10.508(4)			N	1.978(4,6)	O,N	95.9(1,2.0)	
	8	16.989(5)					O,O	175.6(2)	
							N,N	177.6(1)	
$Cu(Pheph)_2$	or	18.10(–)		CuO_2N_2	O	1.94(–4)	O,O	162(2)	363b
(purple)	$P2_12_12_1$	8.37(–)			N	2.09(–4)	O,N	88.00(–,9)[e]	
	4	12.81(–)						92.00(–,9)	
							N,N	178(2)	
$Cu(Et_2ala)_2$	tr	7.754(3)	118.69(4)	CuO_2N_2	O	1.910(2)	O,N	84.1(1)[e]	363c
(red)	P–1	8.092(3)	93.78(3)		N	2.023(2)		95.9(1)	
	1	8.210(2)	100.46(3)						
Cu(py)(OHcpb)(ph)	or	9.808(1)		CuO_2N_2	O	1.88(1,2)	O,O	175.7(5)	363d
(not given)	$Pna2_1$	11.430(3)			N	2.06(3)	O,N	106.1(6)[d]	
	4	13.436(2)			pyN	2.035(7)		72.6(6)[e]	
								91.0(5,5)	
							N,N	160.9(7)	
$[Cu(C_{23}H_{28}NO_3)_2]$	m	20.97(3)		CuO_2N_2	O	1.99(–)		not given	364
$[Cu(C_{42}H_{50}N_2O_4)]_2^m$	$P2_1/a$	21.89(5)	90.16(2)		N	1.98(–)			
(not given)	2	14.90(3)		CuO_2N_2					
$Cu(peph)_2](peph)\cdot 2H_2O$	m			CuO_2N_2	O	1.91(2,2)	O,N	87(–,1)[e]	365
(pale violet)	$P2_1$	not given			N	2.02(2,1)	O,N	95(–,4)	
	not given								
$Cu(C_{20}H_{25}N_2O_2)_2$	tr	13.91(1)	85.52(8)	CuO_2N_2	O	1.88(1,0)	O,N	91(1,1)[d]	366
(not given)	P–1	11.662(8)	109.7(2)		N	1.975(10,5)	O,N	93.5(10,1.5)	
	2	12.301(8)	103.40(5)						
$Cu(C_{16}H_{34}N_2O_3)_2$	m	9.871(3)		CuO_2N_2	O	1.871(–)		not given	367
(dark blue)	$P2_1/c$	8.208(8)			N	1.998(–)			
	2	18.230(4)							
$Cu(i\text{–}eph)_2$	h	11.89(–)		CuO_2N_2	O	1.88(–)	O,N	84.5(–)[e]	368
(deep violet)	P321	11.89(–)			N	2.05(–)	O,N	95.5(–)	
	3	15.32(–)							
$Cu(bz\text{–}L\text{–}prol)_2$	or	24.031(8)		CuO_2N_2	O	1.86(2,1)	O,N	86(1,0)[e]	369
(not given)	$P2_12_12_1$	8.679(3)			N	2.07(2,3)	O,N	94(1,1)	
	4	10.580(4)							
Cu(bz–L–prol).	m	8.857(5)		CuO_2N_2	O	1.95(2)	O,N	88(–)[e]	370
(bz–D–prol)	$P2_1/b$	2.739(5)	97.1(1)		N	1.92(2)	O,N	92(–)	
(violet)	2	10.061(5)					O,O	180(–)	
							N,N	180(–)	

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*		*L-Cu-L*		*Ref.*
$[Cu(bz-L-val)_2]\cdot 2H_2O$	m	13.026(8)		CuO_2N_2	O	1.933(8)	O,N	85.0(3)[e]	371
(red)	$P2_1/c$	8.612(4)	99.60(3)		N	1.997(9)	O,N	95.0(3)	
	2	11.270(8)					O,O	180.0(3)	
							N,N	180.0(3)	
$Cu(bzacac)_2(NH_3)$	m	7.628(2)		CuO_2N_2	O	1.920(2,10)	O,N	82.1(1)[e]	372
(not given)	$P2_1/c$	12.062(3)	103.95(2)		N	1.916(3)	O,N	94.6(1)[d]	
	4	14.365(5)			H_3N	1.983(3)	O,N	91.7(1,2.6)	
							O,O	176.0(1)	
							N,N	not given	
$[Cu(pan)(H_2O)](Cl0_4)$	tr	10.38(–)	85.3(–)	CuO_2N_2	O	1.97(1)	O,N	83(–)[e]	373
(not given)	P–1	8.22(–)	96.8(–)		N	1.96(1,1)	N,N	80(–)[e]	
	2	9.35(–)	93.3(–)	H_2O		1.98(1)	O,O	99(–)	
							N,O	98(–)	
$[Cu(C_5H_{11}N_3OS)NO_3]$	tr	9.001(3)	90.465(38)	CuO_2N_2	O	1.896(16)	O,N	92.0(7)[d]	374
$[Cu(C_5H_{11}N_3OS)(H_2O)]NO_3$	P–1	11.890(5)	112.954(32)	N		1.931(18,3)	N,N	81.9(7)[e]	
(greenish gray)	4	13.924(7)	105.099(32)	O_2NO		1.959(15)	N,O	96.0(7)	
							O,O	89.8(7)[d]	
				CuO_2N_2	O	1.888(16)	O,N	92.2(7)[d]	
					N	1.924(18,2)	N,N	81.9(7)[e]	
				H_2O		1.954(15)	N,O	92.5(7)	
							O,O	93.5(7)	
[Cu(gly–L–tryp)(H_2O)]·	or	7.74(4)		CuO_2N_2	O	1.960(–)	O,O	92.2(5)	375
$2H_2O$	$P2_12_12_1$	13.78(3)	H_2O			1.935(–,13)	O,N	98.8(6)	
(deep blue)	4	14.81(3)			N	1.959(14,80)	O,N	85.1(5)[e]	
							N,N	85.2(6)[e]	
$[Cu(_{17}H_{17}N_2O_2)(MeCO_2)]$	tr	8.157(7)	78.62(7)	CuO_2N_2	O	1.898(2)	O,O	85.63(9)	376a
(dark green)	P–1	10.651(7)	85.814(14)		MeO	1.988(2)	O,N	90.42(9)	
	2	10.900(7)	101.914(13)		N	1.975(3,15)	O,N	92.30(10)[d]	
							N,N	92.51(10)[d]	
$[Cu(C_{20}H_{24}N_4O_3)]\cdot$	tr	12.144(4)	97.13(4)	CuO_2N_2	O	1.96(1,1)	O,O	87.9(4)[p]	376b
$0.5CHCl_3$[g]	P–1	12.315(7)	106.92(4)		N	1.94(1,1)	O,N	83.6(5,2)[e]	
(green brown)	4	16.063(8)	100.01(4)					171.2(5,4)	
							N,N	104.9(5)	
				CuO_2N_2	O	1.968(10,9)	O,O	88.3(4)[p]	
					N	1.91(1,2)	O,N	83.9(5,2.1)[e]	
								170.3(5,2)	
							N,N	105.8(5)	
$2[Cu(C_{23}H_{28}NO_3)_2]$	m	20.97(3)		CuO_2N_2	O	1.99(–)	O,O	not given	376c
$4[Cu(C_{21}H_{25}NO_2)_2]$	$P2_1/a$	21.89(5)	90.16(2)		N	1.98(–)			
(not given)	2+4	14.90(3)							
$[Cu(pypn)](ClO_4)_2$	m	6.968(1)		CuO_2N_2	O	1.901(5,9)	O,O	92.2(2)	376d
(dark red)	$P2_1/n$	12.696(2)	97.04(1)		N	1.935(7,6)	O,N	92.15(3,65)[d]	
	4	23.122(5)						173.5(3);175.4(3)	
							N,N	83.9(4)[e]	
$Cu(C_{16}H_{18}N_4O_4)$	m	13.177(3)		CuO_2N_2	O	1.994(1)	O,N	90.2(1)[d]	376e
(green)	$P2_1/a$	10.137(2)	103.78(2)		N	1.949(2)		89.8(1)	
	2	6.650(1)							
$Cu(sal_2tmput)$[g]	m	14.374(7)		CuO_2N_2	O	1.897(40,4)	O,O	89.2(3)	377
(brown)	Cc	14.508(3)	94.33(8)		N	1.98(9,0)	O,N	95.6(3,1)[d]	
	8	19.370(3)					N,N	101.9(3)	
							O,N	143.2(4,4)	
				CuO_2N_2	O	1.90(3,2)	O,O	87.8(3)	
					N	1.98(3,1)	O,N	94.6(3,7)[d]	
							N,N	101.81(3)[h]	
							O,N	146.0(3,6)	

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
Na[Cu(Meoxazaoxam)	m	21.705(2)		CuO_2N_2	O	1.932(2,52)	O,O	95.1(1)	378
(H_2O)].0.33 H_2O[f]	$P2_1/n$	9.380(1)	101.17(1)		N	1.907(3,16)	N,O	89.6(1,6.7)[d]	
(brown)	4	19.131(2)					N,N	85.7(1)[e]	
							N,O	173.3(1,4.8)	
				CuO_2N_2	O	1.934(2,50)	O,O	95.0(1)	
					N	1.909(3,15)	N,O	90.1(1,7.3)[d]	
							N,N	84.9(1)[e]	
							N,O	172.2(1,4.6)	
				CuO_2N_2	O	1.938(3,53)	O,O	95.6(1)	
					N	1.910(4,24)	N,O	90.1(2,7)[d]	
							N,N	84.7(2)[e]	
							N,O	170.8(1,4.4)	
$Cu(C_{17}H_{16}N_2O_3)$	tr	9.620(2)	104.66(2)	CuO_2N_2	O	1.901(2,1)	O,N	94.3(1,3)[d]	379
(not given)	P-1	10.685(3)	95.50(2)		N	1.942(3,5)	O,N	154.0(1,5)	
	2	7.728(1)	91.66(9)				O,O	91.6(1)	
							N,N	91.5(1)	
Cu(boxamtsulf)	tr	5.279(1)	89.08(2)	CuO_2N_2	O	1.956(3,7)	O,O	86.5(1)	380
(green)	P1	11.388(3)	82.62(2)		N	1.956(4,7)	N,O	82.8(1,1)[e]	
	2	11.943(4)	86.44(2)				N,N	107.0(2)[d]	
							O,N	166.8(2,1.8)	
Cu{Pr(acac)$_2$}[g]	or	12.452(6)		CuO_2N_2	O	1.912(4,2)	O,N	93.9(2,3)[d]	381
(green brown)	$P2_12_12_1$	21.032(12)			N	1.930(5,5)	N,N	85.9(2)[e]	
	8	10.766(7)					O,O	87.2(2)	
							O,N	not given	
				CuO_2N_2	O	1.920(4,2)	O,N	93.9(2,4)[d]	
					N	1.937(4,9)	N,N	85.7(2)[e]	
							O,O	87.2(2)	
							O,N	not given	
$Cu(C_{22}H_{22}N_2O_2)$	m	10.971(4)		CuO_2N_2	O	1.908(6,6)	O,N	93.4(3,3)[d]	382
(brick red)	$P2_1/n$	7.878(2)	96.31(2)		N	1.928(6,4)	N,N	86.5(3)[e]	
	4	21.972(4)					O,O	86.7(2)	
							N,O	178.2(2,5)	
Cu{en(tmp)$_2$}	m	11.628(4)		CuO_2N_2	O	1.901(5,3)	O,N	93.4(2,3)[d]	383
(not given)	$P2_1/a$	13.233(3)	91.60(3)		N	1.932(6,15)	N,N	85.7(2)[e]	
	4	14.451(4)					O,N	174.1(2,4)	
							O,O	not given	
[Cu(l-eph)] $2H_20$	or	8.431(-)		CuO_2N2	O	1.90(-,1)	O,N	88.7(-,4)[e]	384
(blue)	$P2_12_12_1$	15.92(-)			N	2.01(-,2)	N,N	85.1(-)[e]	
	4	16.70(-)					O,O	100.6(-,1)	
[Cu(pba)]	tr	13.196(3)	116.39(2)	CuO_2N_2	O	1.940(4,22)	O,N	84.3(1,8)[e]	385
[Cu(Me_2tn)$_2$(H_2O)]·	P-1	11.088(2)	116.89(3)		N	1.913(4,24)	N,N	97.9(1)[d]	
$3H_2O$	2	11.501(2)	79.52(2)				O,O	93.4(1)	
(blue)				CuN_4O		see Table 2			
Cu(hapt)	m	17.746(6)		CuO_2N_2	O	1.88(2,1)	O,N	93.2(8,4)[d]	386
(dark green)	Cc	9.467(2)	114.06(2)		N	1.96(2,2)	N,N	93.0(6)[d]	
	4	10.646(4)					O,O	91.2(6)	
							O,N	155.2(7,2)	
[Cu($Me_2H_2Me_2$malox]	m	8.866(1)		CuO_2N_2	O	1.919(3,3)	O,N	94.5(1,2)[d]	387
(not given)	$P2_1c$	16.029(1)	97.57(2)		N	1.940(3,0)	N,N	86.4(1)[e]	
	4	9.106(1)					O,O	84.6(1)	
($Cu_{20}H_{14}N_2O_2S_2$)	m	8.7320(15)		CuO_2N_2	O	1.923(6,9)	O,N	94.0(2,5)[d]	388
(not given)	$P2_1/c$	19.045(5)	111.18(-)		N	1.949(7,0)	N,N	83.4(3)[e]	
	4	11.250(7)					O,O	88.6(2)	
Cu{en(ba)$_2$(C_2H_2)$_2$}	m	19.863(9)		CuO_2N_2	O	1.941(8,10)	O,O	91.5(3)	389
(dark green)	$P2_1/n$	12.184(8)	98.4(1)		N	1.955(7,8)	O,N	91.5(3,40)[d]	
	4	9.379(6)					N,N	86.2(3)[e]	

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore*	*Cu-L*		*L-Cu-L*		*Ref.*
[Cu(mnpgly)]	or	6.197(1)		CuO_2N_2	O	1.925(3,2)	O,O	92.7(1)	390
(blue needles)	$P2_12_12_1$	12.772(1)			N	1.983(3,6)	O,N	85.2(1)[e]	
	4	13.717(1)					N,N	97.3(1)[d]	
							O,N	174.8(1.8)	
[Cu{(R,S) –mnpala}]	tr	8.015(2)	80.47(1)	CuO_2N_2	O	1.929(1,6)	O,O	91.6(0)	390
(blue prisms)	P–1	9.297(1)	71.33(2)		N	1.994(1,2)	O,N	83.5(0)[e]	
	2	9.401(2)	79.78(2)				N,N	100.7(0)[d]	
							O,N	173.8(0,5)	
[Cu{(S,S) –mnpala}]·H_2O	m	9.532(2)		CuO_2N_2	O	1.916(3,5)	O,O	92.2(1)	390
(blue needles)	$P2_1$	6.371(1)	104.89(1)		N	1.983(3,3)	O,N	84.7(1)[e]	
	2	11.832(2)					N,N	98.2(1)[d]	
							O,N	174.2(1,4)	
$Cu(C_{12}H_{17}N_3O_3)$	tr	12.11(1)	102.1(1)	CuO_2N_2	O	1.907(13,20)	O,O	87.6(2)	391
(dark red)	P–1	8.15(1)	109.6(1)		N	1.937(14,0)	O,N	92.9(2,14)[d]	
	2	7.92(1)	105.6(1)				N,N	86.5(2)[e]	
[Cu(Et(salnim)$_2$)]·	tr	7.95(1)	130.33(25)	CuO_2N_2	O	1.896(–,10)	O,O	87.8(–)	392
p–NO_2phenol	P–1	11.72(3)	96.42(33)		N	1.916(–,12)	O,N	94.9(–,7)[d]	
(dark red)	2	14.67(3)	95.00(33)				N,N	82.7(–)[e]	
$Cu(C_{16}H_{14}N_2O_4)$	or	19.381(5)		CuO_2N_2	O	1.894(9,2)	O,O	87.8(4)	393
(brown)	Pnca	15.327(4)			N	1.94(1,1)	O,N	93.7(5,1)[d]	
	8	10.158(4)					N,N	85.0(5)[e]	
$Cu(C_{17}H_{16}N_2O_2)$	or	11.925(11)		CuO_2N_2	O	1.868(11,11)	O,O	82.25(4)	394
(not given)	$Pm2_1a$	6.890(6)			N	1.948(12,10)	N,O	92.7(5,5)[d]	
	4	17.780(8)					N,N	91.31(46)[d]	
							O,N	167.0(8,7.1)	
[$Cu(C_{16}H_{14}N_2O_2)$]·tu	tr	10.72(1)	87.9(1)	CuO_2N_2	O	1.891(5,1)	O,O	90.3(2)	395
(brown violet)	P–1	8.76(1)	80.0(1)		N	1.932(6,14)	O,N	94.1(2,6)[d]	
	2	9.64(1)	75.6(1)				N,N	84.8(2)[e]	
[$Cu(C_{20}H_{14}N_2O_2)$]·tu[g]	tr	11.46(1)	74.3(1)	CuO_2N_2	O	1.898(6,5)	O,O	87.4(2)	395
(dark brown)	P–1	16.87(2)	85.7(1)		N	1.951(7,9)	O,N	94.2(3,1)[d]	
	4	10.941(1)	80.6(1)				N,N	84.3(3)[e]	
				CuO_2N_2	O	1.901(6,2)	O,O	88.1(2)	
					N	1.958(6,12)	O,N	94.5(2,5)[d]	
							N,N	84.2(2)[e]	
Cu{bph(salaldim)$_2$}	m	11.30(2)		CuO_2N_2	O	1.90(1,0)	O,O	88.9(–)	396
(not given)	Pc	10.00(2)	118.1(–)		N	1.95(1,1)	O,N	93.6(–,0)[d]	
	2	12.04(2)					N,N	96.1(–)[h]	
$Cu(C_{16}H_{17}N_2O_2)_2$	m	13.246(5)		CuO_2N_2	O	1.878(2)	O,N	90.4(1)[d]	397
(not given)	$P2_1/n$	7.155(3)	92.25(4)		N	1.996(3)	O,N	89.6(1)	
	2	15.123(4)					O,O	180.1(6)	
							N,N	180.1(6)	
[Cu(salphen)]$_2$·tcnq	tr	11.970(4)	130.44(2)	CuO_2N_2	O	1.895(3,5)	O,O	88.8(1)	398
(blue black)	P–1	12.567(4)	92.35(2)		N	1.943(3,4)	O,N	93.8(1,1)[d]	
	1	7.020(2)	92.48(2)				N,N	83.8(1)[e]	
[$Cu(C_{23}H_{21}N_3O_3)$]·	m	13.788(4)		CuO_2N_2	O	1.903(5,3)	O,O	87.8(2)	399
1.5 H_2O	$P2_1/c$	7.881(1)	100.74(3)		N	1.952(5,21)	O,N	94.1(2,5)[d]	
(dark brown)	4	19.899(6)					N,N	94.4(2)[d]	
							O,N	155.2(2,6)	
$Cu(C_{18}H_{17}N_3O_2S)$	or	10.85(3)		CuO_2N_2	O	1.93(–)		not given	400
(not given)	Pbca	15.82(5)			N	1.95(–)			
	8	20.83(6)							
[$Cu(C_{12}H_{18}N_2O_2)$]·	or	17.04(4)		CuO_2N_2	O	1.920(10,6)	O,O	86.2(5)	401
0.5 H_2O	Pbcn	8.06(2)			N	1.919(10,3)	O,N	93.9(5,1)[d]	
(violet)	8	19.64(4)					N,N	86.1(5)[e]	

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$Cu(C_{12}H_{18}N_2O_2)$	m	11.77(2)		CuO_2N_2	O	1.92(–,2)	O,N	93.8(–,3)[d]	402
(not given)	$P2_1/m$	7.25(20)	93.50(25)		N	1.93(–,0)	N,N	86.4(–)[e]	
	2	10.89(2)					O,O	86.0(–)	
							O,N	179.9(–,1)	
$Cu(C_{12}H_{18}N_2O_2)$	m	11.02(4)		CuO_2N_2	O	1.94(–,2)	O,N	93.05(–,1.5)[d]	403
(violet)	$P2_1/c$	8.97(3)	94.0(–)		N	1.97(–,2)	N,N	86.0[e]	
	4	13.10(4)					O,O	88.7(–)	
$Cu(C_{23}H_{24}N_2O_2)$	m	13.022(2)		CuO_2N_2	O	1.900(5,3)	O,O	86.9(2)	404
(dark green)	$P2_1/c$	11.794(3)	104.93(2)		N	1.930(6,4)	N,N	84.6(2)[e]	
	4	13.749(3)					O,N	94.2(3,1)[d]	
[Cu(tn)]·2tcnq	m	37.343(8)		CuO_2N_2	O	1.948(7)	O,N	90.0(3)[d]	405
(black)	C2/c	7.717(1)	96.26(1)		N	1.948(8)	N,N	91.3(3)[d]	
	4	13.888(2)					O,O	94.5(3)	
$Cu(C_{12}H_{16}O_4N_4)$	m	25.528(5)		CuO_2N_2	O	1.892(3)	O,N	92.9(1)[d]; 173.4(1)	406
(dark brown)	C2/c	7.284(1)	92.719(16)		N	1.922(3)	N,N	87.9(1)[e]	
	4	7.109(1)					O,O	87.2(1)	
Cu{(S)-bap-(S)-val}	or	12.846(2)		CuO_2N_2	N	1.939(7,80)			407
(not given)	$P2_12_12_1$	19.427(3)			O	1.925(4)		not given	
	4	9.464(2)							
$Cu(C_{31}H_{30}N_4O_4)$	m	12.069(7)		CuO_2N_2	O	1.910(6,1)	O,N	93.7(3,1)[d]	408
(red brown)	$P2_1/c$	20.909(29)	113.95(5)		N	2.015(7,2)	O,N	89.9(3,6)	
	4	11.958(14)					O,O	156.8(3)	
							N,N	162.8(3)	
$Cu(C_{16}H_{22}N_2O_4)$	tr	10.915(1)	104.87(7)	CuO_2N_2	O	1.906(3,6)	O,O	87.41(12)	409
(mauve)	P–1	8.689(10)	89.66(3)		N	1.928(3,2)	O,N	93.71(13,31)[d]	
	2	9.593(8)	106.342(11)				N,N	86.27(13)[e]	
							O,N	172.04(13,70)	
$Cu(C_{21}H_{20}N_2O_4)$	m	23.098(18)		CuO_2N_2	O	1.940(18,6)	O,O	82.1(7)	410
(red)	C2/c	9.529(5)	104.15(5)		N	1.944(27,45)	O,N	91.4(10,10)[d]	
	8	18.046(8)					N,N	97.6(11)[d]	
							O,N	165.8(10,2)	
$Cu(C_{26}H_{28}N_2O_4)$[g]	tr	13.143(8)	67.36(6)	CuO_2N_2	O	1.910(9,41)	O,O	90.6(4)	411
(green)	P–1	14.279(8)	71.18(7)		N	1.919(11,32)	N,O	92.8(4,5)[d]	
	4	14.298(14)	91.36(5)				N,N	85.9(5)[e]	
							N,O	168.0(4,5)	
				CuO_2N_2	O	1.898(10,8)	O,O	90.2(4)	
					N	1.926(10,26)	N,O	93.4(4,1)[d]	
							N,N	84.6(4)[e]	
							N,O	169.8(4,6)	
[Cu(cbp-phen-sal)]·	tr	8.666(4)	103.01(3)	CuO_2N_2	O	1.886(2,22)	O,O	89.95(9)	412
MeOH	P–1	10.061(4)	104.38(4)		N	1.933(2,35)	N,O	94.9(1)[d]	
(not given)	2	14.104(8)	93.07(2)				N,N	84.0(1)[e]	
							O,N	171.30(10,1.40)	
[Cu(cbp-phen-OMe-sal)]·	tr	8.973(3)	98.80(4)	CuO_2N_2	O	1.824(5,18)	O,O	84.5(2)	412
MeOH	P–1	10.148(9)	118.35(3)		N	1.861(6,26)	N,O	94.3(2)[d]	
(not given)	2	15.836(5)	95.18(5)				N,N	87.2(2)[e]	
							O,N	173.8(2,2)	
[Cu(cbp-phen-Clsal)]·	m	15.296(6)		CuO_2N_2	O	1.880(8,13)	O,O	87.1(3)	412
H_2O	$P2_1/c$	7.166(2)	107.68(3)		N	1.936(9,7)	N,O	95.2(4)[d]	
(not given)	4	25.288(6)					N,N	87.0(4)[e]	
							O,N	170.9(4,1.0)	
$Cu(en)(tfpd)_2$	m	10.665(5)		CuO_2N_2	O	1.909(3,3)	O,O	87.2(1)	413
(not given)	$P2_1/c$	16.131(9)	106.43(5)		N	1.939(3,6)	N,N	85.4(1)[e]	
	not given	9.050(4)					N,O	94.3(1,4)[d]	
							O,N	171.0(1,3.4)	

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$[Cu(C_{25}H_{20}N_2O_2)_2]\cdot$ 0.5 dmso (purple)	m C2/c 8	23.416(11) 9.24(1) 20.194(11)	102.1(1)	CuO_2N_2	O N	1.911(11,7) 1.980(3,9)	O,O N,N O,N O,N	80.5(4) 98.7(5)[d] 90.5(5,2)[d] 170.2(5,3)	414
$[Cu(H_2O)_2Cl_2]\cdot(Ph_3PO)_4$ (dark blue)	m $P2_1/c$ 2	14.038(4) 9.826(2) 27.544(9)	122.540(1)	CuO_2Cl_2	O Cl	1.90(–) 2.23(–)	O,O Cl,Cl O,Cl	180(–) 180(–) 90(–,3)	415
$Cu(dmso)_2Cl_2$ (green)	or Pnma 4	8.0542(13) 11.5464(105) 11.3670(82)		CuO_2Cl_2	O Cl	1.955(4) 2.287(2,3)	Cl,Cl O,O Cl,O	146.13(9) 173.01(26) 90.73(12,2.00)	416
$Cu(Ph_3PO)_2Cl_2$ (not given)	or Fdd 8	31.961(–) 220.839(–) 9.886(–)		CuO_2Cl_2	O Cl	1.96(–) 2.17(–)	O,O Cl,Cl O,Cl	93(–) 102(–) 117(–,12)	417
$Cu(4\text{–}MepyNO)_2Cl_2$ (green)	m $P2_1/c$ 2	6.28(1) 10.663(5) 11.453(5)	101.45(10)	CuO_2Cl_2	O Cl	1.949(6) 2.227(3)	O,O Cl,Cl O,Cl	180.0(2) 180.0(2) 90.0(2,3.6)	418
$Cu(2,6\text{–}Me_2pyNO)_2Cl_2$ (yellow)	or $Pma2_1$ 4	13.88(1) 7.677(5) 16.23(1)		CuO_2Cl_2	O Cl	1.95(1,2) 2.234(4,13)	Cl,Cl O,O O,Cl	100.8(2) 86.7(5) 99.1(4,1)	419
$Cu(nicOH)_2Cl_2$ (yellow)	m $P2_1/c$ 2	6.019(4) 13.16(1) 10.418(8)	115.80(5)	CuO_2Cl_2	O Cl	1.962(3) 2.241(1)	O,O Cl,Cl O,Cl	180.00(8) 180.00(8) 90.00(8,3.08)	420
$[Cu(nitphen)_2Cl_2]$ (brown)	m $P2_1/n$ 2	11.988(4) 10.878(3) 11.788(4)	106.14(2)	CuO_2Cl_2	O Cl	1.989(1) 2.184(1)	O,O Cl,Cl O,Cl	180.00(1) 180.00(1) 90.00(4,3.87)	421
$Cu(pyzNO)_2Cl_2$ (not given)	m $P2_1/n$ 2	7.212(–) 12.500(–) 7.133(–)	114.22(–)	CuO_2Cl_2	O Cl	1.984(–) 2.245(–)	Cl,O	90.9(–)	422a
$Cu(nitph)_2Cl_2$ (not given)	m $P2_1/n$ not given	11.988(4) 10.878(3) 14.286(6)	127.57(8)	CuO_2Cl_2	O Cl	1.985(54) 2.189(18)	O,Cl	86.5(3) 93.5(3)	422b
$Cu(C_2H_8NOS)_2$ (not given)	m $P2_1/c$ 2	4.177(1) 10.562(3) 9.964(3)	93.15(5)	CuO_2S_2	O S	1.913(5) 2.268(2)	O,S O,S O,O S,S	87.7(1)[e] 92.3(1) 180.0(1) 180.0(1)	423
$[Cu(HOMePyS)_2]\cdot 2dmf$ (brown)	m $P2_1/c$ 2	8.599(2) 13.574(3) 9.432(2)	94.33(2)	CuO_2S_2	O S	1.906(4) 2.292(2)	O,O S,S O,S O,S	180.0(1) 180.0(1) 88.5(1)[e] 91.5(1)	424
$[Cu(thiox)_2].1.6H_2O$ (yellow)	m $P2_1/n$ 4	15.016(8) 16.501(1) 3.754(2)	90.65(5)	CuO_2S_2	O S	1.947(4,0) 2.273(1,7)	O,S O,O S,S	88.3(1,1)[e] 85.3(1) 97.8(1)	425
$Cu(Et_2bzthiour)_2$ (olive black)	m $P2_1/c$ 4	8.871(2) 29.492(5) 12.281(2)	124.50(2)	CuO_2S_2	O S	1.927(4) 2.243(2)	O,S S,S O,O	95.3(1,1)[d] 89.6(1) 89.2(2)	426
$[Cu(Et_2bzthioacam)_2$[g] (olive black)	tr P–1 3	10.709(2) 12.150(2) 15.651(4)	90.13(2) 103.73(2) 98.30(1)	CuO_2S_2	O S	1.898(4,14) 2.240(2,4)	O,S O,S S,S	94.5(1,0)[d] 82.2(2) 88.8(1)	427
				CuO_2S_2	O S	1.910(4) 2.254(1)	O,S O,S	95.4(1)[d] 84.6(1)	
$[Cu(H_2O)_2Br_2]\cdot H_2O$ (dark green)	m $P2_1/a$ 2	12.013(3) 7.330(4) 4.116(2)	105.44(3)	CuO_2Br_2	O Br	1.93(2) 2.426(2)	Br,Br O,O O,Br	180.0(7) 180.0(4) 90.0(4,1.4)	428

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$Cu(Ph_3PO)_2Br_2$ (red brown)	or $Pca2_1$ 4	17.193(6) 10.226(4) 19.052(4)		CuO_2Br_2	O Br	1.94(2,3) 2.311(3,9)	O,O Br,Br O,Br O,Br	98.7(5) 103.9(1) 100.0(5,9) 128.9(4,2.8)	429
$Cu(py)_2Cl_2$ (greenish blue)	m $P2_1/n$ 2	17.00(–) 8.59(–) 3.87(–)	91.52(–)	CuN_2Cl_2	N Cl	2.02(–) 2.28(4)	N,Cl	90.1(–)	430
$Cu(py)_2Cl_2$ (not given)	m $P2_1/n$ not given	16.967(3) 8.5596(4) 3.8479(7)	91.98(2)	CuN_2Cl_2	N Cl	2.004(5) 2.298(2)1	Cl,N	90.4(1)	431
$Cu(2\text{–}Mepy)_2Cl_2$ (dark blue)	tr P–1 2	8.58(5) 9.20(5) 10.99(5)	86.8(5) 110.1(5) 12.3(1)	CuN_2Cl_2	N Cl	2.000(12,20) 2.24(5,3)	N,Cl	90.1(9,5)	432
$Cu(4\text{–}Etpy_4)_2Cl_2$ (blue green)	m $P2_1/c$ 2	11.36(2) 4.00(1) 17.58(2)	112.8(2)	CuN_2Cl_2	N Cl	2.00(1) 2.280(5)	N,N Cl,Cl N,Cl	180.0(5) 180.0(5) 90.0(5,1.1)	433a
$Cu(2,6\text{–}Me_2py)_2Cl_2$ (not given) 295K	tr P–1 1	8.068(2) 8.024(2) 7.646(2)	93.84(2) 113.44(2) 117.11(2)	CuN_2Cl_2	N Cl	2.011(3) 2.264(2)	Cl,N	90.0(2,6)	433b
$Cu(2,3\text{–}Me_2py)_2Cl_2$ (not given)	m $P2_1/c$ 2	7.461(4) 14.80(1) 7.879(6)	110.11(5)	CuN_2Cl_2	Cl N	2.254(2) 1.977(6)	Cl,Cl Cl,N N,N	180.0 90.0(3,6) 180.0	433c
$Cu(4\text{–}vipy)_2Cl_2$ (turquoise)	m $P2_1/n$ 2	8.68(–) 3.91(–) 21.11(–)	90.0(–)	CuN_2Cl_2	N Cl	2.01(1) 2.38(2)		not given	434
$Cu(Meim)_2Cl_2$ (not given)	tr P–1 2	7.632(3) 8.166(9) 10.232(3)	87.84(5) 82.77(2) 76.12(5)	CuN_2Cl_2	N Cl	1.969(5,7) 2.258(3,2)	N,N Cl,Cl N,Cl	149.7(1) 143.57(6) 94.7(1,7)	435
$Cu(C_{11}H_{16}N_2)_2Cl_2$ (not given)	m C2 2	23.110(5) 7.533(1) 7.041(1)	105.25(2)	CuN_2Cl_2	N Cl	1.949(2) 2.250(1)	N,N Cl,Cl N,Cl	142.4(2) 135.2(1) 97.1(1,1.7)	436
$Cu(C_7H_8N_4O_2)_2Cl_2$ (red brown)	m C2/c 4	20.328(10) 6.871(5) 14.374(12)	107.83(7)	CuN_2Cl_2	N Cl	2.004(13) 2.234(5)	N,N Cl,Cl N,Cl	97.0(6) 97.9(2) 118.2(5,22.8)	437
$Cu(2,7\text{–}Me_2\text{–}1,8\text{–}nphpy)_2Cl_2$ (green brown)	m $P2_1/n$ 2	10.515(2) 11.095(3) 8.677(2)	102.00(4)	CuN_2Cl_2	N Cl	1.982(9) 2.279(3)	N,N N,Cl Cl,Cl	180.0(3) 90.0(3,1.2) 180.0(3)	438
$Cu(2,4\text{–}Me_2thz)_2Cl_2$ (purple)	m C2/c 4	12.320(13) 8.760(7) 14.592(11)	105.81(6)	CuN_2Cl_2	N Cl	1.985(4) 2.261(2)	N,N N,Cl Cl,Cl	179.0(1) 90.0(1,4) 178.36(8)	439
$Cu(Ettraz)_2Cl_2$ (not given)	m $P2_1/a$ 2	7.462(3) 7.061(3) 12.788(5)	103.39(3)	CuN_2Cl_2	N Cl	1.961(3) 2.3186(8)	N,Cl Cl,Cl	89.66(9) 84.99(2)	440
$Cu(PhMe_2pz)_2Cl_2$ (dark green)	m $P2_1/c$ 2	13.121(5) 10.610(2) 13.973(5)	145.51(1)	CuN_2Cl_2	N Cl	1.979(1) 2.268(1)	N,N N,Cl Cl,Cl	180.00(4) 90.00(4,77) 180.00(4)	441
$[Cu(xan)_2Cl_2]\cdot 2H_2O$ (green)	tr P–1 1	3.647(5) 9.849(2) 12.763(4)	72.41(2) 81.07(6) 82.93(6)	CuN_2Cl_2	N Cl	2.004(3) 2.289(2)	N,N N,Cl Cl,Cl	180.0(1) 90.0(1,2) 180.0(1)	442
$[Cu(diazepam)_2Cl_2]\cdot 2H_2O\cdot 0.33CHCl_3$ (not given)	rh R3bar not given	18.645(2)	117.52(1)	CuN_2Cl_2	N Cl	1.990(8) 2.27(20)	N,Cl	90.9(1,3)	443

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$[Cu(azaH)_2Cl_2]$	or	26.5580(6)		CuN_2Cl_2	N	2.096(20,73)	N,N	160.6(8)	444
$[Cu(azaH)_4]$	Fddd	23.750(2)			Cl	2.270(2)	N,Cl	91.4(6,11.0)	
(green)	8	12.7271(8)				2.819(5)	Cl,Cl	93.63(12)	
				CuN_4	N	2.030(8,83)	N,N	90.2(4)	
$Cu(2,2'-bpy)Cl_2$	tr	7.288(2)	55.36(3)	CuN_2Cl_2	N	2.053(3,26)	N,N	80.0(1)[e]	445
(not given)	P-1	9.640(2)	69.29(2)		Cl	2.267(1,0)	N,Cl	92.71(3);172.09(8,52)	
	2	9.771(2)	70.48(3)				Cl,Cl	92.71(3)	
$Cu(2-ampy)Cl_2$	m	7.932(2)		CuN_2Cl_2	N	1.993(2,5)	N,N	82.98(9)[e]	446
(deep blue)	$P2_1/m$	6.257(1)	112.97(2)		Cl	2.255(1,15)	N,Cl	92.57(7,4.66)	
	2	9.435(2)						175.34(7,4.45)	
							Cl,Cl	91.88(3)	
$Cu(dmaep)Cl_2$	tr	7.348(3)	74.69(2)	CuN_2Cl_2	N	2.003(3,5)	N,N	95.34(9)[d]	447
(bright green)	P-1	8.875(4)	99.06(2)		Cl	2.233(2,8)	N,Cl	98.01(7,69)	
	2	9.982(4)	109.65(2)					134.07(7,1.35)	
$Cu(Et_4en)Cl_2$	m	15.302(9)		CuN_2Cl_2	N	2.074(2)	N,N	85.1(1)[e]	448
(blue)	C2/c	7.890(4)	90.19(5)		Cl	2.246(1)	N,Cl	91.8(1)	
	4	11.645(8)						171.8(1)	
							Cl,Cl	92.2(1)	
$Cu(Me_4Phdiam)Cl_2$	m	10.424(3)		CuN_2Cl_2	N	2.069(2,2)	N,N	83.55(9)[e]	449
(not given)	$P2_1/n$	8.993(2)	90.41(2)		Cl	2.277(1,14)	N,Cl	89.39(9,5.84)	
	4	13.567(4)					N,Cl	169.26(8,8.14)	
							Cl,Cl	91.71(4)	
$Cu\{Ph(bzS)_2\}Cl_2$	m	8.408(1)		CuN_2Cl_2	N	2.017(2,7)	N,N	84.66(9)[h]	450
(dark green)	$P2_1/n$	15.819(1)	93.19(1)		Cl	2.217(1,1)	N,Cl	171.59(7,1.43)	
	4	14.229(2)					Cl,Cl	94.40(3)	
$Cu(Mepzimid)Cl_2$	m	14.177(5)		CuN_2Cl_2	N	2.005(2,4)	N,N	80.75(9)[e]	451
(brown)	C2/c	17.821(4)	106.13(2)		Cl	2.212(1,24)	N,Cl	101.26(8,1.64)	
	8	12.119(2)					N,Cl	140.27(8,8.26)	
							Cl,Cl	100.39(4)	
$Cu(C_{15}H_{26}N_2)Cl_2$	or	11.397(16)		CuN_2Cl_2	N	1.994(6,0)	N,N	90.6(2)[d]	452
(yellow green)	$P2_12_12_1$	11.560(10)			Cl	2.225(4,0)	N,Cl	111.88(2,2.68)	
	4	12.639(17)					Cl,Cl	116.0(1)	
$Cu(bddo)Cl_2$	m	9.019(2)		CuN_2Cl_2	N	2.014(9,12)	N,N	161.0(2)	453
(green)	$P2_1/n$	28.671(5)	113.65(2)		Cl	2.238(3,3)	N,Cl	91.6(2,2.0)	
	4	8.431(2)					Cl,Cl	160.4(1)	
$Cu(bddo)Cl_2$	or	9.397(4)		CuN_2Cl_2	N	1.986(9)	N,N	96.5(2)	453
(red)	Pbcn	15.093(4)			Cl	2.228(3)	N,Cl	114.7(2,16.0)	
	4	15.142(4)					Cl,Cl	105.7(1)	
$Cu(Me_2Ph_2bpd)Cl_2$	m	7.924(1)		CuN_2Cl_2	N	1.98(1)	N,N	83.3(4)[d]	454
(not given)	$P2_1/n$	20.628(4)	97.58(2)		Cl	2.222(5,40)	N,Cl	114.5(3,10.1)	
	4	12.712(3)					Cl,Cl	110.9(2)	
$[Cu(salampH)Cl_2]\cdot$	m	9.959(1)		CuN_2Cl_2	N	2.019(4,15)	N,N	81.6(1)[e]	455
$MeOH\cdot H_2O$	$P2_1/c$	9.924(1)	103.20(2)		Cl	2.273(1,14)	N,Cl	92.58(1,3.58)	
(green)	4	18.197(2)						171.06(1,6.64)	
							Cl,Cl	93.05(4)	
$Cu(C_7H_7N_3O)Cl_2$	m	15.449(11)		CuN_2Cl_2	N	2.063(9,65)	N,N	81.8(3)[e]	456
(not given)	$P2_1/c$	8.955(8)	104.3(1)		Cl	2.235(3,6)	N,Cl	92.9(3,4.0)	
	4	7.365(13)						168.2(4,1.7)	
							Cl,Cl	93.2(1)	
$Cu(C_{14}H_{16}N_4S_4)Cl_2$	or	8.571(1)		CuN_2Cl_2	N	2.028(4)	N,N	87.7(2)	142
(bright green)	Pnma	16.104(3)			Cl	2.246(2)	N,Cl	88.8(1)	
	4	13.961(2)					Cl,Cl	94.39(8)	
$Cu(C_{10}H_{11}N_2S)_2$	tr	12.024(8)	77.81(4)	CuN_2S_2	N	2.017(7,28)	N,N	108.7(3)	457
(not given)	P1	12.021(6)	64.22(4)		S	2.221(3,4)	N,S	85.9(2,2)[e]	
	2	8.238(6)	85.72(4)					141.1(2,4.6)	
							S,S	105.2(1)	

TABLE I *(Continued)*

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$Cu(C_{16}H_{15}N_2OS)_2$	m	45.000(1)		CuN_2S_2	N	2.046(7)	N,N	180.0(4)	458
(not given)	C2/c	4.354(2)	142.51(2)		S	2.279(6)	N,S	83.4(4)[e]	
	4	25.060(9)						96.6(4)	
							S,S	180.0(4)	
$Cu(Me_2Sdaz)_2$	not given	not given		CuN_2S_2	N	2.08(2)	N,S	85.0(–)[e]	459
(not given)					S	2.224(8)			
$Cu(Et_2SPhbz)_2$	or	27.792(16)		CuN_2S_2	N	1.97(1,1)	N,N	98.7(5)	460
(black)	Pbca	19.197(11)			S	2.229(4,6)	N,S	95.6(3,21)[d]	
	8	12.325(10)					S,S	90.7(2)	
$Cu(Spican)_2$	m	6.027(1)		CuN_2S_2	N	2.031(5)	N,N	180.0(2)	461
(red brown)	$P2_1/b$	8.526(2)			S	2.262(2)	N,S	86.0(2)[e]	
	2	23.547(5)	117.42(8)					94.0(2)	
							S,S	180.0(2)	
$Cu(Mequin)_2$	m	7.444(4)		CuN_2S_2	N	2.040(–)	N,N	180.0(–)	462
(not given)	$P2_1/b$	16.09(3)			S	2.278(–)	N,S	85.5(–)[e]	
	2	7.990(5)	105.3(1)					94.5(–)	
							S,S	180.0(–)	
$Cu(chSpam)_2$	tr	5.223(7)	111.2(1)	CuN_2S_2	N	2.048(4)	N,S	85.7(1)[e]	463
(bronze red)	P–1	10.600(4)	96.8(1)		S	2.252(2)	N,S	not given	
	1	11.573(4)	92.0(1)						
$Cu(Me_2Etecys)_2$	tr	5.508(1)	102.23(2)	CuN_2S_2	N	2.031(13,29)	N,N	87.2(5)[e]	464
(red brown)	P1	12.402(2)	90.14(2)		S	2.246(5,16)	N,S	89.1(4,7)[e]	
	1	5.500(6)	77.75(2)					163.9(4,1.3)	
							S,S	98.6(2)	
$Cu\{Etox(ts)_2\}$	tr	9.306(6)	90.63(5)	CuN_2S_2	N	1.970(5,11)	N,N	79.9(1)[e]	465
(not given)	P–1	10.443(7)	114.25(5)		S	2.265(1,2)	N,S	84.1(6,2)[e]	
	2	7.479(5)	98.42(5)				N,S	162.9(2,9)	
							S,S	112.3(5)	
Cu(EtSacac)	m	11.278(10)		CuN_2S_2	N	1.983(8, 5)	N,N	86.3(3)[e]	466
(not given)	$P2_1/c$	7.472(5)	91.45(6)		S	2.233(3, 7)	N,S	96.6(3,4)[d]	
	4	16.562(17)						159.4(2,7)	
							S,S	88.0(1)	
$Cu(C_{17}H_{24}N_2S_4)$	m	16.722(2)		CuN_2S_2	N	1.9498(–,30)	N,N	93.13(19)[j]	467
(dark brown)	C2/c	8.401(1)	108.34(1)		S	2.2225(–,11)	N,S	97.98(9)[d]	
	4	14.551(2)						143.61(10)	
							S,S	93.32(6)	
Cu(EtcpS)	or	7.739(1)		CuN_2S_2	N	1.946(14,21)	N,N	84.7(7)[e]	468
(not given)	$P2_12_12_1$	13.893(2)			S	2.251(5,8)	N,S	96.6(5,10)[d]	
	4	17.096(3)						166.5(5,5)	
							S,S	85.3(2)	
$Cu(Me_4cpS)$	m	16.728(5)		CuN_2S_2	N	1.955(5)	N,N	98.3(2)	469
(dark brown)	C2/c	8.626(2)	105.83(2)		S	2.221(2)	N,S	99.1(2)[d]	
	4	14.621(5)					N,S	138.6(1)	
$Cu(C_{34}H_{26}N_6S_2)$	m	20.334(3)		CuN_2S_2	N	1.984(3)	N,N	94.7(2)[d]	470
(violet)	C2/c	9.716(2)	127.55(1)		S	2.245(1)	N,S	101.1(1)[d]	
	4	19.717(4)					S,S	87.5(1)	
$Cu(Py)_2Br_2$	m	8.424(2)		CuN_2Br_2	N	2.013(5)	N,Br	90.1(1)	431
(not given)	$P2_1/n$	17.599(9)	97.12(2)		Br	2.451(1)			
	(not given)	4.0504(8)							
$Cu(2\text{–}Mepy)_2Br_2$	tr	8.777(5)	74.75(7)	CuN_2Br_2	N	1.983(6,3)	N,N	176.2(1)	471
(blue)	P–1	11.738(13)	60.73(4)		Br	2.420(3,7)	Br,Br	176.2(3)	
	2	8.494(5)	70.52(7)				Br,N	90.1(2,4)	

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*		*L-Cu-L*		*Ref.*
$Cu(2,3\text{–}Me_2py)_2Br_2$	m	7.566(5)		CuN_2Br_2	N	1.976(9)	N,N	180(–)	433c
(not given)	$P2_1/c$	15.33(2)	109.72(6)		Br	2.392(2)	Br,Br	180(–)	
	2	7.899(6)					Br,N	90.0(4,1)	
$Cu(2,6\text{–}Me_2py)_2Br_2$	tr	7.999(2)	94.37(2)	CuN_2Br_2	N	1.997(4)	Br,N	90.0(2,4)	433b
(not given)	P–1	7.921(2)	112.85(2)		Br	2.425(1)			
295K	1	7.849(2)	115.99(2)						
$Cu(Meim)_2Br_2$	m	4.130(1)		CuN_2Br_2	N	1.953(5)	N,N	180.0(2)	472
(not given)	$P2_1/c$	13.899(4)	99.00(4)		Br	2.494(1)	N,Br	90.0(2, 2)	
	2	10.529(3)					Br,Br	180.0(2)	
$Cu(bzim)_2Br_2$	m	13.794(5)		CuN_2Br_2	N	1.961(7,15)	N,N	154.6(3)	473
(dark brown)	$P2_1/c$	7.875(2)	105.82(5)		Br	2.424(1,22)	Br,Br	139.0(1)	
	4	14.510(6)					Br,N	94.4(2,7)	
$Cu(bzim)_2Br_2$	m	13.78(2)		CuN_2Br_2	N	1.955(3,4)	N,N	155.8(1)	474
(dark brown)	$P2_1/c$	7.861(2)	105.59(1)		Br	2.425(1,22)	Br,Br	138.8(10)	
(at 163K)	4	14.309(2)					Br,N	94.2(1,8)	
$Cu(3,5\text{–}Ph_2pz)_2Br_2$	m	14.644(3)		CuN_2Br_2	N	2.016(10,11)	N,N	92.4(4)	475
(dark purple)	$P2_1/n$	11.679(2)	108.82(2)		Br	2.368(2,8)	Br,Br	96.3(1)	
	4	16.640(3)					Br,N	92.0(3,5);(152.7(3,0)	
$[Cu(adeH)_2Br_2]Br_2$	m	18.649(3)		CuN_2Br_2	N	2.013(5)	N,N	95.1(2)	476
(dark brown)	C2/c	8.731(2)	113.14(2)		Br	2.361(1)	Br,Br	95.81(5)	
	4	12.028(2)					Br,N	95.1(2);144.7(2)	
$Cu(bpy)Br_2$	m	16.966(4)		CuN_2Br_2	N	2.030(6)	N,N	80.22(36)[e]	445
(not given)	C2/c	9.287(2)	111.60(2)		Br	2.410(1)	Br,Br	91.06(6)	
	4	7.490(2)					Br,N	94.45(18)	
$Cu(phen)Br_2$	m	10.005(2)		CuN_2Br_2	N	2.041(8,8)	N,N	81.2(3)[e]	477
(not given)	$C2_1$	6.256(2)	117.52(1)		Br	2.398(1,12)	Br,Br	91.79(6)	
	2	10.314(2)					Br,N	93.5(2,5);174.8(3,5)	
$Cu(C_6H_{10}N_2O_2)Br_2$	tr	7.702(1)	70.05(2)	CuN_2Br_2	N	1.995(8,5)	N,N	77.0(3)[e]	478
(dark green)	P–1	7.942(2)	68.98(2)		Br	2.348(2,3)	Br,Br	98.1(1)	
	2	10.500(3)	63.37(2)				Br,N	92.4(3,1);168.9(2,6)	
$Cu(bispyam)Br_2$	m	14.44(5)		CuN_2Br_2	N	1.96(3)	N,N	94.8(1,5)[d]	479
(dark brown)	C2	7.93(2)	94.7(5)		Br	2.41(1)	Br,Br	98.3(1,5)	
	2	5.26(3)					Br,N	101.2(10);133.8(12)	
$Cu(Me_4tu)_2Cl_2$	m	9.464(2)		$CuCl_2S_2$	Cl	2.238(6,4)	Cl,Cl	145.0(3)	480
(ruby red)	$P2_1$	8.550(1)	105.56(4)		S	2.315(7,1)	S,S	140.1(3)	
	2	11.532(2)					Cl,S	100.1(2,2.5);91.7(3,9)	
$Cu(dth)Cl_2$	m	6.875(2)		$CuCl_2S_2$	Cl	2.244(1,14)	Cl,Cl	98.4(1)	481
(dark green)	$P2_1/n$	8.963(2)	90.48(2)		S	2.321(1,16)	S,S	89.7(1)[e]	
	2	14.513(4)					S,Cl	91.1(1,8);154.0(1,7.9)	
$[Cu(salbh)Cl]\cdot H_2O$	m	16.201(21)		CuO_2NCl	O	1.927(8,36)	O,O	171.8(3)	482a
(dark green)	$P2_1/a$	7.107(10)	89.87(9)		N	1.933(9)	O,N	81.3(4)[e];91.9(4)[d]	
	4	12.540(18)			Cl	2.211(4)	O,Cl	93.8(3)	
$Cu(3,5\text{–}I_2tyr)Cl$	or	8.405(2)		CuO_2NCl	O	1.975(20,10)	O,O	85.2(8)	482b
(dark blue)	$P2_12_12_1$	20.694(3)			N	1.97(3)	O,N	164.9(9)	
	4	7.532(3)			Cl	2.231(8)		82.7(9)[e]	
							O,C	97.7(6);174.2(6)	
							N,Cl	95.1(8)	
$[Cu(pyoxts)(H_2O)]Cl\cdot H_2O$	tr	9.732(2)	95.73(3)	CuO_2NS	H_2O	1.941(5)	O,O	85.4(2)	483
	P–1	9.491(3)	101.65(3)		O	1.875(4)	O,N	94.5(2)[d];174.1(2)	
(green)	2	7.894(2)	79.30(2)		N	1.943(6)	N,S	86.3(1)[e]	
							O,S	93.5(1);176.3(1)	
Cu(salalgly)(tu)	m	18.599(–)		CuO_2NS	O	2.03(–,14)	O,N	89.4(–)[e];93.3(–)[d]	484
(black green)	C2/c	14.275(–)	138.64(-)		N	1.94(–)	O,S	92.5(–,8.2)	
	8	13.617(–)			tuS	2.27(–)			

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$[Cu(C_{12}H_{11}N_3O)Cl]\cdot H_2O$[g]	or	18.952(9)		CuN_2OCl	N	1.980(5,8)	N,N	92.6(2)[d]	485
(dark green)	Pccn	19.680(9)			O	1.906(2)	N,O	92.32(9)[d];158.1(2)	
	16	15.028(8)			Cl	2.281(1)	N,Cl	92.9(2);167.47(9)	
							O,Cl	86.80(7)	
				CuN_2OCl	N	1.982(13,5)	N,N	91.9(5)[d]	
					O	1.911(10)	N,O	93.0(5)[d];156.1(5)	
					Cl	2.321(12)	N,Cl	93.0(5);171.4(5)	
							O,Cl	85.3(4)	
Cu(salMetsc)Cl[g]	tr	10.261(4)	96.01(3)	CuN_2OCl	N	1.96(1,2)	N,N	81(1)[e]	486
(not given)	P-1	11.025(3)	111.58(3)		O	1.91(1)	N,O	91(1)[d];170(1)	
	4	12.249(6)	112.77(3)		Cl	2.233(5)	N,Cl	96(1);173.4(7)	
							O,Cl	92(1)	
				CuN_2OCl	N	1.94(2,2)	N,N	81(1)[e]	
					O	1.91(1)	N,O	91(1)[d];170(2)	
					Cl	2.233(1)	N,Cl	95(1);172.4(7)	
							O,Cl	93(1)	
Cu(salenEt$_2$)Cl	m	7.294(3)		CuN_2OCl	N	2.01(-,7)	N,N	84.6(-)[e]	487
(not given)	$P2_1/c$	12.324(6)	108.87(2)		O	1.90(-)	N,O	92.6(-)[d]	
	4	16.500(8)			Cl	2.237(-)	N,Cl	95.8(-)	
							O,Cl	94.1(-)	
Cu(salenEt$_2$)Br	or	11.623(3)		CuN_2OCl	N	2.01(-,7)	N,N	84.4(-)[e]	487
(not given)	Pbca	27.843(6)			O	1.90(-)	N,O	92.3(-)[d]	
	8	11.578(3)			Cl	2.235(-)	N,Cl	94.2(-)	
							O,Cl	90.0(-)	
[Cu(Me$_4$Brsaldim)Cl]	or	12.2720(6)		CuN_2OCl	N	2.03(2,9)	N,N	79.8(5)[e]	488
(green)	$Pna2_1$	9.5690(5)			O	1.90(2)	N,O	92.2(5)[d]	
	4	14.6585(7)			Cl	2.22(1)	N,Cl	94.5(5)	
							O,Cl	95.1(5)	
$[Cu(C_7H_{11}N_3OS_2)(H_2O)]$	m	7.748(1)		CuN_2OS	N	1.949(4,13)	N,N	82.6(3)[e]	489
(dark red)	$P2_1/b$	8.884(2)			S	2.262(1)	N,S	85.1(2)[e]	
	4	17.120(7)	92.22(3)		H_2O	1.949(1)	N,O	95.5(3)	
							O,S	96.7(2)	
$[Cu(C_6H_{10}N_4OS)(H_2O)]\cdot dmf$	m	7.140(3)		CuN_2OS	N	1.950(3,14)	N,N	83.0(2)[e]	490
(brown)	$P2_1/b$	8.933(5)			S	2.256(1)	N,S	85.2(2)[e]	
	4	24.214(9)	109.05(8)		H_2O	1.952(3)	N,O	96.2(2)	
							O,S	95.6(2)	
$[Cu(C_{16}H_{20}N_2OS)(NH_3)]$[g]	tr	16.363(7)	89.973(7)	CuN_2OS	H_3N	2.11(1)	N,N	175.7(6)	491
(not given)	P-1	5.075(1)	107.53(1)		N	1.99(1)	N,O	86.9(5)[d]	
	2	22.198(9)	98.94(3)		O	2.01(1)	N,O	91.7(5)	
					S	2.366(6)	N,S	93.3(4)[e]	
							N,S	88.2(5)	
							O,S	178.2(4)	
				CuN_2OS	H_3N	2.02(1)	N,N	175.1(6)	
					N	1.89(1)	N,O	83.5(4)[d]	
					O	2.01(1)	N,O	82.5(5)	
					S	2.149(6)	N,S	97.1(5)	
							N,S	97.0(5)	
							O,S	178.2(4)	
$[Cu(C_8H_9N_3OS)(im)]ClO_4$	m	9.863(3)		CuN_2OS	imN	1.956(4)	N,O	91.1(1)[d]	492
(dark green)	$P2_1/n$	11.155(3)	99.59(2)		N	1.945(4)	N,S	86.2(1)[e]	
	4	16.057(5)			O	1.935(3)	N,O	87.5(1)	
					S	2.251(1)	N,S	95.1(1)	
$Cu(C_{14}H_{10}N_2OS)(EtNH)$	m	7.877(2)		CuN_2OS	N	1.933(5)	N,O	93.9(2)[d]	493
(not given)	$P2_1/n$	19.948(6)	108.8(2)		EtHN	2.002(6)	N,S	85.5(2)[e]	
	4	10.379(2)			O	1.893(4)	N,S	91.2(2)	
					S	2.253(2)	O,N	89.6(2)	

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*	*L-Cu-L*			*Ref.*
$[Cu(C_{14}H_{16}N_3OS)]ClO_4$[g]	m	10.32(3)		CuN_2OS	N	1.909(9,19)	N,O	97.2(4)[d]	494
(brown green)	$P2_1/c$	11.41(3)	89.33(5)		O	1.873(8)	N,O	94.9(4)	
	2	14.34(4)			S	2.428(6)	N,S	84.1(3)[e]	
				CuN_2OS	N	1.909(9,19)	N,O	97.2(4)[d]	
					O	1.873(8)	N,O	94.9(4)	
					S	2.409(6)	N,S	85.4(3)[e]	
							N,S	84.1(3)	
$[Cu(C_{21}H_{17}N_4OS)]NO_3$	m	10.337(4)		CuN_2OS	N	1.976(6,2)	N,N	94.6(4)[d]	495
(black)	$P2_1/b$	21.010(8)			O	1.885(5)	N,O	95.7(4)[d]	
	4	9.748(3)	94.73(4)		S	2.297(2)	N,S	85.3(3)[e]	
							O,S	84.2(3)	
							N,S	176.2(4)	
							N,O	169.0(5)	
$[Cu(salenEt_2)Br]\cdot CHCl_3$	or	11.683(5)		CuN_2OBr	N	2.02(–,8)	N,N	85.4(–)[e]	487
(not given)	Pbca	28.160(10)			O	1.89(–)	N,O	92.1(–)[d]	
	8	11.746(5)			Br	2.38(–)	N,Br	93.8(–)	
							O,Br	90.0(–)	
[Cu(HOEten)Br]Br	or	16.922(5)		CuN_2OBr	N	1.979(14,29)	N,N	81.0(5)[e]	496
(not given)	$Pna2_1$	8.862(3)			O	2.038(15)	N,O	85.3(6)[e]	
	4	6.356(2)			Br	2.362(3)	N,Br	95.8(4)	
							O,Br	96.7(4)	
$Cu(C_6H_{10}N_3OS_2)Cl$	m	8.101(2)		CuN_2ClS	N	1.984(5,28)	N,N	77.2(3)[e]	497
(dark green)	$P2_1/n$	8.025(2)			S	2.264(7)	N,S	85.3(2)[e]	
	4	18.026(8)	109.68(3)		Cl	2.251(1)	N,Cl	93.4(2)	
							Cl,S	103.0(1)	
$[Cu(Hin)Cl_2]\cdot HCl$	or	9.575(–)		$CuCl_2ON$	Cl	2.248(–,11)	Cl,Cl	95.43(–)	498
(green)	$P2_12_12_1$	14.855(–)			O	2.039(–)	Cl,O	94.24(–)	
	4	7.056(–)			N	2.016(–)	Cl,N	89.23(–)	
							O,N	80.12(–)[e]	
$Cu(Me_2pyzNO)Cl_2$	m	9.340(–)		$CuCl_2ON$	Cl	2.183(–,2)	Cl,Cl	101.8(–)	422
(not given)	$P2_1/m$	6.470(–)	104.76(–)		N	2.142(–)	Cl,O	91.8(–)	
	4	7.848(–)			O	1.998(–)	Cl,N	102.2(–)	
							O,N	64.2(–1)	
$Cu(Hbz)Cl_2$	or	21.396(1)		$CuCl_2ON$	Cl	2.249(1)	Cl,Cl	97.08(4)	499
(not given)	Pbca	12.049(3)			O	1.988(3)	Cl,O	92.84(9)	
	8	7.678(3)			N	1.989(4)	Cl,N	88.5(1)	
							O,N	81.1(1)[e]	
$Cu(C_8H_{12}N_4O_5)Cl_2$	or	6.535(1)		$CuCl_2ON$	Cl	2.228(2)	Cl,Cl	95.33(6)	500
(blue)	$P2_12_12_1$	8.423(1)			O	2.045(4)	Cl,O	92.63(11)	
	4	23.313(2)			N	1.960(4)	Cl,N	91.28(3)	
							O,N	80.81(16)[e]	
$Cu(tsc)Cl_2$	m	9.161(3)		$CuCl_2NS$	Cl	2.257(1)	Cl,Cl	94.49(5)	501
(green)	$P2_1/n$	6.980(3)	99.50(4)		N	2.002(4)	Cl,S	92.02(4)	
	4	10.437(4)			S	2.266(1)	Cl,N	89.58(9)	
							N,S	86.2(1)[e]	
$Cu(tcaz)Cl_2$	tr	8.310(6)	103.9(2)	$CuCl_2NS$	Cl	2.249(5)	Cl,Cl	94.7(1)	502
(green)	P–1	8.566(5)	99.2(2)		N	2.033(7)	Cl,N	90.2(2)	
	2	5.902(5)	83.1(2)		S	2.271(5)	Cl,S	89.2(1)	
							N,S	85.3(2)[e]	
$[Cu(C_3H_6N_4S)Cl_2]\cdot H_20$	or	16.256(1)		$CuCl_2NS$	Cl	2.257(2)	Cl,Cl	94.66(6)	503
(light green)	Pbca	15.511(2)			N	2.033(5)	Cl,N	85.15(15)	
	8	7.327(1)			S	2.301(2)	Cl,S	91.74(6)	
							N,S	87.99(14)[e]	
[Cu(thiocarb)(H_2O)]	m	8.383(1)		CuS_2ON	S	2.279(2)	S,N	87.9(–,1.3)[e]	504
$(NO_3)_2\cdot H_2O$	Cc	11.024(1)	93.85(1)		N	1.945(5)	S,O	92.6(–,1.2)	
(not given)	4	18.036(3)			H_2O	1.960(6)	S,S	174.4(–)	
							O,N	177.4(–)	

TABLE I (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore*	*Cu-L*		*L-Cu-L*		*Ref.*
$Cu(tmpo)Br_2$	or	13.205(5)		$CuBr_2ON$	Br	2.270(2,0)	Br,Br	106.5(1)	505
(dark brown)	Pnma	10.200(4)			O	1.860(5)	O,N	39.3(2)[o]	
	not given	9.796(3)			N	1.998(7)			
Cu(thpuan)Cl	m	7.472(3)		CuONClS	O	2.006(8)	O,N	80.3(6)[e]	506
(green)	$P2_1/n$	8.240(4)			N	1.975(9)	O,Cl	91.4(3)	
	4	22.317(9)	114.90(4)		S	2.255(4)	N,S	84.1(4)[e]	
					Cl	2.255(3)	Cl,S	102.8(2)	

[a] Where more than one chemically equivalent distance or angle is present the mean value is tabulated. The first number in paranthesis is e.s.d. and the second is a maximum deviation from the mean value.
[b] The chemical identity of coordinated atom/ligand is specified in these columns.
[c] There are square planar (c_1) and tetrahedral (c_2) entities.
[d] Six-membered metallocyclic ring.
[e] Five-membered metallocyclic ring.
[f] There are three crystallographically independent molecules.
[g] There are two crystallographically independent molecules.
[h] Seven-membered metallocyclic ring.
[i] Eight-membered metallocyclic ring.
[j] Nine-membered metallocyclic ring.
[k] There are four crystallographycally independent molecules.
[l] Four-membered metallocyclic ring.
[m] There are monomer and dimer in the same crystal.
[n] There are tetra- and pentacoordinate species.
[o] Three-membered metallocyclic ring.

For the five-membered metallocyclic rings, the L-Cu-L angles range from 81° to 89° (mean 85°) when L = O donor ligands, from 74° to 81.5° (mean 79.5°) when L = N donor ligands with unsaturation and from 81° to 91° (mean 85.5°) when the N donor ligands are saturated. For S-donor ligands the intra-ligand angles range from 90° to 94° (mean 92°) and for a Se-donor ligand the angle is 95°.

For the six-membered metallocyclic rings, the L-Cu-L angles range from 90° to 95° (mean 93°) when L = O donor ligands and from 87° to 111° (mean 93.5°) when L = N donor ligands. The metallocyclic intraligand L-Cu-L ring angle opens with increasing size of the ring, for example for L = O donor ligands: 64.3° (four-membered) < 84.9° (five-membered) < 92.9° (six-membered); for L = N donor ligands; 67.4° (four-membered) < 79.5° (five-membered, unsaturated N) < 85.5° (five-membered, saturated N) < 93.3° (six-membered) < 96.0° (seven-membered) < 98.8° (eight-membered) < 109.5° (nine-membered).

Interestingly, in the series of copper(II) compounds in which all four-coordinate sites are occuppied by four oxygen donor atoms, only a square-planar arrangement about copper(II) is observed. There is a tendency of an elongated Cu-O bond distance with a decrease in denticity of the respective oxygen donor ligands. The mean Cu-O bond distance increases in the sequence: 1.90Å (tetradentate) < 1.92Å (bidentate) < 1.94Å (unidentate). The sum of all interatomic Cu-O bond distances follow the same trend, with the values: 7.61Å < 7.66Å < 7.75Å, respectively.

On the other hand, when nitrogen-donor atoms are present, square-planar as well as tetrahedral configurations about copper(II) atoms are formed. In the series of square-planar species, we can see the same trend of an elongated Cu-N bond distance as found for CuO_4 species, with the mean values: 1.97Å (tetradentate) < 1.99Å (bidentate) < 2.00 (unidentate). Again, the sum of all four interatomic Cu-N bond distances follow the same trend, with the mean values: 7.89Å (tetradentate) < 7.97Å(bidentate) < 8.00Å (unidentate). In the series of bi- and tetradentate N-donor ligands, Cu-N bond distances are somewhat shorter when unsaturated ligands are bonded (σ and π); than those with saturated (only σ-bonding).The mean Cu-N bond distances are: 1.94Å (tetra-unsaturated) < 1.945Å (bi-unsaturated); 2.00Å (tetra-saturated) < 2.03Å (bi-saturated). The sum of all four interatomic distances are: 7.77 *vs.* 8.00Å for the former and 7.80 *vs.* 8.11Å for the latter.

In the series of tetrahedral arrangements for copper(II) with the chromophore CuN_4 it was found that mean Cu-N bond distance increases in the sequence: 1.95Å (bidentate; unsaturated) < 1.97Å (unidentate) < 2.04Å (bidentate; saturated). The sum of all four interatomic Cu-N bond distances, follow the same trend as expected, with the values: 7.83, 7.87 and 8.08Å, respectively.

A square-planar as well as a tetrahedral arrangement was also found for $CuCl_4$ complex anions. The mean values of Cu-Cl bond distance and sum of all four interatomic distances are 2.264Å and 9.07Å for the former and 2.250Å and 9.00Å for the latter.

When sulfur-donor ligands are coordinated to copper(II), the mean values of the Cu-S and CuS_4 chromophore are 2.300Å and 9.20Å for the square-planar configuration, somewhat larger than those of 2.283 and 9.13Å found for the tetrahedral species.

However, when all four donors are bromides ($CuBr_4$) only a tetrahedral configuration about copper(II) atom is found with the mean values of Cu-Br and $CuBr_4$ chromophore of 2.394 and 9.58Å, respectively.

In complexes with mixed coordination about copper(II), the mean values of the sum of all four interatomic Cu-L bond distances for square-planar complexes for tetrahedral complexes increase with increasing covalent radius of coordinated atoms. For example: 8.15 *vs.* 8.22Å for CuN_3Cl; 8.19 *vs.* 8.26Å for CuN_3S; 7.83 *vs.* 7.81Å for CuO_2N_2; 8.55 *vs.* 8.47Å for CuN_2Cl_2; 8.58 *vs.* 8.43Å for CuN_2S_2 and 8.83 *vs.* 8.75Å for CuN_2Br_2.

There are four types of homo-donor ligands: uni-, bi-, tri- and tetradentate. The mean Cu-L bond distance in the series of unidentate ligands, increases in the sequence: 1.96Å(O) < 2.00Å(N) < 2.17Å(P) < 2.24Å(S) < 2.25Å(Cl) < 2.40Å(Br) and in the series of bidentate ligands in the order: 1.91Å(O) < 2.00Å(N) < 2.29Å(S) < 2.63Å(Se). Tri- and tetradentate ligands are only found for nitrogen-donors with mean values of 2.03 and 1.97Å, respectively.

Finally, there are three types of hetero-donor ligands: bi-, tri- and tetradentate. The mean Cu-L bond distance for bidentate ligand are: 1.91 and 2.00Å (O and N); 1.92 and 2.26Å (O and S); 2.01 and 2.25Å (N and S). For complexes of tridentate ligands

TABLE IA Summary of the mean Cu(I) —L and Cu(II) —L bond lengths [Å] in tetra - coordinates derivatives

Ligand Donor	*Atom LX Donor*	*Coval. Radius [Å]*	*Unidentate Cu(I)/Cu(II)*	*Bidentate Cu(I)/Cu(II)*	*Tridentate Cu(I)/Cu(II)*	*Tetradentate Cu(I)/Cu(II)*
L – O	0.73	2.245/1.96	2.17/1.91			
L – N	0.75	2.04/2.00	2.03/1.99	2.08/2.03	2.055/1.97	
Cl	0.99	2.34/2.25				
L – S	1.02	2.34/2.24	2.34/2.29	2.331–	2.30/–	
L – P	1.06	2.30/2.17	2.32/–	2.29/–		
Br	1.14	2.48/2.40				

the values are: 1.98 and 1.94Å (two O and N); 1.91 and 2.00Å (O and two N); 1.96 and 2.26Å (two N and S); 1.95 and 2.28Å (N and two S); and 1.92, 1.95 and 2.25Å (O, N and S). For tetradentate ligands the values are: 1.91 and 1.95Å (pairs of O and N) and 1.88, 1.93 and 2.38Å (O, two N and S).

A summary of the mean Cu(I)-L and Cu(II)-L distances are gathered in Table IA. In general, the mean Cu(I)-L bond distances are longer than those of Cu(II)-L. This reflects the difference in Pauling ionic radii of Cu(I) (0.96Å) and Cu(II) (0.70Å).

Some four-coordinate copper(II) compounds were studied at two different temperature, $Cu(NCS)_2(4\text{-Mepy})_2$,[70] $[Cu(Et_2en)_2]\ (ClO_4)_2$,[79] $(MePhEtNH)_2[CuCl_4]$[162] and $Cu(C_{21}H_{26}NO_3)_2$.[307–308] The $Cu(NCS)_2(4\text{-Mepy})_2$ complex which contains three crystallographically independent molecules was studied[70] at room temperature and at 180K. The mean Cu-N bond distances decrease with decreasing temperature. The values are 1.95Å (NCS) and 2.04Å (pyridine) at room temperature and 1.93 and 2.02Å at 180K. Interestingly, the $[Cu(Et_2en)_2]\ (ClO_4)_2$ complex[79] at 298K is triclinic but at 333K is monoclinic. The mean Cu-N bond distance is the same for both forms (2.03Å).

The $(MePhEtNH)_2[CuCl_4]$ complex[162] is square-planar at 298K (mean Cu-Cl, 2.265(1) Å), but when the temperature increases (353K) the Cu(II), becomes tetrahedral with a mean Cu-N bond distance of 2.219(4) Å.

Finally, the complex $Cu(C_{21}H_{26}NO_3)_2$ was studied at 173K[307] and at 223K[308] at the higher temperature, two crystallographically independent molecules are present. The mean Cu-O and Cu-N distances (values of 1.90 and 2.02Å at 173K) are somewhat longer than those observed at 1.88 and 2.00Å at 223K.

There is an example, $[Cu(H_2bim)_2]Cl_2[Cu(H_2bim)Cl_2]_2$[113] which contains a monomeric complex with the CuN_4 chromophore and a dimeric form with the CuN_2Cl_2 chromophore.

Two monomers, with the chromophores CuN_4 and CuN_2Cl_2, were found in $[Cu(azaH)_4][Cu(azaH)_2Cl_2]$.[444]

Some four-coordinate copper(II) compounds occur in two isomeric forms which differ primarily by degree of distortion involving both Cu-L distances and L-Cu-L angles.[50–53, 76, 108, 147, 148, 183, 195, 361, 453] Two independent molecules have been found to be

present in one crystal in several cases.[101, 104, 112, 123, 149, 171, 175,176, 187, 194, 200, 201, 210, 230, 261, 271, 293, 303, 304, 308, 310, 321, 326, 334, 345, 361, 377, 381, 395, 411, 427, 485, 491, 494] In some cases three such independent molecules have been found[69, 70, 378] and even four.[187] There is one example of a complex which exhibits *cis*- and *trans*- isomerism.[144, 146]

Another two examples[162, 163] exhibit configuration isomerism between square planar and tetrahedral.

3 PENTACOORDINATE COPPER(II) COMPLEXES

Crystallographic and structural data for penta-coordinate copper(II) compounds are given in Table II. Two types of geometry are observed, the more common square pyramidal and the less common trigonal bipyramidal. There are almost four hundred examples of square pyramidal complexes (Table IIA). The square pyramidal environments around Cu(II) are built up from unidentate ligands to pentadentate ligands. The apical position of the square pyramid is occupied by 'hard' donor ligands; oxygen donors, nitrogen donors or chloride atoms; by 'borderline' bromide atoms and by 'soft' donor ligands; sulphur donors, carbon donors and iodide atoms. Oxygen donor ligands are most common. The mean Cu-L(apical) distance of unidentate ligands increases in the sequence: 2.098Å(CN) < 2.263Å(NL) < 2.330Å(OL) < 2.514Å(Cl) < 2.627Å(Br) < 2.652Å(SL) < 2.883Å(I). In general, the mean Cu-L(apical) bond distances are longer than Cu-L(equatorial) bond distances and increase in the sequence: 1.974Å(N) < 1.976Å(O) < 2.273Å(S) < 2.285Å(Cl) < 2.408Å(Br) < 2.563Å(I).

In general, the mean Cu-L(equatorial) bond distances are somewhat shorter than those for Cu-L(apical). The mean Cu-N(equatorial) *vs.* Cu-N(apical) bond distances for ligands of different denticity are: 1.974 *vs.* 2.263Å (unidentate), 2.003 *vs.* 2.204Å (tetradentate); 2.005 *vs.* 2.254Å (tridentate): 2.015 *vs.* 2.220Å (bidentate); 2.022 *vs.* 2.183Å (pentadentate).

There is a correlation between the Cu-L(apical) distance and the displacement of the Cu(II) atom from the basal plane of the square planar donor atoms towards the apical ligand. When the displacement increases, the Cu-L(apical) decreases, when L is Cl, S or I. For example, 0.2 and 2.635(1) Å,[363] 0.24 and 2.633 (2) Å,[627] 0.27 and 2.404(3) Å,[628] 0.46 and 2.399(1) Å,[625] 0.55 and 2.37Å,[626] when L is a chloride; 0.13 and 2.88(1) Å,[633] 0.37 and 2.607(2) Å,[632] 0.43 and 2.424(1) Å,[631] when L is unidentate S donor; and 0.1 and 2.806(2) Å,[641] 0.31 and 2.785(1) Å,[639] and 0.38 and 2.742(2) Å,[640] when L is an iodide atom.

However, when L is an oxygen or nitrogen donor ligand, no such correlation was found. There are at least two reasons for this, the denticity of the ligands vary from uni- to pentadentate and the ligands vary from 'pure' σ-donor to π-acceptor as well.

The displacement of the Cu(II) atom from the basal plane ranges from 0.01 to 0.53Å, when the apical ligand is an oxygen donor and from 0.05 to 0.96Å, when the apical ligand is a nitrogen donor (Table IIA).

TABLE II Crystallographic and structural data for penta-coordinated copper(II) compounds[a]

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
A: SQUARE-PYRAMIDAL									
$[Cu(C_5H_6N_2O)_5](ClO_4)_2$ (blue)	tr P–1 2	15.635(2) 9.343(1) 12.273(1)	98.16(1) 120.26(1) 106.05(1)	CuO_5 0.12	O_{eq} O_{ap}	1.945(6,10)[b] 2.239(6)	O_{eq},O_{eq} O_{eq},O_{ap}	89.8(3,4.9)[b] 172.0(3,5) 93.4(3,3.3)	507
$Cu(Cl_3ac)_2(H_2O)_3$ (blue)	m C2/c 4	23.082(3) 6.253(1) 9.726(2)	 94.67(1) 	CuO_5 0.11	O_{eq} H_2O_{eq} H_2O_{ap}	1.954(4,0) 1.968(4,0) 2.183(5)	O_{eq},O_{eq} O_{eq},O_{ap}	89.9(2,7) 173.6(2,4.8) 93.2(2,2.4)	508
$[Cu3\text{–}OHbenz)_2 \cdot (H_2O)_3] \cdot 5H_2O$ (not given)	or $Cmc2_1$ 4	24.24(2) 11.47(1) 7.265(1)	 	CuO_5 0.015	O_{eq} H_2O_{eq} H_2O_{eq}	1.947(5,0) 1.963(6,0) 2.341(12)	O_{eq},O_{eq} O_{eq},O_{ap}	91.2(4,2.5) 161.5(4,7.3) 97.2(4,18.8)	509
$Cu(phex)_2(H_2O)_3$[c] (green blue)	tr P–1 4	6.40(1) 9.28(2) 32.01(6)	100.7(10) 78.5(1) 90.12(10)	CuO_5 CuO_5	O_{eq} H_2O_{eq} H_2O_{ap} O_{eq}	1.972(15,13) 2.029(14,9) 2.261(15) 1.958(16.4)	O_{eq},O_{eq} O_{eq},O_{ap} O_{eq},O_{eq}	90.2(6,3.7) 172.8(6,4.0) 92.1(5,8.2) 90.2(6,2.4)	510
					H_2O_{eq} H_2O_{ap}	2.071(13,3) 2.280 (17)	 O_{eq},O_{ap}	172.3(6,4.3) 92.2(6,7.9)	
$Ba[Cu(pth)_2(H_2O)_2] \cdot 2H_2O$ (light blue)	m $P2_1$ 2	9.155(9) 7.831(8) 13.498(14)	 95.1(1) 	CuO_5	O_{eq} H_2O_{eq} H_2O_{ap}	1.942(9.35) 1.971(10,0) 2.289(9)	O_{eq},O_{eq} O_{eq},O_{ap}	84.0(3)[d] 91.0(3,3.8) 166.5(3,1.1) 96.5(3,6.8)	511
$Cu(faxy)_2(bpyO)_2 \cdot (H_2O)$ (green)	tr P–1 2	11.944(6) 10.731(5) 8.643(4)	112.35(2) 100.45(2) 92.14(2)	CuO_5	O_{eq} $bpyO_{eq}$ H_2O_{ap}	1.95(2x) 1.98(–,1) 2.31(1)	O_{eq},O_{eq} O_{eq},O_{ap}	95.6(1,2.7) 166.5(1) 86.6(1,4.4)	512
$Cu(F_3acac)_2(Menit)$ (red)	tr P–1 2	10.119(5) 12.159(6) 11.814(5)	115.13(1) 85.30(1) 68.42(1)	CuO_5 0.14	O_{eq} O_{ap}	1.925(4,17) 2.303(3)	O_{eq},O_{eq} O_{eq},O_{ap}	92.4(1,7)[e] 87.1(1,1) 171.3(1,3.7) 94.3(1,5.3)	513
$Cu(ftbd)_2(Me_2SO)$ (not given)	tr P–1 2	9.940(3) 10.497(2) 11.907(2)	82.58(2) 84.04(2) 77.93(2)	CuO_5	O_{eq} Me_2SO_{ap}	1.928(5,17) 2.265(5)		not given	514
$Cu(F_6acac)_2(tmpo)$ (not given)	tr P–1 2	9.900(1) 11.862(2) 13.416(3)	87.34(1) 99.72(1) 122.95(1)	CuO_5 1.01	$tmpoO_{eq}$ O_{eq} O_{ap}	1.920(5) 1.959(6,49) 2.162(6)	O_{eq},O_{eq} O_{eq},O_{ap}	91.1(2)[e] 89.9(1,1.7) 163.6(2,14.2) 86.5(2)[e] 89.1(2,3.1) 123.9(2)	515
$Cu(F_6acac)(Phnit)$[c] (dark brown)	tr P–1 4	11.346(5) 14.115(6) 20.129(9)	70.12(3) 76.68(4) 75.20(3)	CuO_5 CuO_5	$nitO_{eq}$ O_{eq} O_{ap} $nitO_{eq}$	1.932(4) 1.930(5,25) 2.167(7) 1.948(7)	O_{eq},O_{eq} O_{eq},O_{ap} O_{eq},O_{ap}	92.0(3)[e] 89.3(2,4.3) 168.4(2,8.5) 89.2(2)[e] 108.2(3,8)	516
					O_{eq} O_{ap}	2.022(7,39) 1.908(9,5)	 O_{eq},O_{ap} O_{ap},O_{ap}	143.5(2) 91.3(3,1.1)[e] 88.1(3,3.7) 175.5(3)	
$(C_4H_{16}N_3)[Cu(ox)_2 \cdot (NO_3)] \cdot 2H_20$ (blue)	m $P2_1/c$ 4	10.235(2) 11.077(3) 14.885(4)	 104.10(2) 	CuO_5	oxO_{eq} O_2NO_{ap}	1.938(3,4) 2.467(4)	O_{eq},O_{eq}	85.5(1,6)[d]	56g
$K[Cu(NH_3)_5](PF_6)_3$ (not given)	or Imma 4	14.90(1) 11.79(1) 10.57(1)	 	CuN_5	H_3N_{eq} H_3N_{ap}	2.029(19,19) 2.193(22)	N_{eq},N_{eq} N_{eq},N_{ap}	89.0(2) 94.6(7,4)	517a

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(im)_5][PPhO_3]\cdot 4H_2O$ (dark blue)	m $P2_1/c$ 4	14.134(5) 9.229(3) 24.150(8)		CuN_5 9 0.21	Neq N_{ap}	2.041(5,21) 2.230(5)	N_{eq},N_{eq} N_{eq},N_{ap}	89.4(2,2.7) 168.0(2,6) 95.9(2,1.4)	517b
$Cu(pys)_2(NH_3)_2$ (dark green)	or $Pn2_1a$ 4	13.915(5) 14.356(5) 12.659(5)		CuN_5	H_3Neq Neq N_{ap}	1.989(11,95) 2.275(18.204) 2.377(10)	N_{eq},N_{eq} $N_{eq}N_{ap}$	62.0(5)[g] 96.1(5,9.5) 151.4(5,6.9) 100.0(4,16.9)	518a
$Cu(3\text{–}Mepy)_3(NCS)_2$ (green)	m Pc 2	9.027(7) 9.021(7) 14.958(50)	114.08(4)	CuN_5	N_{eq} SCN_{eq} SCN_{ap}	2.03(1,3) 1.97(1) 2.19(1)	N_{eq},N_{eq} N_{ap},N_{eq} N_{ap},N_{eq}	89.35(40,45) 167.75(40,3.15) 95.33(40,1.57) 98.7(4)	518b
$Cu(3,4\text{–}Me_2py)_3(NCS)_2$ (green)	m Pc 2	9.825(7) 9.740(7) 14.130(60)	108.80(40)	CuN_5	N_{eq} SCN_{eq} SCN_{ap}	2.017(1,37) 1.98(1) 2.22(2)	N_{eq},N_{eq} N_{ap},N_{eq}	89.68(50,1.25) 171.05(50,55) 94.77(50,2.47)	518b
$[Cu(en)_2(NCS)]Br$ (dark violet)	or Pnam 4	7.224(5) 15.573(12) 10.429(5)		CuN_5	N_{eq} SCN_{ap}	2.015(10,5) 2.67(1)	N_{eq},N_{eq}	85.1(1.0,0)[d]	519
$[Cu(Meen)_2(NCS)](NCS)$ (not given)	m $P2_1/n$ 4	12.038(4) 14.080(6) 8.805(3)	98.98(3)	CuN_5 0.18	N_{eq} SCN_{ap}	2.054(13,25) 2.238(14)	N_{eq},N_{eq}	84.35(5,5)[d]	520
$[Cu(apip)_2(NCS)]\cdot(C10_4)$ (blue)	or $P2_12_12_1$ 4	14.721(2) 15.652(2) 7.754(1)		CuN_5 0.16	N_{eq} SCN_{ap}	2.036(8,7) 2.239(8)	N_{eq},N_{eq} N_{eq},N_{ap}	89.7(3,5.4) 94.5(3,3.3)	521
$[Cu(phen)_2\cdot(3,5\text{–}Me_2py)](C10_4)_2$ (blue)	m $P2_1/n$ 4	18.430(3) 9.122(2) 18.744(8)	97.92(3)	CuN_5 0.256	Me_2pyN_{eq} $phenN_{eq}$ $phenN_{ap}$	2.036(10) 2.046(13,73) 2.134(13)	N_{eq},N_{eq} N_{eq},N_{ap}	81.3(5)[d] 91.9(4,2.4) 165.0(5,5.4) 77.1(5)[d] 104.0(5,7.7)	522
$[Cu(bpy)_3](ClO_4)_2$ (purple blue)	tr P–1 2	7.904(1) 11.029(2) 18.741(4)	79.69(2) 89.88(1) 82.15(2)	CuN_5 0.15	N_{eq} N_{ap}	2.026(6,12) 2.222(7)	N_{eq},N_{eq} N_{eq},N_{ap}	170.2(3,5.4) 78.0(3)[d] 97.9(3,5.3)	523
Cu(dpt)$(NCS)_2$ (blue)	m $P2_1/a$ 2	7.58(2) 14.12(2) 13.58(2)	113.2(3)	CuN_5	N_{eq} SCN_{eq} SCN_{ap}	2.03(1,5) 2.04(1) 2.14(1)	N_{eq},N_{eq} N_{eq},N_{ap}	91.8(4,1)[e] 86.3(4,8) 162.4(4,8.6) 99.2(4,7.5)	524
Cu(den)$(NCS)_2$ (blue)	m $P2_1/n$ 4	11.24(2) 14.02(2) 7.32(2)	97.5(3)	CuN_5 0.17	N_{eq} SCN_{eq} SCN_{ap}	2.02(1,2) 1.97(1) 2.26(1)	N_{eq},N_{ap} N_{eq},N_{ap}	82.8(6,5)[d] 96.4(6,8) 94.9(6,3.2)	525
Cu(pzmet)$(NCS)_2$ (green)	or $P2_12_12_1$ 4	15.795(3) 20.433(3) 9.618(1)		CuN_5	SCN_{eq} N_{eq} N_{ap}	1.97(6,1) 1.998(5,4) 2.246(6)	N_{eq},N_{eq} N_{eq},N_{ap}	90.0(2,2.1) 165.7(2,13.4) 89.7(2)[e] 103.9(2,3.0)	526
Cu(terpy)$(N_3)_2$ (not given)	m $P2_1/n$ 4	8.071(3) 11.893(2) 16.318(6)	100.23(3)	CuN_5 0.25	N_{eq} $(N_3)_{eq}$ $(N_3)_{ap}$	2.019(14,8) 1.960(17) 2.207(16)	N_{eq},N_{eq} N_{eq},N_{ap}	79.4(5,1.0)[d] 98.8(6,4.7) 160.1(6,3.6) 97.2(6,2.9)	527
$Cu(9\text{–}aneN_3)(N_3)_2$ (green)	m $P2_1/n$ 4	13.626(3) 7.875(2) 14.415(5)	113.11(2)	CuN_5	$(N_3)_{eq}$ N_{eq} N_{ap}	1.987(2,4) 2.054(2,19) 2.238(2)	N_{eq},N_{eq} N_{eq},N_{ap}	84.5(1)[d] 91.8(1,3.4) 82.3(1,4)[d] 106.9(2,8.5)	528a
$[Cu(terpy)(NCO)_2]_2\cdot 2H_2O$ (not given)	tr P–1 2	8.864(3) 9.485(6) 10.774(7)	83.58(5) 87.21(4) 68.44(3)	CuN_5	N_{eq} OCN_{eq} OCN_{ap}	2.015(7,58) 1.904(7) 2.188(7)	N_{eq},N_{eq} N_{eq},N_{ap}	79.3(3,9)[d] 88.9(3,10.5) 98.3(3,4.1) 158.0(3,1.2)	528b

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(dien)(tph)]\cdot 2H_2O$ (dark blue)	m $P2_1/c$ 4	18.379(3) 8.263(4) 15.958(8)	99.98(3)	CuN_5 0.248	N_{eq} $pthN_{eq}$ $pthN_{ap}$	2.036(3,16) 2.007(3) 2.391(3)	N_{eq},N_{eq} N_{eq},N_{ap}	83.4(2,2)[d] 95.5(2,1.2) 164.3(2,10.6) 97.9(2,10.6)	529
$Cu(Me_5dien)(ncb)_2$ (blue)	or Pbca 8	14.749(2) 17.604(3) 13.907(3)		CuN_5 0.363	N_{eq} $ncbN_{eq}$ $ncbN_{ap}$	2.057(3,45) 1.980(4) 2.153(3)	N_{eq},N_{eq} N_{eq},N_{ap}	85.5(1,3)[d] 91.6(1,7) 159.7(1,7.8) 100.1(1,7.0)	530
$[Cu(den)(bpy)](NO_3)_2\cdot 2H_2O$ (blue–black)	m $P2_1/c$ 4	10.29(5) 7.60(5) 28.59(5)	106.9(5)	CuN_5 0.24	N_{eq} $bpyN_{eq}$ $bpyN_{ap}$	2.026(6,24) 2.012(6) 2.192(6)	N_{eq},N_{eq} N_{eq},N_{ap}	84.9(2,1.3)[d] 94.0(2,2) 165.3(2,7.5) 78.4(2)d 103.6(2,5.7)	531
$[Cu(den)(phen)](NO_3)_2$ (blue)	m C2/c 8	25.97(5) 8.13(5) 19.72(5)	100.0(5)	CuN_5 0.24	N_{eq} $phenN_{eq}$ $phenN_{ap}$	1.988(22,15) 2.058(18) 2.224(20)	N_{eq},N_{eq} N_{eq},N_{ap}	85.2(9,4)[d] 93.8(8,2.8) 164.8(8,9.4) 77.8(8)[d] 103.7(9,7.2)	531
[Cu(bipyam)·(dpt)]$(NO_3)_2$ (black blue)	m $P2_1/a$ 4	16.8(5) 12.33(5) 10.42(5)	99.(5)	CuN_5 0.32	N_{eq} $bipN_{eq}$ N_{ap}	2.028(15,19) 2.034(15) 2.164(15)	N_{eq},N_{eq} N_{eq},N_{ap}	85.1(6)[d] 93.9(6)[e] 87.7(6,2.8) 161.8(6,2.9) 89.2(6)[e] 102.1(6,9.4)	532
$[Cu(dpt)(bpy)](NO_3)_2$ (black–blue)	or Pbca 8	13.96(5) 13.02 22.58(5)		CuN_5 0.28	N_{eq} $bpyN_{eq}$ $bpyN_{ap}$	2.024(15,12) 2.033(15) 2.218(15)	N_{eq},N_{eq} N_{eq},N_{ap}	86.3(6)[d] 93.1(6)[e] 89.8(6,8) 163.8(6,12.9) 77.0(6)[d] 104.4(6,8.8)	532
[Cu(dien)(bipyam)]·$Cl_2.2H_2O$ (not given)	m $P2_1/c$ 4	7.78(2) 9.75(3) 28.01(5)	115.0(5)	CuN_5 0.32	N_{eq} $bipN_{eq}$ $bipN_{ap}$	2.009(14,21) 1.955(13) 2.125(13)	N_{eq},N_{eq} N_{eq},N_{ap}	85.1(6,3)[d] 92.0(6,4) 160.8(5,1.8) 90.4(5)[e] 102.5(5,4.5)	533
[Cu(dien)(bipyam)]·$(ClO_4)_2.H_2O$ (not given)	m $P2_1/c$ 4	15.683(5) 7.621(5) 21.044(9)	121.42(2)	CuN_5 0.34	N_{eq} $bipN_{eq}$ $bipN_{ap}$	2.033(7,18) 1.994(6) 2.169(5)	N_{eq},N_{eq} N_{eq},N_{ap}	84.3(3,5)[d] 93.0(3,2.1) 159.9(1,8.0) 90.2(3)[e] 103.1(3,1.8)	533
$(Cu(ibo)_2]Cl_2$ (dark blue)	m $P2_1/c$ 4	13.453(2) 16.121(2) 8.835(1)	114.66(1)	CuN_5 0.18	N_{eq} N_{ap}	1.975(3,39) 2.357(4)	N_{eq},N_{eq} N_{eq},N_{ap}	81.0(1,1.1)[d] 98.2(1,9) 165.6(2,8.1) 76.5(1)[d] 102.9(1,7.1)	534
$[Cu(tmbc)(N_3)](ClO_4)$ (green)	tr P–1 2	15.649(3) 10.463(3) 7.531(2)	88.71(1) 100.37(1) 91.5(1)	CuN_5 0.210	N_{eq} $(N_3)_{ap}$	2.084(4,9) 2.160(5)	N_{eq},N_{eq} N_{eq},N_{ap}	83.3(2,3)[d] 95.6(2,1)[e] 168.3(2,6) 95.8(2,4.0)	535
[Cu(doct)(NCS)]·(ClO_4)[c] (not given)	or $Pca2_1$ 8	23.90(4) 8.56(2) 14.71(3)		CuN_5	N_{eq} SCN_{ap}	2.04(3,6) 2.12(3)	N_{eq},N_{eq} N_{eq},N_{ap}	86(1,3)[d] 95(1) 155(1,11) 102(1,14)	536
				CuN_5	N_{eq} SCN_{ap}	2.04(3,6) 2.19(3)	N_{eq},N_{eq} N_{eq},N_{ap}	85(1,3)[d] 97(1) 157(1,10) 101(1,6)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
[Cu(tim)(NCS)](PF$_6$)	or	12.003(4)		CuN_5	N_{eq}	1.942(8,22)	N_{eq},N_{eq}	82.2(4,2)[d]	537
(deep-blue)	Pnam	15.365(6)			SCN_{ap}	2.384(13)		97.7(3)	
	4	11.500		0.07				176.5(4)	
							N_{eq},N_{ap}	91.7(4,2.0)	
Cu(tim)(1-Meim)]·(PF$_6$)$_2$	not given			CuN_5	N_{eq}	1.988(3,0)	N_{eq},N_{eq}	80.46(15)[d]	538
					imN_{ap}	2.139(3)		94.00(14)	
(blue)				0.44				162	
Cu(cyclopsf)(NCO)	m	13.552(4)		CuN_5	N_{eq}	2.001(7,11)	N_{eq},N_{eq}	79.7(2,1)[d]	539
(dark green)	$P2_1/c$	11.818(4)	113.69(1)		OCN_{ap}	2.038(6)		90.6(3,2.5)[e]	
	4	11.634(5)		0.96			N_{eq},N_{ap}	107.0(3,4.3)	
[Cu($C_{23}H_{31}N_5$)](C10$_4$)$_2$	m	9.170(4)		CuN_5	N_{eq}	1.961(17,1)	N_{eq},N_{eq}	88.1(7,1.6)[d]	540a
(blue-purple)	$P2_1/c$	17.059(6)	111.91(5)			2.063(22,6)		158.0(7,6.5)	
	2	19.024(6)			N_{ap}	2.220(13)	N_{eq},N_{ap}	94.8(6,3.8)[e]	
								107.0(7,2.8)	
[Cu(quep)](C10$_4$)$_2$	tr	14.196(8)	74.16(2)	CuN_5	$quepN_{eq}$	1.999(1,80)	N_{eq},N_{eq}	90.0(7)[e]	540b
(blue-black)	P-1	10.958(6)	75.55(2)		$quepN_{ap}$	2.134(1)		81.9(7,4.2)[d]	
	2	9.177(6)	88.95(2)					88.9(7,12.9)	
								158.8(7,3.6)	
							N_{eq},N_{ap}	90.0(7)[e]	
								99.6(7,16.7)	
[Cu(dap)](C10$_4$)$_2$	or	17.358(4)		CuN_5	N_{eq}	2.049(13,31)	N_{eq},Neq	86.3(5)[d]	541
(blue)	Pbca	14.262(3)			N_{ap}	2.251(12)		92.6(6,2.4)[e]	
	8	16.533(4)		0.116				87.8(5)	
								173.1(7,2)	
							N_{eq},N_{ap}	82.8(6,1.9)[d]	
								103.5(6,1.9)	
[Cu(Me$_4$rol)](C1O$_4$)$_2$·	or	17.332(5)		CuN_5	N_{eq}	2.063(8,48)	N_{eq},N_{eq}	85.9(3,7)[d]	542
H_2O	$P2_12_12_1$	15.448(5)			N_{ap}	2.082(8)		146.5(3,12.1)	
(blue)	4	9.066(4)					N_{eq},N_{ap}	106.8(3,12.1)	
[Cu($C_{17}H_{20}ON_7$)](ClO$_4$)·	m	25.6516(21)		CuN_5	N_{eq}	1.975(5,23)	N_{eq},N_{eq}	80.6(2,1)[d]	543
1.61H_2O	C2/c	8.0487(7)	118.114(5)			2.069(5,56)		92.5(2)[e]	
(blue)	8	23.7624(17)		0.062	N_{ap}	2.167(6)		101.2(2)	
								152.8(2,8.2)	
							N_{eq},N_{ap}	91.4(2)[e]	
								105.0(2,17)	
Cu(p-3a)[c]	tg	17.075(9)		CuN_5	N_{eq}	2.00(3,14)	N_{eq},N_{eq}	80(1,2)[d]	544
(dark-blue)	$P3_121$				N_{ap}	2.23(3)		95(1)	
	6	21.289(11)						159(1,1)	
							N_{eq},N_{ap}	102(1,8)	
				CuN_5	N_{eq}	2.04(3,24)	N_{eq},N_{eq}	79(1,2)[d]	
					N_{ap}	2.31(3)		96(1)	
							N_{eq},N_{ap}	103(1,9)	
[Cu(diaza)](PF$_6$)$_2$	m	14.145(11)		CuN_5	N_{eq}	1.930(14)	N_{eq},N_{eq}	84.3(8,3.7)[d]	545
(not given)	$P2_1/c$	9.030(6)	90.9(3)			2.096(25,49)		109.2(6)	
	4	16.743(11)		0.17	N_{ap}	2.133(18)		157.0(8,5.9)	
							N_{eq},N_{ap}	84.2(6,5)[d]	
								110.8(7,12.9)	
[Cu(penoc)](PF$_6$)$_2$	or	12.931(8)		CuN_5	N_{eq}	1.90(1)	N_{eq},N_{eq}	83.0(8,2.7)[d]	546a
(not given)	$P2_12_12_1$	16.604(12)				2.05(1,5)		110.2(6)	
	4	11.441(9)			N_{ap}	2.10(1)		157.1(8,6.2)	
							N_{eq},N_{ap}	83.9(8,2)[d]	
								114.2(8,10.3)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(C_{19}H_{23}N_7)]\cdot(BF_4)_2$ (blue green)	m $P2_1/c$ 4	12.431(9) 14.024(6) 14.296(11)		CuN_5	N_{eq} N_{ap}	2.02(1,9) 2.20(2)	N_{eq},N_{eq}	78.7(6,1.6)[d] 92.4(6)[e] 89.2(6,17.9) 154.4(6,3.2)	546b
							N_{eq},N_{ap}	81.5(6)[e] 99.4(6,17.9)	
$[Cu(C_{13}H_{18}N_7OBr)]BF_4$ (deep blue)	or Pbca 8	15.041(8) 17.733(7) 15.206(6)		CuN_5 0.23	N_{eq} N_{ap}	2.08(3,22) 2.19(2)	N_{eq},N_{eq}	74.2(9,8.5)[d] 91.6(9)[e] 117.5(8) 159(1,2)	547
							N_{eq},N_{ap}	83.8(7)[d] 101.8(7,5.5)	
$[Cu(17\text{–}aneN_5)][CuBr_4]$ (dark blue)	m Pn 2	9.088(2) 11.692(1) 9.832(5)	90.28(3)	$CuBr_4$		Br not given			232
				CuN_5	N_{eq} N_{ap}	2.07(2,5) 2.29(4)	N_{eq},N_{eq}	85.3(8,4)[d] 99.7(9)	
							N_{eq},N_{ap}	83.3(8)[d] 91.6(10)	
(ampi)$[CuCl_5]\cdot 2H_2O$ (dark green)	m $P2_1/a$ 4	17.991(6) 9.249(3) 9.560(3)	98.14(5)	$CuCl_5$	Cl_{eq} Cl_{ap}	2.312(2,28) 2.570(2)	Cl_{eq},Cl_{eq}	89.0(3,1.4) 165.0(1,1)	548a
							Cl_{eq},Cl_{ap}	97.4(3,2.8)	
$Cu(bs\text{–}glyNO)(H_2O)_3$ (pale blue)	m $P2_1/c$ 4	12.736(4) 10.292(5) 10.402(3)	109.41	CuO_4N 0.21	O_{eq} N_{eq} H_2O_{eq} H_2O_{ap} O_{ap}	1.936(3) 1.966(4) 1.947(3,3.8) 2.270(3)	O_{eq},O_{eq} O_{eq},N_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	88.7(1,1.9) 83.6(1)[d] 96.3(1) 93.4(1,6.4) 105.1(1)	363
$Cu(tsgly)(H_2O)_3$ (blue)	m $P2_1/c$ 4	13.690(1) 10.333(1) 10.556(1)	109.03(1)	CuO_4N 0.22	N_{eq} O_{eq} H_2O_{eq} H_2O_{ap}	1.964(6) 1.931(4) 1.970(4,34) 2.259(4)	O_{eq},O_{eq} N_{eq},O_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	87.4(2) 167.2(2) 83.3(2)[d] 89.6(2,6.3) 167.7(2) 92.3(2,6.1) 106.8(2)	548b
$[Cu(napox)(H_2O)_3]\cdot 2H_2O$ (brown)	tr P–1 2	7.387(5) 11.543(6) 8.953(7)	93.95(5) 104.05(8) 92.60(5)	CuO_4N	N_{eq} O_{eq} H_2O_{eq} H_2O_{ap}	1.963(7) 1.951(5) 1.462(7,6) 2.257(5)	N_{eq},O_{eq} O_{eq},O_{eq} N_{eq},O_{ap} O_{eq},O_{ap}	82.7(2)[d] 92.4(3) 102.1(3) 93.5(3,1.3)	549
Cu(Mephimac) $(H_2O)_2$ (blue green)	or $P2_1/c$ 4	12.523(2) 7.481(2) 15.126(4)		CuO_4N 0.13	H_2O_{eq} O_{eq} N_{eq} H_2O_{ap}	1.962(4) 1.935(4,3) 2.049(5) 2.424(4)	O_{eq},N_{eq} O_{eq},O_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	85.3(1,6)[d] 94.3(1,2.6) 92.5(2,3.3) 102.3(2)	550
$[Cu(acrp)_2(py)]\cdot H_2O$ (green)	or Pnma 4	14.275(2) 13.095(2) 14.904(2)		CuO_4N	O_{eq} pyN_{ap}	1.909(5,2) 2.310(8)	O_{eq},O_{eq}	90.0(2,0)[e] 89.4(2,8) 167.2(2,1.0)	551
							O_{eq},N_{ap}	96.4(2,6)	
Cu(4–Mequinox)$_2$(py) (dark red)	m $P2_1/c$ 4	8.192 14.717 15.734	101.2	CuO_4N	O_{eq} pyN_{ap}	1.983(–,20) 2.161	not given		552
$Cu(camph)_2(2\text{–}Mepy)$ (not given)	or $P2_12_12_1$ 4	16.660(3) 14.172(2) 10.979		CuO_4N 0.11	O_{eq} pyN_{ap}	1.964(13,17) 2.203(14)	O_{eq},O_{eq}	93.1(5,6)[e] 88.5(5,4.7)	553
							O_{eq},N_{ap}	98.7(5,10.0)	
$Cu(acac)_2(4\text{–}NH_2py)$ (green)	m $P2_1/c$ 4	8.36(3) 14.75(3) 14.35(3)	112.14(20)	CuO_4N 0.22	pyN_{eq} O_{eq} O_{ap}	2.010(8) 1.943(7,9) 2.165(6)	O_{eq},O_{eq} O_{eq},N_{eq} O_{eq},O_{ap}	89.5(3,4.3) 91.8(3)[e] 88.6(3) 92.4(2)[e] 97.8(2,5.4)	554
							N_{eq},O_{ap}	92.7(3)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$Cu(acac)_2(qu)$	tr	14.23(3)	94.0(2)	CuO_4N	$acacO_{eq}$	1.96(1,2)	O_{eq},O_{eq}	93.5(5,4)[e]	555
(blue)	P-1	8.66(2)	89.4(2)		quN_{ap}	2.36(1)		90.7(5,5.6)	
	2	8.02(2)	110.8(2)	0.2			O_{eq},N_{ap}	93.8(5,3.6)	
$[Cu(Me_2enO)(ox)] \cdot 2H_2O$	tr	6.207(3)	103.32(7)	CuO_4N	oxO_{eq}	1.963(4,3)	O_{eq},O_{eq}	84.1(1)[d]	556
(blue-violet)	P-1	8.960(7)	94.44(7)		$enOO_{eq}$	1.947(4)		86.7(2,2.6)	
	2	11.627(12)	104.38(6)	0.06	$enON_{ap}$	1.984(5)	N_{eq},O_{eq}	96.1(2)[e]	
								93.5(2,2.6)	
							$O_{eq}O_{ap}$	91.2(2,4.5)	
							$N_{eq}O_{ap}$	93.2(2)	
$Cu(slth)(H_2O)_2$[c]	m	6.68(4)		CuO_4N	O_{eq}	1.94(1,2)	O_{eq},O_{eq}	90.1(5,1.3)	557
(green)	$P2_1$	13.640(4)	90.88(4)		N_{eq}	1.95(1)	O_{eq},N_{eq}	83.2(5)[d]	
	4	14.646(8)		0.17	H_2O_{eq}	1.96(1)		89.3(5,6.1)	
					H_2O_{ap}	2.42(1)		95.3(5)[e]	
							O_{eq},O_{ap}	96.5(4,1.3)	
							N_{eq},O_{ap}	91.2(4)	
				CuO_4N	O_{eq}	1.95(1,3)	O_{eq},O_{eq}	90.3(4,1.2)	
					N_{eq}	1.93(1)	O_{eq},N_{eq}	83.2(5)[d]	
				0.18	H_2O_{eq}	1.97(1)		88.8(5,5.6)	
					H_2O_{ap}	2.34(1)		94.3(4)[e]	
							O_{eq},O_{ap}	96.0(4,2.6)	
							N_{eq},O_{ap}	93.6(4)	
$Cu(niphen)_2(2\text{-}Mepy)$	tr	10.537(10)	93°18′(10)	CuO_4N	O_{eq}	1.93(7,3)	O_{eq},O_{eq}	87.0(6)	558
(deep green)	P-1	8.624(10)	94°20′(10)		pyN_{eq}	1.98(7)		88.5(6,2.5)	
	2	12.089(10)	92°21′(10)	0.17	O_{ap}	2.16(7)		91.0(6)[e]	
							N_{eq},O_{eq}	91.0(6,4.0)	
							O_{eq},O_{ap}	87.0(6)[e]	
							N_{eq},O_{ap}	95.0(6)	
$Cu(salam)(H_2O)$[c]	m	12.30(1)		CuO_4N	N_{eq}	1.966(10)	O_{eq},O_{eq}	90.2(4,1.3)	559
(green)	$P2_1/c$	8.45(1)	91.0(5)		O_{eq}	1.931(10,17)	O_{eq},N_{eq}	84.2(4)[d]	
	8	23.84(2)		0.198	H_2O_{eq}	1.996(9)		89.5(4,5.3)	
					O_{ap}	2.385(11)		94.7(4)[e]	
							O_{eq},O_{ap}	96.0(4,10.2)	
							O_{ap},N_{eq}	92.1(4)	
				CuO_4N	N_{eq}	1.956(10)	O_{eq},O_{eq}	90.7(4,1.6)	
					O_{eq}	1.926(10,16)	O_{eq},O_{eq}	84.2(4)[d]	
				0.198	H_2O_{eq}	1.982(9)		89.3(4,5.1)	
					O_{ap}	2.302(10)		94.4(4)[e]	
							O_{eq},O_{ap}	96.6(4,13.0)	
							O_{ap},N_{eq}	91.8(4)	
$[Cu(bgH)_2][Cu(acac) \cdot Cl]_2$	or	15.218(2)		CuO_4Cl	O_{eq}	1.925(2,8)	O_{eq},O_{eq}	93.8(1,1)[e]	363
	Pbca	15.986(3)			Cl_{ap}	2.635(1)		85.1(1,5)	
(blue green)	4	14.565(3)		0.2			O_{eq},Cl_{ap}	95.8(1,1.1)	
				CuN_4	N	1.936(3,3)	N,N	88.2(1)[e]	
								91.8(1)	
$[Cu(pyrem)(pz)(BF_4)] \cdot BF_4$	tr	8.489(1)	100.01(2)	CuN_4F	N_{eq}	1.983(4,67)	N_{eq},N_{eq}	81.9(2,1)[d]	560
	P-1	8.829(2)	106.19(2)		pzN_{eq}	1.948(4)		98.3(2,6)	
(blue)	2	13.189(4)	96.42(1)		F_{ap}	2.517(3)	N_{eq},F_{ap}	89.5(2,3.05)	
$[Cu(NH_3)_4(H_2O)] \cdot (18\text{-crown-}6)(PF_6)_2$	or	19.275(2)		CuN_4O	H_3N_{eq}	2.035(10.5)	not given		561
	Cmcm	10.018(1)			H_2O_{ap}	2.29(1)			
(not given)	4	14.672(1)							
$[Cu(NH_3)_4SO_4] \cdot H_2O$	or	10.6509(7)		CuN_4O	H_3N_{eq}	2.032(6,1)	N_{eq},N_{eq}	90.7(1,3.8)	562a
(deep blue)	Pnma	11.9860(16)			O_3SO_{ap}	2.339(9)	N_{eq},O_{ap}	94.0(1,2.6)	
	4	7.0690(3)		0.2					
$[Cu(3,5\text{-}Me_2pz)_4 \cdot (H_2O)] \cdot (ClO_4)_2$[c]	m	19.783(5)		CuN_4O	pzN_{eq}	2.03(2)	N_{eq},N_{eq}	89(2)	562b
	C2	16.271(6)	134.98(3)		H_2O_{ap}	2.26(2)			
(violet)	4	13.994(6)							
				CuN_4O	pzN_{eq}	1.97(2)	N_{eq},N_{eq}	91(2)	
					H_2O_{ap}	2.30(2)			

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$Cu(fuc)_2(NH_3)_2(H_2O)$	m	5.705(1)		CuN_4O	H_3N_{eq}	1.991(2,14)	N_{eq},N_{eq}	90.3(–,1.2)	563
(blue)	$P2_1/m$	7.590(2)			$fucN_{eq}$	2.046(2,0)		165.9(1)	
	2	16.240(4)	92.78(4)	0.085	H_2O_{ap}	2.509(2)	O_{ap},N_{eq}	96.8(1,8.1)	
$[Cu(3,5\text{-}Me_2py)_2 \cdot$	tr	9.391(2)	74.8(2)	CuN_4O	pyN_{eq}	2.008(2,2)	N_{eq},N_{eq}	81.3(1)[d]	564
$(phen)(H_2O)](ClO_4)_2$	P–1	12.457(2)	87.95(2)		$phenN_{eq}$	2.024(2,8)		89.2(1,7.9)	
(purple)	2	13.448(3)	79.46(1)	0.237	H_2O_{ap}	2.238(2)		165.6(1,8)	
							N_{eq},O_{ap}	96.7(1,6.0)	
$Cu(pq1)_2(H_2O)$	tr	12.20(1)	91.7(1)	CuN_4O	N_{eq}	1.994(4,27)	N_{eq},N_{eq}	82.1(3)[d]	565
(green)	P–1	13.91(1)	112.7(1)		H_2O_{eq}	2.014(4)		87.8(3,5.7)	
	2	7.35(1)	103.9(1)	0.17	N_{ap}	2.245(4)	O_{eq},N_{eq}	91.7(3,6)	
							N_{eq},N_{ap}	76.9(2)[d]	
								90.8(3,13.9)	
							N_{ap},O_{eq}	95.1(3)	
$Cu(dgx)_2(H_2O)$	tr	10.190(5)	105.75(1)	CuN_4O	N_{eq}	1.944(19,23)	N_{eq},N_{eq}	79.9(6,8)[d]	566
(not given)	P–1	10.851(4)	96.76(4)		H_2O_{ap}	2.141(14)		88.9(7,9.8)	
	2	13.883(6)	115.26(4)				O_{ap},N_{eq}	98.0(7.5.0)	
$[Cu(pcx)_2(HO)]Cl_2$	m	16.854(7)		CuN_4O	N_{eq}	1.990(3,19)	N_{eq},N_{eq}	79.6(1)[d]	567
(green)	C2/c	7.091(3)	106.39(4)		H_2O_{ap}	2.248(4)		102.1(1)	
	4	14.879(8)		0.289			N_{eq},O_{ap}	94.8(1,8.4)	
$[Cu(pad)_2(H_2O)]Cl_2$	m	21.672(1)		CuN_4O	N_{eq}	1.985(2,16)	N_{eq},N_{eq}	79.7(1,0)[d]	568
(dark green)	C2/c	4.615(1)	106.58(1)		H_2O_{ap}	2.238(4)	N_{eq},O_{ap}	94.9(1,8.3)	
	8	13.398(1)		0.11					
$[Cu(zimid)_2(H_2O)]Cl_2 \cdot$	tr	10.020(2)	104.63(2)	CuN_4O	N_{eq}	2.004(8,34)	N_{eq},N_{eq}	82.1(4,3)[d]	569
$2H_2O$[c]	P–1	14.384(2)	111.04(1)		H_2O_{ap}	2.208(12)		89.4(4,8.4)	
(blue)	2	7.205(1)	84.93(2)					165.8(4,7.8)	
							O_{ap},N_{eq}	97.5(4,4.7)	
				CuN_4O	N_{eq}	2.002(9,32)	N_{eq},N_{eq}	81.0(4,2)[d]	
					H_2O_{ap}	2.202(12)		89.5(4,8.7)	
								166.2(4,7.9)	
							O_{ap},N_{eq}	96.9(4,5.0)	
$Cu(pspz)_2(H_2O)] \cdot$	m	25.176(7)		CuN_4O	N_{eq}	2.005(9,12)	N_{eq},N_{eq}	89.0(4)[e]	570
$(ClO_4)_2 \cdot 3.3H_2O$	C2/c	12.642(1)	122.63(2)		H_2O_{ap}	2.136(11)		89.4(4,4)	
(blue)	4	13.908(4)						165.9(4,7.0)	
							O_{ap},N_{eq}	97.1(3,3.5)	
$[Cu(Me_2tn)_2(H_2O)] \cdot$	tr	13.196(3)	116.39(2)	CuN_4O	N_{eq}	2.013(3,48)	N_{eq},N_{eq}	91.6(1,1.2)[e]	385
$[Cu(pba)] \cdot 3H_2O$	P–1	11.088(2)	116.89(3)		H_2O_{ap}	2.357(3)		89.3(1,1.1)	
(blue)	2	11.6501(2)	79.52(2)					166.15(1,8.95)	
							N_{eq},O_{ap}	94.6(1,14.1)	
				CuO_2N_2	O	1.940(4,22)	O,O	93.4(1)	
					N	1.913(4,24)	N,N	97.9(1)[e]	
							O,N	84.3(1,8)[d]	
$[Cu(C_7H_{18}N_2)_2(H_2O)] \cdot$	m	10.257(2)		CuN_4O	N_{eq}	2.007(3,3)	not given		91
$(HCO_3)_2 \cdot 0.5H_2O$	$P2_1/n$	13.196(2)	102.20(1)			2.116(4,5)			
(blue)	4	17.124(3)			H_2O_{ap}	2.209(3)			
$[Cu(C_7H_{18}N_2)_2 \cdot$	m	8.633(3)		CuN_4O	N_{eq}	2.054(17,45)	not given		91
$(C_4H_4O_5)] \cdot 2H_2O \cdot MeOH$	$P2_1/c$	18.399(8)	91.55(3)		O_{ap}	2.225(9)			
(blue)	4	17.458(7)							
$[Cu(Me\text{-}tsc)_2(SO_4)] \cdot$	m	11.080(3)		CuN_4O	N_{eq}	1.990(–,41)	N_{eq},N_{eq}	81.2(2,8)[d]	571
$2H_2O$[c]	$P2_1/a$	17.688(5)			O_3SO_{ap}	2.023		89.6(2,9.0)	
(blue)	8	15.293(4)	98.07(2)				N_{eq},O_{ap}	95.4(2,12.3)	
				CuN_4O	N_{eq}	1.979(–,41)	N_{eq},N_{eq}	82.1(2,3)[d]	
					O_3SO_{ap}	2.516		89.7(2,9.1)	
							N_{eq},O_{ap}	94.2(2,11.2)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(Me\text{-}1,3\text{-}pn)_2(NO_3)]\cdot NO_3$ (blue)	tr P-1 2	7.855(6) 9.145(4) 12.494(7)	103.39(4) 94.73(5) 113.51(4)	CuN_4O 0.21	N_{eq} O_2NO_{ap}	2.038(2,29) 2.330(2)	N_{eq},N_{eq}	91.4(1,9)[e] 89.9(1,2.3) 167.9(1,10.6)	572
							N_{eq},O_{ap}	96.0(1,10.9)	
$Cu(1,3\text{-}pn\text{-}2\text{-}o1)_2\cdot(Cl_2ac)$ (dark blue)	or Cmca 8	11.170(8) 26.482(12) 12.794(7)		CuN_4O 0.31	N_{eq} O_{ap}	2.026(13,4) 2.268(15)	N_{eq},N_{eq}	88.8(5,0)[e] 89.4(5.6) 165.0(5)	573
							N_{eq},O_{ap}	97.5(5,6.2)	
$[Cu(pmdp)_2(trt)]\cdot C_3H_6O$ (not given)	tr P1 1	8.253(4) 8.402(3) 10.428(6)	83.63(3) 94.68(6) 106.44(4)	CuN_4O 0.186	Neq $trtO_{ap}$	2.055(50,25) 2.23(4)	N_{eq},N_{eq}	83.6(4,4)[d] 89.8(4,9.4) 168.7(3,7.0)	574
							N_{eq},O_{ap}	95.3(3,7.8)	
$[Cu(bpy)_2(imsuc)]\cdot 0.5fH\cdot 5H_2O$ (blue)	tr P-1 2	12.649(3) 12.161(2) 13.431(2)	115.51(1) 110.66(2) 90.01(2)	CuN_4O 0.18	imO_{eq} N_{eq} N_{ap}	1.996(7) 2.01(1,3) 2.17(1)	N_{eq},N_{eq}	81.6(4)[d] 87.4(4,5.8)	575
							O_{eq},N_{eq}	92.9(4,1.1)	
							O_{eq},N_{ap}	96.4(4)	
							N_{eq},N_{ap}	93.9(4,23.9)	
$[Cu(pmdp)_2(lac)]lac\cdot H_2O$ (dark blue)	m $P2_1$ 2	8.764(3) 18.571(7) 8.617(2)	100.69(2)	CuN_4O 0.33	N_{eq} $pmdpN_{eq}$ O_{ap}	2.054(11,45) 2.067(10,42) 2.157(8)	N_{eq},N_{eq}	83.3(4,3)[d] 88.7(4,5.7)	576
							N_{eq},O_{ap}	99.4(4.4.9)	
$Cu(azam)(NCS)_2$ (blue)	m $P2_1/n$ 4	9.548(2) 15.814(3) 10.660(2)	91.89(2)	CuN_4O 0.14	O_{eq} N_{eq} SCN_{eq} SCN_{ap}	2.012(4) 2.013(5,42) 1.962(4) 2.328(4)	O_{eq},N_{eq}	90.2(2)[e] 89.3(2,1.01)	577
							N_{eq},N_{eq}	87.1(2)[d] 90.2(2,5.2)	
							O_{eq},N_{ap}	98.5(2)	
							N_{eq},N_{ap}	92.9(2)	
$[Cu(dien)(4,4'\text{-}bpy)\cdot(H_2O)](ClO_4)_2$ (dark blue)	tr P-1 2	16.221(4) 10.270(3) 6.975(8)	105.53(5) 97.96(5) 74.75(3)	CuN_4O 0.068	$dienN_{eq}$ pyN_{eq} H_2O_{ap}	2.019(7,24) 2.023(6) 2.351(7)	N_{eq},N_{eq}	83.9(3,1)[d] 88.0(3,8.1) 169.9(3,8.8)	578
							N_{eq},O_{ap}	91.0(3)	
$[Cu(dien)(thym)(H_2O)]\cdot Br\cdot 2H_2O$ (purple)	m $P2_1/n$ 4	6.341(1) 12.840(8) 20.805(12)	95.50(3)	CuN_4O 0.159	$dienN_{eq}$ $thymN_{eq}$ H_2O_{ap}	2.017(3,23) 1.989(3) 2.465(3)	N_{eq},N_{eq}	84.0(1,4)[d] 89.7(1,7.5) 168.5(1,5.8)	579
							O_{ap},N_{eq}	94.3(1,6.0)	
$Na[Cu(dien)(5\text{-}imp)\cdot(H_2O)]\cdot 9H_2O$ (purple)	or $P2_12_12_1$ 2	8.706(4) 21.074(12) 12.171(7)		CuN_4O	$dienN_{eq}$ $impN_{eq}$ H_2O_{ap}	1.946(11,105) 1.917(5) 2.875(8)	N_{eq},N_{eq}	85.0(4,7.4)[d] 92.9(4,5) 174.3(3)	580
							N_{eq},O_{ap}	88.8(4,3.6)	
$[Cu(bpy)(Im)]NO_3\ H_2O$ (not given)	or $Pna2_1$ 4	11.437(3) 23.849(4) 6.680(1)		CuN_4O 0.10	$bpyN_{eq}$ N_{eq} O_{ap}	1.990(10,27) 1.982(9.8) 2.316(9)	N_{eq},N_{eq}	81.5(4)[d] 91.7(4,10.2) 157.8(4,9.8)	581
							N_{eq},O_{ap}	78.6(4)[d] 94.9(4,23.2)	
$[Cu(phen)(saltb)]NO_3$ (not given)	m $P2_1/n$ 4	13.055(3) 9.722(4) 17.633(4)	103.03(3)	CuN_4O	$salthN_{eq}$ $salthO_{eq}$ N_{eq} N_{ap}	1.966(5.5) 1.927(5) 2.024(5) 2.261(6)	N_{eq},N_{eq}	79.5(2,9)[d] 83.8(2,8.8)	582
							N_{eq},O_{eq}	91.5(2)[e] 93.1(2.1.6)	
							O_{eq},N_{ap}	96.0(2)	
							N_{eq},N_{ap}	102.7(2,2.8)	
$[Cu(phen)(ggly)]\cdot 3H_2O$ (deep blue)	tr P-1 2	7.842(1) 9.395(2) 13.763(4)	74 64(2) 72.00(2) 75.76(2)	CuN_4O 0.15	$gglyN_{eq}$ $gglyO_{eq}$ N_{eq} N_{ap}	1.971(5,69) 2.008(4) 2.009(5) 2.275(5)	N_{eq},N_{eq}	82.9(2)[d] 91.4(2,8.5)	583
							N_{eq},O_{eq}	82.0(2)[d] 88.1(2,6.1)	
							N_{eq},N_{ap}	78.3(2)[d] 94.6(2,16.4)	
							O_{eq},N_{ap}	96.2(2)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
[Cu(2,9–Me_2phen) · (gly)] · 5H_2O (deep blue)	m P2/c 4	9.591(4) 14.478(3) 17.238(5)	 114.79(2) 	CuN_4O 0.25	$glyN_{eq}$ $glyO_{eq}$ N_{eq} N_{ap}	1.975(2,75) 2.033(2) 2.013(2) 2.263(2)	N_{eq},N_{eq} O_{eq},N_{eq} N_{eq},N_{ap} N_{ap},O_{eq}	82.58(9)[d] 90.3(9,7.7) 81.67(8)[d] 78.47(7)[d] 95.9(1,17.4) 99.7(1,5.1)	584
Cu(tppb)(pt) (green)	tr P–1 2	11.835(2) 12.062(2) 12.831(2)	66.91(1) 83.68(1) 77.10(1)	CuN_4O 0.38	ptN_{eq} ptO_{eq} N_{eq} N_{ap}	2.033(3) 1.968(2) 2.003(3,17) 2.218(2)	N_{eq},N_{eq} N_{eq},N_{ap} O_{eq},N_{eq}	92.05(9)[c] 92.6(1,5.5) 92.05(9)[c] 92.7(9,1.3) 83.10(9)[d] 86.7(9,3.6) 89.8(3,11.0)	585
Cu(ggly)(ctd)[e] (not given)	m $P2_1$ 4	4.716(3) 26.86(6) 14.761(14)	 90.63(6) 	CuN_4O 	$glyN_{eq}$ N_{eq} O_{ap}	1.96(–,9) 2.01 2.74		not given	586
Cu(hepor)(H_2O) (not given)	or Pbca 8	8.795(3) 19.515(5) 23.658(6)	 	CuN_4O 0.09	N_{eq} H_2O_{ap}	2.05(1,5) 2.33		not given	587
[Cu(edp)(H_2O)] ·H_2O[e] (violet blue)	m $P2_1/c$ 8	17.298(15) 13.505(9) 14.119(22)	 115.8(2) 	CuN_4O CuN_4O	N_{eq} H_2O_{ap} N_{eq}	1.920(7,6) 2.056(7,4) 2.361(8) 1.920(7,9)	N_{eq},N_{eq} N_{eq},O_{ap} N_{eq},N_{eq}	82.0(3,4)[d] 81.2(3,5) 159.7(3,2.0) 99.8(3,14.9) 82.1(3,7)[d]	588
					H_2O_{ap}	2.050(7,9) 2.317(8)	N_{eq},O_{eq}	81.1(3,4) 158.1(3,3.2) 99.4(3,15.0)	
Cu(pcxb)(H_2O) (dark green brown)	tr P–1 2	7.443(3) 9.560(2) 11.197(4)	92.63(2) 100.02(2) 84.50(2)	CuN_4O 0.19	N_{eq} H_2O_{ap}	1.987(2,47) 2.286(2)	N_{eq},N_{eq} N_{eq},O_{ap}	82.5(1,3)[d] 91.7(1,19.7) 162.2(1,1.1) 96.4(1,8.0)	589
[Cu(pcxt)(H_2O)] ·2H_2O (blue violet)	m $P2_1/c$ 4	9.094(10) 17.620(7) 12.141(7)	 91.9(1) 	CuN_4O 0.19	N_{eq} H_2O_{ap}	1.980(6,48) 2.338(5)	N_{eq},N_{eq} N_{eq},O_{ap}	82.15(20,5)[d] 89.5(2,20.7) 162.45(20,2.05) 95.75(20,3.75)	590
[Cu(Me_3pcx)(H_2O)] · 2H_2O (not given)	m $P2_1/c$ 4	11.730(5) 13.097(7) 12.668(5)	 119.59(3) 	CuN_4O 0.263	N_{eq} H_2O_{ap}	1.999(5,69) 2.369(1)	N_{eq},N_{eq} O_{ap},N_{eq}	81.3(6,1)[d] 94.4(6)[e] 97.7(2,9.8)	591
[Cu(mecyclo)(H_2O)] · 0.5$HClO_4$ ·0.5H_2O (violet)	m C2/c 8	38.317(2) 9.701(2) 15.734(7)	 97.81(2) 	CuN_4O 0.07	N_{eq} H_2O_{ap}	2.057(18,50) 2.552(16)	N_{eq},N_{eq} O_{ap},N_{eq}	86.6(8,1.0)[d] 93.4(8,1.4)[e] 90.0(8,4.8) 92.0(7,3.3)	592
α–[Cu(bppn)(H_2O) · 2H_2O (deep blue)	m $P2_1/c$ 4	11.719(2) 13.092(2) 12.663(2)	 119.56(1) 	CuN_4O 0.27	N_{eq} H_2O_{ap}	1.997(2,63) 2.361(2)	N_{eq},N_{eq} N_{eq},O_{ap}	81.15(10,5)[d] 94.5(1)[e] 89.3(1,11.0) 97.8(1,9.8)	593
β–[Cu(bppn)(H_2O) · 2H_2O (deep blue)	m $P2_1/n$ 4	6.939(9) 12.615(16) 19.472(20)	 97.15(8) 	CuN_4O 0.24	N_{eq} H_2O_{ap}	2.009(5,65) 2.268(4)	N_{eq},N_{eq} O_{ap},N_{eq}	81.1(2,1)[d] 93.7(2)[e] 89.2(2,8.2) 96.9(2,5.9)	594
[Cu(pcxc)(H_2O) ·H_2O (blue violet)	m C2/c 8	19.985(8) 11.114(3) 17.581(5)	 112.5(1) 	CuN_4O 0.19	N_{eq} H_2O_{ap}	1.980(8,55) 2.382(7)	N_{eq},N_{eq} O_{ap},N_{eq}	82.4(3,1.5)[d] 89.5(3,21.5) 96.7(3,13.7)	595
(Cu(pcxt)(H_2O)] ·H_2O (violet blue)	m C2/c 8	19.239(9) 12.136(4) 16.351(6)	 108.5(1) 	CuN_4O 0.21	N_{eq} H_2O_{ap}	1.986(9,59) 2.303(8)	N_{eq},N_{eq} N_{eq},O_{ap}	82.1(3,1.4)[d] 81.7(3,1) 96.9(3,6.8)	596

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(Meimol)(H_2O)] \cdot (ClO_4)_2$ (blue green)	tr P–1 2	11.343(5) 11.770(4) 8.452(2)	109.71(2) 91.25(2) 98.24(3)	CuN_40 0.185	N_{eq} H_2O_{ap}	1.999(3,9) 2.341(3)	N_{eq},N_{eq}	82.2[d] 92.2[e] 92.1(–,9.9) 168.3(–,3.1)	597
							N_{eq},O_{ap}	94.5(–,6.6)	
$[Cu(texa)(H_2O)] \cdot (ClO_4)_2$ (red)	or Pnma 4	18.683(2) 8.897(1) 13.558(2)		CuN_40 0.25	N_{eq} H_2O_{ap}	1.992(4,2) 2.342(6)	N_{eq},N_{eq}	84.3(3,3.1)[d] 100.5(3)[e] 93.4(3,12.2) 162.7(3)	598
							N_{eq},O_{ap}	97.7(2,6.7)	
$[Cu(texa)(NO_3)](ClO_4)$ (blue)	or Pnma 4	20.417(5) 9.033(4) 10.870(2)		CuN_40 0.34	N_{eq} O_2NO_{ap}	2.001(10,6) 2.20(2)	N_{eq},N_{eq}	83.8(6,4.0)[d] 98.2(5)[e] 93.4(3,12.2) 162.7(3)	598
							N_{eq},O_{ap}	97.7(2,6.7)	
$[Cu(niaza)(H_2O)] \cdot (ClO_4)$ (blue)	or Pbca 8	14.625(4) 19.083(2) 17.476(4)		CuN_4O 0.25	N_{eq} H_2O_{ap}	2.048(9,12) 2.215(9)	N_{eq},N_{eq}	73.3(3)[d] 94.4(4,4.9)[e] 89.2(4,15.9) 164.8(4,1.7)	599
							N_{eq},O_{ap}	97.2(4,4.3)	
$[Cu(C_8H_{16}N_4O_2)(H_2O)] \cdot H_2O$ (violet)	m $P2_1/c$ 4	6.795(7) 16.872(8) 12.103(13)	118.02(8)	CuN_4O	N_{eq} H_2O_{ap}	1.992(7,48) 2.772(6)	N_{eq},N_{eq}	84.6(2)[d] 92.4(2,6)[e] 90.5(2,5.9)	600
$[Cu(pqp)(H_2O)](ClO_4)_2$ (not given)	or Pbca 8	24.671(6) 13.938(5) 15.376(6)		CuN_4O 0.14	N_{eq} H_2O_{ap}	2.025(6,1) 2.307(6)	N_{eq},N_{eq}	80.8(2,1.1)[d] 89.7(2,26.7) 159.9(2,1)	601
$[Cu(niaza)(H_2O)] \cdot (ClO_4)_2 \cdot H_2O$ (purple)	or Pbca 8	19.144(8) 17.499(5) 14.635(5)		CuN_4O	N_{eq} H_2O_{ap}	2.056(9,16) 2.259(8)	N_{eq},N_{eq}	73.0(3)[d] 94.5(4,5.0)[e] 89.1(4,6.1) 163.2(3,1.8)	602
							O_{ap},N_{eq}	97.4(3,4.6)	
$[Cu(pyram)(H_2O)] \cdot (BF_4)_2$ (blue)	tr P–1 2	9.967(6) 12.957(3) 9.473(3)	91.24(3) 103.46(4) 106.70(3)	CuN_4O 0.178	N_{eq} H_2O_{ap} N_{ap}	2.029(2,85) 2.070(2) 2.172(2)	N_{eq},N_{eq} N_{eq},O_{eq} N_{ap},O_{eq} N_{eq},N_{ap}	93.49(8,6.23)[e] 97.35(9,10.1) 88.19(8,1.8) 92.27(8) 95.55(9,3.03)	603
$[Cu(C_{14}H_{32}N_4)(H_2O)] \cdot (ClO_4)_2 \cdot H_2O$ (dark blue)	m $P2_1/c$ 4	9.784(3) 14.081(3) 16.958(5)	91.26(3)	CuN_4O 0.22	N_{eq} H_2O_{ap}	2.075(6,34) 2.398(3)	N_{eq},N_{eq}	85.6(2,7)[d] 94.1(2,1)[e] 89.8(2,4.3) 166.4(2,11.8)	604
							N_{eq},O_{ap}	96.8(2,10.1)	
$[Cu(quen)(H_2O)] \cdot (ClO_4)_2$ (blue–black)	m Cc 4	18.657(9) 9.951(5) 17.157(8)	128.59(2)	CuN_4O	N_{eq} H_2O_{ap}	1.990(3,46) 2.394(3)	N_{eq},N_{eq}	82.6(3)[d] 90.0(3,7)[e] 90.3(3,8.3) 167.2(3,2.8)	540b
							O_{ap},N_{eq}	92.3,(3,9.8)	
$[Cu(quen)(H_2O)](BF_4)_2$ (blue–black)	trg $P3_2$ 3	10.180(3) 20.322(7)		CuN_4O	N_{eq} H_2O_{ap}	1.985(1,74) 2.375(1)	N_{eq},N_{eq}	82.9(5)[d] 90.4(5,4)[e] 90.4(5,7.5) 167.1(3,3.8)	540b
							O_{ap},N_{eq}	92.3(5,6.8)	
$[Cu(amet)(ClO_4)ClO_4 \cdot 0.5H_20$ (blue)	or Pbca 8	13.939(3) 16.169(6) 15.325(5)		CuN_4O	N_{eq} O_3ClO_{ap}	2.023(8,27) 2.539(7)	$N_{eq}N_{eq}$	85.1(3)[d] 91.7(4,1.6)[e] 90.1(4,5.0) 177.8(4,1.5)	605
							O_{ap},N_{eq}	90.2(3,5.9)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(tepa)(NO_2)]PF_6$ (green)	m $P2_1/c$ 4	11.817(8) 13.124(6) 15.692(7)	 92.39(4) 	CuN_4O	ONO_{eq} N_{eq} N_{ap}	2.012(5) 2.057(5,26) 2.253(5)	N_{eq},N_{eq} O_{eq},N_{eq} N_{eq},N_{ap} O_{eq},N_{ap}	91.8(2,2.4) 170.1(2) 87.3(2,6) 166.9(2) 93.9(2,4.5)[e] 94.6(2)	606
$[Cu(tepa)(NO_3)]NO_3$ (not given)	m $P2_1/c$ 4	13.706(3) 7.837(3) 20.963(2)	 90.29(4) 	CuN_4O	O_2NO_{eq} N_{eq} N_{ap}	2.044(11) 2.050(13,52) 2.202(12)	N_{eq},N_{eq} N_{eq},N_{ap} N_{eq},O_{eq} O_{eq},N_{ap}	91.4(5,2.7)[e] 170.5(5) 100.9(5)[e] 87.5(5,4) 166.4(5) 92.4(4)	607
$[Cu(12\text{-}aneN_4)(NO_3)] \cdot NO_3$ (not given)	m $P2_1/n$ 4	12.00(1) 13.76(1) 8.86(2)	 90.10(3) 	CuN_4O 0.5	Neq O_2NO_{ap}	2.016(6,7) 2.183(4)	N_{eq},N_{eq} N_{eq},O_{ap}	86.3(2,1.3)[d] 150.4(2,1.3) 104.8(2,3.0)	608
$[Cu(tmbc)(ClO_4)]ClO_4$ (blue)	m $P2_1/c$ 4	15.187(1) 10.487(3) 16.668(4)	 100.77(1) 	CuN_4O 0.089	N_{eq} O_3ClO_{ap}	2.072(6,14) 2.219(5)	N_{eq},N_{eq} N_{eq},O_{ap}	84.1(2,2)[d] 95.7(3,1)[e] 174.7(4,5) 92.6(3,3.8)	535
$[Cu(azdec)(ClO_4)]ClO_4$ (blue)	m $P2_1/n$ 4	7.440(1) 14.678(3) 16.903(3)	 90.485(1) 	CuN_4O 0.014	N_{eq} O_3ClO_{ap}	2.043(6,14) 2.530(5)	N_{eq},N_{eq}	92.5(3,2.8)[e] 84.4(2)[d] 90.0(2,5.6)	609a
$[Cu(beeda)(ClO_4)]ClO_4$ (blue)	m $P2_1/n$ 4	10.985(4) 24.497(6) 9.784(4)	 112.89(3) 	CuN_4O	N_{eq} O_3ClO_{ap}	1.98(3,5) 2.61(5)	N_{eq},N_{eq}	92.0(9,5.8)[d] 93.1(9,6.9) 151.5(3,4.5)	609b
$[Cu(diclo)(dmf)].(ClO_4)_2$ (not given)	m P2/c 4	19.806(6) 11.422(3) 16.401(4)	 95.26(3) 	CuN_4O	N_{eq} $dmfO_{ap}$	2.039(10,32) 2.205(12)		not given	610
$[Cu(pea)(N_3)]H_2O$ (black)	m $P2_1/c$ 4	9.529(4) 18.950(21) 13.829(5)	 109.38(5) 	CuN_4O 0.23	$(N3)_{eq}$ N_{eq} O_{eq} N_{ap}	2.004(26) 2.077(23,50) 1.928(14) 2.162(24)	N_{eq},N_{eq} N_{eq},N_{ap} N_{eq},O_{eq} O_{eq},N_{ap}	89.0(8)[d] 91.4(9,2.4) 90.6(9)[e] 96.4(11,6.6) 95.2(8)[e] 87.2(9.8.0) 98.1(7)	611
$Cu(C_{24}H_{36}N_{10}O_6) \cdot H_2O$ (green)	or $Cmc2_1$,Cmcm 4	16.331(2) 15.319(2) 15.336(4)	 	CuN_4O 0.17	N_{eq} H_2O_{ap}	1.892(3,5) 2.67(1)	N_{eq},N_{eq} N_{eq},O_{ap}	84.7(6)[d] 93.9(518)[e] 89.3(6,4.6) 167.1(8) 96.4(6,5.9)	612
$[Cu(C_{16}H_{34}N_{10}O_3(H_2O)] \cdot 4H_2O.3/4NH_4ClO_4$ (purple)	m $P2_1/c$ 4	9.373(2) 14.34(2) 26.129(4)	 105.25(1) 	CuN_4O 0.15	N_{eq} H_2O_{ap}	1.87(1,2) 2.74(1)	N_{eq},N_{eq} N_{eq},O_{ap}	84.8(8,13)[d] 94.6(9,2)[e] 89.7(9,5.2) 170.8(11,1.7) 94.6(8,2.0)	612
$[Cu(buox)(H_2O)]_2 \cdot [(buox)_2](ClO_4)_4$[c] (not given)	m $P2_1/c$ 8	13.425(2) 21.446(3) 14.349(4)	 104.4.(5) 	CuN_4O 0.27 CuN_4O	N_{eq} H_2O_{ap} N_{eq} H_2O_{ap}	2.001(7,43) 2.287(4) 1.996(4,46) 2.300(4)	N_{eq},N_{eq} N_{eq},O_{ap} N_{eq},N_{eq} N_{eq},O_{ap}	80.0(2,4)[d] 104.6(2)[h] 89.7(2,14.9) 92.8(3) 79.3(2.7)[d] 94.5(2) 106.7(2)[h] 93.9(2,6.0)	613
$[Cu(procyclo)](ClO_4)_2$ (not given)	m $P2_1/n$ 4	9.685(9) 17.339(6) 15.437(4)	 92.99(4) 	CuN_4O 0.21	N_{eq} O_{ap}	2.074(3,10) 2.224(11)	N_{eq},N_{eq} O_{ap},N_{eq}	167.2(5,12.7) 95.6(5,9.8) 88.5(4)[e]	614

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(phcyclo)](ClO_4)_2 \cdot 0.5H_2O$ (not given)	m C2/c 8	27.450(8) 16.495(3) 16.783(3)	 125.46(3) 	CuN_4O 0.30	N_{eq} O_{ap}	2.080(12,16) 2.161(9)	N_{eq},N_{eq} O_{ap},N_{eq}	163.4(5,13.5) 92.7(4)[e] 98.3(5,9.9)	614
$[Cu(toxa)][(ClO_4)_2$ (purple blue)	or Pbca 8	16.494(3) 18.188(3) 14.330(2)	 	CuN_4O 0.033	N_{eq} O_{ap}	2.037(8,28) 2.335(6)	N_{eq},N_{eq} N_{eq},O_{ap}	84.6(4,1.7)[d] 94.5(3,1.6)[e] 90.3(4,5.7) 172.0(4,1.4) 81.9(3,3)[d] 90.8(3,16.2)	615
$[C(azaxa)](ClO_4)_2$ (redish blue)	m $P2_1/n$ 4	13.880(2) 15.122(3) 10.463(20)	 97.95(1) 	CuN_4O 0.039	N_{eq} O_{ap}	2.040(14,19) 2.275(9)	N_{eq},N_{eq} N_{eq},O_{ap}	86.2(6.1)[d] 93.8(5,9)[e] 90.0(6,4.7) 177.8(6,3) 81.3(5,1.0)[d] 91.0(5,10.7)	615
$[Cu(hyaza)](ClO_4)_2$ (purplish blue)	m $P2_1/c$ 4	10.367(3) 13.104(5) 16.079(6)	 93.28(3) 	CuN_4O 0.111	N_{eq} O_{ap}	2.013(12,31) 2.259(8)	N_{eq},N_{eq} N_{eq},O_{ap}	85.0(4,1.6)[d] 94.8(5,1.1)[e] 89.9(5,6.5) 173.4(7,2.5) 81.7(4,1.7)[d] 93.3(6,15.8)	615
$[Cu(C_{16}H_{27}N_4O)ClO_4 \cdot 4H_2O$ (blue)	m $P2_1/n$ 4	30.943(20) 8.188(4) 7.936(4)	 95.89(5) 	CuN_4O	N_{eq} O_{ap}	2.023(5,20) 2.145(4)	N_{eq},N_{eq} N_{eq},O_{ap}	85.8(2,3)[d] 93.8(2,5)[e] 89.9(2,4.5) 92.8(2,5.3)	616
$[Cu(C_{14}H_{17}N_7O_2Br)]BF_4$ (purple)	m $P2_1/n$ 4	7.793(2) 18.574(6) 13.694(4)	 99.16 	CuN_4O	N_{eq} O_{ap}	1.979(4,100) 2.481(4)	N_{eq},N_{eq} 	81.2(2,3)[d] 96.0(2)[e] 90.2(1,12.4) 164.5(2,3.3)	617
$[Cu(C_{16}H_{36}N_4O_4)](PF_6)_2$ (not given)	m $P2_1c$ 4	15.080(5) 20.406(8) 8.697(3)	 90.16(3) 	CuN_4O 0.1	N_{eq} O_{ap}	2.01(2,6) 2.47(2)	N_{eq},N_{eq} N_{eq},O_{ap}	84.5(1,2.5)[d] 89.9(1,16.1) 166.9(1,7) 81.3(7)[d]	618
[Cu(cyclops)(CN)]. MeOH (deep green)	m $P2_1/c$ 4	12.61(1) 7.674(7) 19.46(1)	 106.38(2) 	CuN_4C 0.05	N_{eq} NC_{ap}	1.984(6,8) 2.042(8)	C_{ap},N_{eq} N_{eq},N_{eq} 	105.9(3,6.4) 80.1(2,1)[d] 85.7(2,7.9) 91.4(2,2.3)[e]	619
$[Cu(pnao)(CN)] \cdot 0.5C_2H_3N$ (deep blue)	or Fdd2 16	18.993(2) 32.352(2) 11.799(1)	 	CuN_4C 0.5	N_{eq} NC_{ap}	2.011(3,64) 2.154(5)	N_{eq},N_{eq} 	79.6(1,1)[d] 92.3(1)[e] 86.5(1,8.0)	620
$[Cu(nuqu)Cl]ClO_4$ (green)	m $P2_1/n$ 4	15.647(3) 9.475(2) 14.156(3)	 107.71(2) 	CuN_4Cl 0.048	Cl_{eq} N_{eq} N_{ap}	2.251(2) 2.038(5,68) 2.243(5)	N_{eq},N_{eq} N_{eq},Cl_{eq} N_{eq},N_{ap} N_{ap},Cl_{eq}	80.7(2,1.6)[d] 83.6(2)[e] 88.0(2,5.7) 92.8(1,1.2) 86.3(2,10.0) 124.1(2)	621
$[Cu(oaoH)(oaoH_2)Cl]$ (dark green)	m $P2_1/c$ 4	8.19(4) 10.746(3) 13.340(7)	 104.94(4) 	CuN_4Cl 0.221	$oaoN_{eq}$ Cl_{ap}	1.989(3,22) 2.625(1)	N_{eq},N_{eq} N_{eq},Cl_{ap}	78.9(1,6)[d] 89.3(1,15.2) 96.6(1,4.1)	622
$[Cu(tmbi)Cl]Cl.H_2O$ (blue)	m $P2_1/n$ 4	11.468(3) 13.482(7) 10.447(3)	 107.82(3) 	CuN_4Cl 0.27	N_{eq} Cl_{ap}	2.017(6,6) 2.502(2)	N_{eq},Cl_{ap} N_{eq},N_{eq} 	97.8(2,2.0) 82.4(2,1)[d] 90.9(2)[e] 88.9(2,10.9)	623

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
[Cu(mehep)Cl]NO_3· $2H_2O$[e] (not given)	tr P–1 1	15.90(5) 14.47(5) 10.39(5)	103.4(2) 88.6(2) 114.4(2)	CuN_4Cl 0.3	N_{eq} Cl_{ap}	1.97(2,9) 2.50(1)	N_{eq},N_{eq}	79.5(8,1)[d] 98.1(8,1)[e] 88.8(8,9.4) 155.3(9,3.3)	624
							N_{eq},Cl_{ap}	99.8(8,8.4)	
				CuN_4Cl 0.3	N_{eq} Cl_{ap}	1.99(2,4) 2.49(1)	N_{eq},N_{eq}	79.0(7,6)[d] 98.6(8,3)[e] 88.8(8,10.4) 154.6(9,3.0)	
							N_{eq},Cl_{ap}	99.9(7,13.1)	
[Cu(tetim)Cl]Cl (blue)	tr P–1 2	7.574(1) 9.548(1) 11.469(1)	96.32(1) 107.19(1) 99.67(2)	CuN_4Cl 0.46	N_{eq} Cl_{ap}	1.967(5,10) 2.399(1)	N_{eq},N_{eq}	80.2(2,1)[d] 92.8(2)[e] 86.6(2,6.5)	625
							N_{eq},Cl_{ap}	104.2(1,6.4)	
[Cu(12–anebN$_4$)Cl]NO_3 (blue)	m $P2_1/c$ 4	20.578 11.476 14.920	93.03	CuN_4Cl 0.55	N_{eq} Cl_{ap}	2.07 2.37	N_{eq},N_{eq} N_{eq},Cl_{ap}	85.76(–,8)[d] 105.8(–,2.7)	626
[Cu(amen-qu)Cl]Cl (blue green)	m C2/c 8	28.268(2) 7.030(1) 26.147(3)	118.87(1)	CuN_4Cl 0.24	N_{eq} Cl_{ap}	2.001(9,23) 2.633(2)	N_{eq},N_{eq}	82.8(3)[d] 91.4(3,1.4)[e] 89.4(3,6.6)	627
							N_{eq},Cl_{ap}	96.9(2,5.7)	
[Cu(tim)Cl]PF_6 (red violet)	not given			CuN_4Cl 0.34	N_{eq} Cl_{ap}	1.955(9) 2.404(3)	N_{eq},N_{eq}	88.3(4,8.8)	628
$Cu(en)_2(S_2O_3)$ (not given)	m $P2_1/c$ 4	6.61 11.88 15.04	112.2	CuN_4S	N_{eq} S_{ap}	2.6(–,5) 2.71	N_{eq},N_{eq}	88.0(–,5)[d]	629
Cu(pytzin)$(NCS)_2$ (dark green)	m $P2_1/n$ 4	14.96(1) 12.23(1) 8.57(1)	106.8(1)	CuN_4S	SCN_{eq} N_{eq} S_{ap}	1.945(–,5) 2.01(–,4) 2.95	N_{eq},N_{eq}	108.1(–1.4) 143.8(3)	630
Cu(ddd)(ClphS) (dark green)	m $P2_1/c$ 4	10.536(2) 12.793(3) 15.061(3)	105.50(1)	CuN_4S 0.43	N_{eq} $ClphS_{ap}$	1.976(1) 2.424(1)	N_{eq},N_{eq}	79.8(1,7)[d] 96.1(1)[e] 87.3(1,8.8)	631
							S_{ap},N_{eq}	102.5(1,4.8)	
Cu(ddd)(phS) (dark green)	or Pbca 8	13.072(2) 14.940(2) 18.786(2)		CuN_4S 0.463	N_{eq} phS_{ap}	1.980(2,9) 2.424(1)	N_{eq},N_{eq}	79.8(1,7)[d] 95.2(1)[e] 86.9(1,8.3)	631
							N_{eq},S_{ap}	103.5(1,6.8)	
[Cu(trien)(SCN)]NCS (blue)	or $P2_12_12_1$ 4	10.803(1) 9.381(1) 13.815(2)		CuN_4S 0.37	N_{eq} NCS_{ap}	2.016(4,14) 2.607(2)	N_{eq},N_{eq}	84.5(3,2)[d] 88.1(3,10.8)	632
							N_{eq},S_{ap}	100.7(2,3.3)	
[Cu(haza)(SCN)]ClO_4 · $2H_2O$ (red)	m $P2_1/n$ 4	8.016(3) 30.109(8) 10.865(2)	104.93(2)	CuN_4S 0.13	N_{eq} NCS_{ap}	2.03(1,1) 2.88(1)	N_{eq},N_{eq}	87.1(2,1)[d] 94.0(2,2)[e] 92.7(2,5.0)	633
							N_{eq},N_{eq}	93.2(1,9.6)	
[Cu(pms)(N_3)]ClO_4 (not given)	m $P2_1/a$ 4	16.316(5) 8.379(1) 14.409(2)	100.69(2)	CuN_4S	$(N3)_{eq}$ N_{eq} S_{ap}	1.945(5) 2.010(5,65) 2.665(2)	N_{eq},N_{eq}	82.9(2,5)[d] 89.9(2,7.6)	634
							N_{eq},S_{ap}	85.5(6)[d] 93.3(6,11.0)	
{Cu(tht)}$(ClO_4)_2$ (blue)	or Pbca 8	20.373(7) 14.205(3) 15.242(3)		CuN_4S	N_{eq} S_{ap}	2.043(7,22) 2.549(2)	N_{eq},N_{eq}	86.4(3,8)[d] 93.1(3,2.1)[e] 89.7(3,5.4)	635a
							N_{eq},S_{ap}	88.5(2,1.6)[d] 93.9(2,8.9)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
[Cu(pmtp)][Cu(pmtp) · (ClO_4)]$(ClO_4)_3$ (greenish blue)	m $P2_1/a$ 4	24.180(7) 31.855(7) 9.760(3)	143.84(1)	CuN_4S	N_{eq} S_{ap} N_{eq}	2.000(14,9) 2.353(6) 2.276(8)	N_{eq},N_{eq}	82.1(6)[d] 90.5(6.8,4) 175.3(4)	635b
							S_{eq},N_{eq}	85.9(5)[d] 165.7(3)	
							N_{eq},N_{ap}	79.9(3)[d] 96.5(3,16.6)	
							S_{eq},N_{ap}	85.1(4)[d]	
[Cu(dpq)$_2$Br]HSO_4 · dpg (green)	m C2/c 8	26.850(6) 13.487(4) 27.295(6)	107.21(2)	CuN_4Br	N_{eq} Br_{ap}	2.041(7,60) 2.446(2)	N_{eq},N_{eq}	78.2(3)[d] 83.1(2) 86.7(3,8.5)	636
							Br_{ap},N_{eq}	103.6(2,7.0)	
[Cu(bnzen)$_2$Br]Br (not given)	m $P2_1/c$ 4	12.872(1) 21.074(2) 12.633(1)	108.19(7)	CuN_4Br	N_{eq} Br_{ap}	2.084(3,28) 2.547(1)	N_{eq},N_{eq}	83.6(1,2)[d] 87.7(1,4.6)	637
							Br_{ap},N_{eq}	102.9(1,10.3)	
[Cu(tim)Br]PF_6 (blue)	not given			CuN_4Br 0.30	N_{eq} Br_{ap}	1.947(16,–) 2.549(11)	N_{eq},N_{eq}	89.0(7,9.3)	628a
[Cu(MeOHbpe)Br]ClO_4 (not given)	m $P2_1/c$ 4	9.28(3) 13.22(4) 16.05(5)	98.3(3)	CuN_4Br 0.36	N_{eq} Br_{eq} N_{ap}	2.024(17,39) 2.423(5) 2.148(17)	N_{eq},N_{eq}	80.8(6,2.0)[d] 160.4(6)	628b
							Br_{eq},N_{eq}	99.5(4,1.2) 146.0(4)	
							N_{eq},N_{ap}	80.6(6)[d] 97.3(6,16.7)	
$Cu(en)_2(SSeO_3)$ (not given)	m $P2_1/c$ 4	6.59 12.10 14.98	110.5	CuN_4Se	N_{eq} Se_{ap}	2.07(–,8) 2.89	N_{eq},N_{eq}	87.5(–,1.5)[d]	629
[Cu($C_{16}H_{32}N_4$)I]I · $2.5H_2O$ (deep violet)	m $P2_1/c$ 4	7.702(2) 20.755(8) 17.295(6)	115.09(2)	CuN_4I	N_{eq} I_{ap}	1.97(2,7) 3.03(7)	N_{eq},N_{eq}	88(1,5)[e] 96(1)[h] 93.8(–,5.8)	638
							N_{eq},I_{ap}	89.8(–,5.6)	
[Cu(abapt)I]I (dark green)	m $P2_1/c$ 4	9.263(2) 18.189(3) 11.740(3)	92.97(9)	CuN_4I 0.311	N_{eq} I_{ap}	2.042(5,28) 2.785(1)	N_{eq},N_{eq}	91.8(2,8.8)[e] 88.7(2,6.6)	639
							N_{eq},I_{ap}	98.8(2,4.6)	
Cu(cyclopsf)(I) (not given)	m $P2_1/c$ 4	10.036(3) 7.399(3) 24.982(8)	106.67(1)	CuN_4I 0.38	N_{eq} I_{ap}	1.956(11,20) 2.742(2)	N_{eq},N_{eq}	80.8(4,2)[d] 87.7(4,4.9) 94.6(4,2.1)[e]	640
							N_{eq},I_{ap}	101.5(3,8.3)	
[Cu(pya–dpt)I]I.MeOH (green)	tr P–1 2	8.398(3) 9.503(3) 12.191(5)	86.96(3) 85.68(3) 78.73(3)	CuN_4I 0.1	N_{eq} I_{ap}	2.055(11,48) 2.806(2)	N_{eq},N_{eq}	78.8(4)[d] 93.7(4,5)[e] 89.0(4,5.4)	641
							N_{eq},I_{ap}	99.1(3,6.5)	
[Cu(13–aneS_4)(H_2O)] · $(ClO_4)_2$[c] (not given)	m $P2_1/c$ 8	18.073(3) 13.607(3) 18.167(3)	119.759(1)	CuS_4O 0.38	S_{eq} H_2O_{ap}	2.327(5,17) 2.14(1)	S_{eq},S_{eq}	87.8(2,1.8)[d] 90.9(2)[e] 161.0(2,4.3)	642
							S_{eq},O_{ap}	99.5(2,5.0)	
				CuS_4O 0.38	S_{eq} H_2O_{ap}	2.322(5,11) 2.16(2)	S_{eq},S_{eq}	87.7(2.1.3)[d] 91.2(2)[e] 161.0(2,3.2)	
							S_{eq},O_{ap}	99.3(2,5.1)	
[Cu(12–aneS_4)(H_2O)] · $(ClO_4)_2$	or $Pbc2_1$ 4	9.010(2) 15.775(3) 13.380(2)		CuS_4O 0.53	S_{eq} H_2O_{ap}	2.333(1,38) 2.11(2)	S_{eq},S_{eq}	87.0(6,7.1)[d] 152.7(4,1)	642
							S_{eq},O_{ap}	103.0(9,4.4)	
[Cu(Me_2Opur)$_2$(H_2O)$_2$ · (NO_3)]NO_3 (not given)	tr P–1 2	13.310(7) 11.127(1) 7.450(1)	96.90(1) 100.76(1) 93.68(1)	CuO_3N_2 0.03	$purN_{eq}$ H_2O_{eq} O_2NO_{eq} H_2O_{ap}	1.986(3,21) 1.948(3) 1.996(3) 2.338(3)	O_{eq},O_{eq} N_{eq},N_{eq} O_{eq},N_{eq} O_{ap},O_{eq} O_{ap},N_{eq}	88.2(1) 92.7(1) 91.2(1,1.4) 89.5(1,12.1) 92.7(1,1.5)	643

TABLE II *(Continued)*

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$Cu(dnsglyNO)_2(py)_2 \cdot (H_2O)$ (blue)	m P2/c 2	21.274(5) 5.719(5) 19.154(5)	 116.9(1) 	CuO_3N_2 0.06	$glyO_{eq}$ pyN_{eq} H_2O_{ap}	1.954(5,0) 2.011(1,0) 2.196(9)	O_{eq},O_{eq} N_{eq},N_{eq} O_{eq},N_{eq} O_{eq},O_{ap} O_{ap},N_{eq}	176.8(3) 166.3(3) 90.2(3,9) 88.4(2) 96.8(3)	644
$Cu(phex)_2(py)_2(H_2O)$ (dark blue)	or $P2_12_12_1$ 4	11.29(3) 37.74(8) 5.87(2)	 	CuO_3N_2 0.08	pyN_{eq} $phexO_{eq}$ H_2O_{ap}	2.04(1,1) 1.975(10,5) 2.24(1)	O_{eq},O_{eq} N_{eq},N_{eq} O_{eq},N_{eq}	177(1) 167(1) 90.8(1,3.8)	645
$Cu(memacet)_2(py)_2 \cdot (H_2O)$[c] (blue)	m $P2_1$ 2	16.112(3) 5.8692(9) 18.130(3)	 75.818(7) 	CuO_3N_2 0.11	pyN_{eq} acO_{eq} H_2O_{ap}	2.042(3,21) 1.945(3,10) 2.202(4)	O_{eq},O_{eq} N_{eq},N_{eq} O_{eq},N_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	179.0(2) 169.2(2) 90.0(1,1.3) 90.5(2,2.3) 95.4(2,8)	646
				CuO_3N_2 0.11	pyN_{eq} acO_{eq} H_2O_{ap}	2.093(5,22) 2.072(5,46) 2.59(1)	O_{eq},O_{eq} N_{eq},N_{eq} O_{eq},N_{eq} N_{eq},O_{ap} O_{eq},O_{ap}	139.7(2) 152.4(2) 85.5(2,6.4) 103.8(4,3.2) 109.4(5,2.1)	
$Cu(bzim)(5'-dqmp) \cdot (H_2O)_3$[c] (blue)	tr P1 2	7.069(6) 13.959(10) 14.204(12)	75.12(6) 94.15(6) 97.98(6)	CuO_3N_2 0.164	$bzimN_{eq}$ $dqmpN_{eq}$ H_2O_{eq} H_2O_{ap}	2.01(1) 1.97(1) 1.975(10,5) 2.23(1)	N_{eq},N_{eq} O_{eq},O_{eq} N_{eq},O_{eq} O_{ap},N_{eq} O_{ap},O_{eq}	170.5(4) 170.1(4) 90.3(4,4.6) 94.8(4,2.2) 87.1(4,1.9)	647
				CuO_3N_2 0.183	$bzimN_{eq}$ $dqmpN_{eq}$ H_2O_{eq} H_2O_{ap}	2.02(1) 1.97(1) 1.97(1,0) 2.23(1)	N_{eq},N_{eq} O_{eq},O_{eq} N_{eq},O_{eq} O_{ap},O_{eq} O_{ap},N_{eq}	157.4(4) 179.5(4) 90.0(4,4.7) 90.2(4,1.7) 102.6(4,9)	
$Cu(anic)_2(CHO_2)_2.H_2O$ (not given)	or Fdd2 8	33.063(9) 18.997(9) 5.540(2)	 	CuO_3N_2 0.17	O_{eq} $anicN_{eq}$ H_2O_{ap}	1.956(7,0) 2.031(9,0) 2.154(15)	N_{eq},O_{ap} O_{eq},O_{ap} N_{eq},O_{eq}	93.7(4) 96.2(3) 89.5(4)	648
$[Cu(tplb)_2(H_2O)_2 \cdot (ClO_4)]ClO_4$ (not given)	m $P2_1$ 2	10.255(1) 20.218(3) 10.316(2)	 106.21(1) 	CuO_3N_2	$tplbN_{eq}$ H_2O_{eq} O_3ClO_{ap}	2.004(4,16) 1.93(4,12) 2.411(3)	N_{eq},N_{eq} N_{eq},O_{eq} N_{eq},O_{ap} O_{eq},O_{eq} O_{eq},O_{ap}	169.89(16) 89.97(17,1.40) 94.95(15,2.84) 178.76(15) 90.36(17,4.67)	649
$Cu(mcpa)_2(py)_2(H_2O)$ (not given)	m C2 2	15.828(9) 5.815(2) 16.591(4)	 110.83(3) 	CuO_3N_2	pyN_{eq} $mepaO_{eq}$ H_2O_{ap}	2.06(1,0) 1.95(1,0) 2.27(2)	O_{eq},O_{eq} N_{eq},N_{eq} O_{eq},N_{eq} N_{eq},O_{ap} O_{eq},O_{ap}	176.5(8) 167.9(7) 90.2(8,5) 96.1(6) 88.3(7)	650
$Cu(py)_2(bz)_2(H_2O)$ (not given)	m Pb_1/n 4	5.993(1) 19.721(4) 18.877(4)	 92.99(1)	CuO_3N_2	pyN_{eq} bzO_{eq} H_2O_{ap}	2.055(10,5) 1.935(10,5) 2.28(1)	O_{eq},N_{eq} N_{eq},N_{eq} O_{eq},O_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	90.1(3,1.9) 168.6(3) 178.6(3) 89.4(3,3) 95.7(3,1.1)	651
$Cu(CHO_2)_2(py)_2(H_2O)$ (not given)	or Pnma,$Pn2_1$ 4	9.734(2) 14.366(2) 10.302(2)	 	CuO_3N_2	pyN_{eq} O_{eq} H_2O_{ap}	2.021(−,0) 1.957(−,65) 2.307	not given		652
$Cu(oflp)_2(py)_2(H_2O)$ (not given)	or P2cb 2	5.621(2) 17.218(7) 13.288(6)	 	CuO_3N_2	$oflpO_{eq}$ pyN_{eq} H_2O_{ap}	1.944(4,0) 2.030(5,0) 2.199(8)	O_{ap},O_{eq} O_{ap},N_{eq} O_{eq},N_{eq} O_{eq},O_{eq} N_{eq},N_{eq}	91.0(2) 95.4(2) 89.9(3,1.2) 178.1(2) 169.3(3)	653

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$Cu(2\text{–}NH_2py)_2(2\text{–}npa)_2 \cdot (H_2O)$ (blue)	m C2/c 4	25.418(9) 5.718(1) 18.785(3)	99.73(2)	CuO_3N_2	$npaO_{eq}$ pyN_{eq} H_2O_{ap}	1.947(5,0) 2.078(5,0) 2.211(7)	O_{eq},N_{eq} O_{eq},O_{ap} O_{eq},O_{eq} N_{eq},O_{ap} N_{eq},N_{eq}	90.15(20,65) 89.0(2) 178.0(3) 98.3(1) 163.5(3)	654
$Cu(2\text{–}Mepy)_2(bz)_2(H_2O)$ (blue)	or $Pn2_1a$ 4	20.387(8) 18.997(6) 6.191(2)		CuO_3N_2	pyN_{eq} bzO_{eq} H_2O_{ap}	2.007(–,16) 1.944(–,20) 2.302	not given		655
$Cu(ma)_2(bz)_2(H_2O)$ blue	or $P2_12_12_1$ 2	22.304(2) 7.633(1) 5.730(1)		CuO_3N_2	bzO_{eq} maN_{eq} H_2O_{ap}	1.972 2.015 2.222	not given		656
$Cu(acpyr)_2(ac)_2 \cdot (H_2O)$ (blue)	m C2/c 4	15.127(2) 6.746(2) 24.483(3)	96.06(1)	CuO_3N_2	$pyrN_{eq}$ acO_{eq} H_2O_{ap}	2.012(5,0) 1.961(5,0) 2.423(7)	O_{eq},O_{eq} N_{eq},N_{eq} N_{eq},O_{eq} N_{eq},O_{ap} O_{eq},O_{ap}	178.3(2) 167.5(2) 90.1(2,2) 96.2(2) 89.2(2)	657
$Cu(phen)(H_2O)_2(C_4O_4)$ (dark brown)	tr P–1 2	10.484(3) 10.368(2) 8.288(2)	95.30(2) 83.48(2) 110.45(2)	CuO_3N_2 0.158	O_{eq} H_2O_{eq} $phenN_{eq}$ H_2O_{ap}	1.976(2) 1.964(2) 2.034(2,15) 2.297(2)	O_{eq},O_{eq} N_{eq},N_{eq} O_{eq},N_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	97.4(1) 81.5(1)[d] 89.9(1,2.0) 167.9(1,2.0) 94.7(1,2.2) 94.4.(1,1.9)	278
$Cu(Me_4en)(Cl_3ac) \cdot (H_2O)$ (not given)	m $P2_1/c$ 4	11.104(7) 17.196(9) 10.769(6)	103.82(4)	CuO_3N_2 0.16	enN_{eq} acO_{eq} H_2O_{ap}	2.047(14,37) 1.979(10,14) 2.302(12)	N_{eq},N_{eq} O_{eq},N_{eq} O_{eq},O_{eq} O_{ap},O_{eq} O_{ap},N_{eq}	85.6(5)[d] 88.2(5,9) 167.7(5,5.2) 97.6(4) 88.0(4,5.7) 101.8(5,1.9)	658
$Cu(bgly)_2(bpy) \cdot (pn\text{–}2\text{–}ol)^c$ (blue)	tr P–1 4	22.199(11) 15.357(6) 10.223(4)	103.78(3) 83.06(4) 88.89(4)	CuO_3N_2 0.171	$bpyN_{eq}$ $bglyO_{eq}$ O_{ap}	1.995(20,15) 1.965(10,5) 2.27(2)	N_{eq},N_{eq} N_{eq},O_{eq} N_{eq},O_{ap} O_{eq},O_{eq} O_{eq},O_{ap}	82.6(6)[d] 91.8(6,1.5) 93.55(70,1.45) 92.4(5) 99.5(6)	659
				CuO_3N_2 0.172	$bpyN_{eq}$ $bglyO_{eq}$ O_{ap}	2.01(2,1) 1.945(10,15) 2.34(1)	N_{eq},N_{eq} N_{eq},O_{eq} N_{eq},O_{ap} O_{eq},O_{eq} O_{eq},O_{ap}	83.1(6)[d] 91.75(60,25) 94.95(6,3.15) 91.9(5) 94.9(5)	
$[Cu(Me_4en)(nmf)_3] \cdot (ClO_4)_2$ (blue)	m $P2_1/c$ 4	8.255(3) 17.951(6) 16.451(4)	91.05(2)	CuO_3N_2 0.185	enN_{eq} $nmfO_{eq}$ $nmfO_{ap}$	2.03(5,2) 1.983(4,2) 2.181(4)	N_{eq},N_{eq} O_{eq},O_{eq} O_{eq},O_{ap} O_{eq},N_{eq} O_{ap},N_{eq}	86.6(2)[d] 90.9(2) 94.5(2,1.2) 89.9(2,1.8) 98.7(2,2.5)	660
$[Cu(bpy)(tsnO)_2(H_2O)] \cdot 2H_2O$ (blue)	tr P–1 2	18.162(4) 14.975(4) 7.272(2)	103.67(6) 87.10(5) 104.48(6)	CuO_3N_2 0.20	$tsnO_{eq}$ $bpyN_{eq}$ H_2O_{ap}	1.933(4,23) 2.002(4,4) 2.309(4)	N_{eq},N_{eq} O_{eq},O_{eq} O_{eq},N_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	80.4(2)[d] 92.9(2) 92.2(2,2.0) 97.1(2,4.2) 94.7(2,1.7)	661
$[Cu(Me_4en)(SO_4) \cdot (H_2O)_2] \cdot 2H_2O$ (blue)	or Pbca 8	12.543(1) 15.782(1) 13.862(1)		CuO_3N_2 0.25	enN_{eq} O_3SO_{eq} H_2O_{eq} H_2O_{ap}	2.025(–,1) 1.986 1.974 2.205	N_{eq},N_{eq} N_{eq},O_{eq} O_{eq},O_{eq} N_{eq},O_{ap} O_{eq},O_{ap}	86.9[d] 91.4(–,3) 87.3 101.7(–,3.1) 92.5(–,1.4)	662
$Cu(mecry)_2(bpy) \cdot (H_2O)$ (blue)	m $P2_1/n$ 4	6.851(1) 17.626(2) 15.553(1)	96.52(1)	CuO_3N_2 0.297	$bpyN_{eq}$ O_{eq} H_2O_{ap}	2.014(3,9) 1.948(2,22) 2.292(2)	N_{eq},N_{eq} O_{eq},O_{eq} O_{eq},O_{ap} O_{eq},N_{eq} O_{ap},O_{eq}	80.2(1)[d] 91.1(1) 97.9(9,2.4) 92.9(1,5) 94.06(10,2.25)	663

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$Cu(dik)(SO_4)(H_2O)_2$ (green)	m $P2_1/n$ 4	11.982(2) 13.803(3) 8.866(2)	107.30(2)	CuO_3N_2	$dikN_{eq}$	1.996(2,1)	N_{eq},N_{eq}	90.25(5)[e]	664
					H_2O_{eq}	1.947(1)	N_{eq},O_{ap}	94.82(6,7.17)	
					O_3SO_{eq}	1.957(2)	N_{eq},O_{eq}	89.10(6,2.40)	
					H_2O_{ap}	2.271(2)	O_{eq},O_{ap}	98.30(6,1.14)	
							O_{eq},O_{eq}	89.79(6)	
[Cu(5′–ump)(im)$_2$· (H_2O)]·$4H_2O$[c] (pale blue)	m $P2_1$ 4	8.585(2) 20.226(2) 13.876(3)	99.22(2)	CuO_3N_2	imN_{eq}	1.98(3,2)	not given		665
					$umpO_{eq}$	2.07(2,6)			
					H_2O_{ap}	2.07(3)			
				CuO_3N_2	imN_{eq}	2.00(3,50)	not given		
					$umpO_{eq}$	2.00(2,3)			
					H_2O_{ap}	2.12(2)			
[Cu(L–ala)$_2$(Meim)$_2$]· EtOH (blue violet)	m $P2_1/c$ 2	11.1119(6) 18.8398(7) 8.9652(5)	105.38(2)	CuO_3N_2	O_{eq}	1.970(4,0)	O_{eq},N_{eq}	90.3(2)	666
					imN_{eq}	1.968(5,9)			
					O_{ap}	2.731(5)			
$Cu(phalan)_2(dmsO)$ (blue)	tr P1 1	5.734(4) 8.359(9) 11.778(10)	97.21(8) 100.07(6) 105.78(7)	CuO_3N_2	O_{eq}	1.956(10,12)	O_{eq},N_{eq}	83.0(4,3)[d]	667
					N_{eq}	2.005(11,10)		172.35(40,25)	
				0.037	$dmsO_{ap}$	2.526(11)	O_{eq},O_{eq}	89.6(4)	
							N_{eq},N_{eq}	104.2(4)	
							O_{eq},O_{ap}	101.15(40,65)	
							N_{eq},O_{ap}	82.3(4,9)	
[Cu(taprop)$_2$$(H_2O)$]· $4H_2O$ (blue violet)	or $P2_12_12_1$ 4	12.582(9) 26.076(15) 6.954(8)		CuO_3N_2	O_{eq}	1.921(4,6)	N_{eq},O_{eq}	85.4(2,2)[d]	668
					N_{eq}	1.992(7,3)		89.9(2,5.5)	
				0.07	H_2O_{ap}	2.440(8)	O_{eq},O_{eq}	172.6(2)	
							N_{eq},N_{eq}	178.3(4)	
							O_{eq},O_{ap}	93.7(3,5.3)	
							O_{ap},N_{eq}	90.7(4.1.3)	
$Cu(But\text{-}Megly)_2(H_2O)$ (dark blue)	or $P2_12_12_1$ 2	7.565(1) 9.378(2) 12.171(2)		CuO_3N_2	N_{eq}	2.081(2,0)	N_{eq},O_{eq}	84.85(7)[d]	669
					O_{eq}	1.922(2,0)		90.02(7,5.17)	
				0.072	H_2O_{ap}	2.464(2)	N_{eq},N_{eq}	171.55(8)	
							O_{eq},O_{eq}	179.40(8)	
							O_{eq},O_{ap}	89.70(6)	
							O_{ap},N_{eq}	94.23(5)	
[Cu(C_3 H_2O_4)(phen)· (H_2O)] ·$1.5H_2O$[c] (not given)	tr P–1 4	12.487(3) 11.717(4) 11.534(2)	109.2(1) 105.4(1) 92.1(1)	CuO_3N_2	$phenN_{eq}$	2.006(6,21)	O_{eq},O_{eq}	94.4(2)[e]	670
					$ma1O_{eq}$	1.912(7,16)	N_{eq},N_{eq}	81.7(2)[d]	
				0.105	H_2O_{ap}	2.304(4)	O_{eq},O_{ap}	98.3(2,1.7)	
							O_{eq},N_{eq}	91.6(2,8)	
							O_{ap},N_{eq}	90.2(2,4.5)	
				CuO_3N_2	$phenN_{eq}$	2.021(6,6)	O_{eq},O_{eq}	94.5(2)[e]	
					$ma1O_{eq}$	1.921(5,9)	N_{eq},N_{eq}	81.4(2)[d]	
				0.112	H_2O_{ap}	2.273(4)	O_{eq},O_{ap}	96.6(2)	
							O_{eq},N_{eq}	90.9(2,1.5)	
							O_{ap},N_{eq}	95.1(2,1.1)	
[Cu(bpy)(ox)(H_2O)]· $2H_2O$ (blue)	tr P–1 2	10.565(3) 7.246(3) 10.806(3)	102.47(3) 62.12(3) 98.13(3)	CuO_3N_2	$bpyN_{eq}$	1.989(5,1)	N_{eq},N_{eq}	81.5(2)[d]	671
					oxO_{eq}	1.953(4,17)	O_{eq},O_{eq}	84.2(2)[d]	
				0.115	H_2O_{ap}	2.341(4)	O_{eq},N_{eq}	97.2(2,2.5)	
							N_{eq},O_{ap}	91.4(2,2.1)	
							O_{eq},O_{ap}	95.4(2,4.4)	
[Cu(sal)(Me_4en)· (EtOH)] (black)	or $P2_12_12_1$ 4	9.252(3) 13.016(6) 14.131(6)		CuO_3N_2	enN_{eq}	2.059(4,9)	O_{eq},O_{eq}	94.1(1)[e]	672
					$sa1O_{eq}$	1.901(4,15)	N_{eq},N_{eq}	85.1(1)[d]	
				0.154	$EtHO_{ap}$	2.520(4)	N_{eq},O_{eq}	89.6(2,2)	
							O_{ap},O_{eq}	94.6(1,3.4)	
							O_{ap},N_{eq}	94.3(1)	
$Cu(C1qO)_2(MeOH)$ (dark brown)	tr P–1 2	12.389(9) 11.730(9) 5.462(3)	87.21(5) 78.48(4) 74.84(5)	CuO_3N_2	$C1qO_{eq}$	1.961(4,1)	O_{eq},N_{eq}	83.3(5,2)[d]	673
					$ClqN_{eq}$	2.001(5.9)		89.9(2.0)	
				0.158	$MeHO_{ap}$	2.274(4)	O_{eq},O_{eq}	169.3(2)	
							N_{eq},N_{eq}	172.7(2)	
							O_{ap},N_{eq}	93.5(2,6.3)	
							O_{ap},O_{eq}	95.3(2,4)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
[Cu(phen)(acac)(H_2O)]·(F_6acac)·H_2O (not given)	tr P–1 2	12.284(6) 14.437(7) 8.020(8)	78.42(1) 109.32(2) 113.07(1)	CuO_3N_2 0.16	acacO_{eq} phenN_{eq} H_2O_{ap}	1.910(4,6) 2.009(5,1) 2.292(3)	N_{eq},N_{eq} O_{eq},O_{eq} O_{eq},N_{eq} N_{eq},O_{ap}	82.0(2)[d] 94.3(2)[e] 91.1(2,7) 167.7(2,2.2) 96.1(2,2.7)	674
Cu(phen)(acac)·(F_6acac) (not given)	tr P–1 2	12.623(6) 11.470(6) 8.111(32)	81.17(4) 92.48(1) 97.69(1)	CuO_3N_2 0.16	acacO_{eq} phenN_{eq} F_6acacO_{ap}	1.9065(50,55) 2.0145(60,5) 2.341(5)	N_{eq},N_{eq} O_{eq},O_{eq} N_{eq},O_{eq} N_{eq},O_{ap} O_{eq},O_{ap}	81.5(2)[d] 95.1(2)[e] 90.9(2,1) 96.9(2,5.6) 93.4(2,4.7)	674
Cu(C_5O_5)(bpy)(H_2O) (green)	tr P–1 2	7.1016(9) 9.3392(9) 11.891(7)	68.94(1) 84.67(1) 68.97(7)	CuO_3N_2 0.16	O_{eq} pyN_{eq} H_2O_{ap}	1.992(1,20 1.979(1,6) 2.270(1)	O_{eq},O_{eq} N_{eq},N_{eq} O_{eq},O_{ap} O_{eq},N_{eq} O_{ap},N_{eq}	85.89(3)[d] 81.80(4)[d] 95.18(4,3.03) 95.51(4,3.42) 94.06(4,17)	675
[Cu(rph)$_2$(H_2O)] ·2H_2O (blue)	m $P2_1/a$ 4	10.29(2) 24.58(9) 7.81(1)	 91.8 	CuO_3N_2 0.16	O_{eq} N_{eq} H_2O_{ap}	1.946(10,10) 2.009(10,1) 2.307(10)	O_{eq},N_{eq} O_{eq},O_{eq} N_{eq},N_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	85.95(50,5)[d] 89.6(5,4.0) 171.7(4) 169.3(5) 94.1(4,7) 95.4(5)	676
Cu(Me_4en)(phenquin)·(phenbq) (green)	m $P2_1/n$ 4	14.331(3) 11.079(3) 18.471(3)	 101.84(3) 	CuO_3N_2 0.17	enN_{eq} bqO_{eq} quinO_{ap}	2.038(4,7) 1.934(3,5) 2.286(3)	O_{eq},O_{eq} N_{eq},N_{eq} O_{eq},N_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	85.7(1)[d] 86.1(2)[d] 93.3(1,4) 87.6(1,6.0) 102.0(1,3.8)	677
[Cu(bpy)(nac)(H_2O)]·H_2O (blue)	tr P–1 2	8.285(11) 9.259(11) 9.744(10)	78.25(9) 73.60(9) 75.9(1)	CuO_3N_2 0.18	bpyN_{eq} nacO_{eq} H_2O_{ap}	2.003(6,9) 1.915(5,2) 2.277(8)	N_{eq},N_{eq} O_{eq},O_{eq} N_{eq},O_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	81.6(2)[d] 94.3(2)[e] 91.1(2,1) 96.1(3,2) 94.2(3,4)	678
[Cu(phen)(nal)(H_2O)]·NO_3·3H_2O (blue)	tr P–1 2	16.654(3) 11.130(2) 7.918(2)	98.53(2) 112.12(2) 89.94(2)	CuO_3N_2 0.185	phenN_{eq} nacO_{eq} H_2O_{ap}	2.007(2,8) 1.924(2,10) 2.277(3)	O_{eq},O_{eq} N_{eq},N_{eq} N_{eq},O_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	93.8(1)[e] 81.9(1)[d] 91.2(1,6) 96.7(1,1.0) 94.1(1,1.6)	679
Na_2[Cu(tsleuNO)$_2$]·2H_2O·MeOH (not given)	m $P2_1$ 2	16.775(2) 11.914(2) 9.053(2)	 100.54(1) 	CuO_3N_2 0.184	O_{eq} N_{eq} H_2O_{ap}	1.972(4,11) 1.987(4,23) 2.353(4)	N_{eq},O_{eq} N_{eq},O_{ap} O_{eq},O_{ap} O_{eq},O_{eq} N_{eq},N_{eq}	82.2(2,1.0)[d] 99.2(2)[e] 90.3(3,8.3) 101.9(2,2.3) 88.7(2,5.5) 176.9(2) 156.1(2)	680
Cu(Me_2ileu)$_2$(H_2O) (blue)	or $P2_12_12_1$ 4	22.154(5) 15.032(4) 6.032(3)	 	CuO_3N_2 0.196	O_{eq} N_{eq} H_2O_{ap}	1.925(5,25) 2.015(5,5) 2.448(6)	N_{eq},O_{eq} O_{eq},N_{eq} N_{eq},O_{ap} O_{eq},O_{ap} O_{eq},O_{eq} N_{eq},N_{eq}	84.9(2,1)[d] 89.33(20,5.83) 94.05(40,3.55) 97.45(20,3.55) 165.1(2) 171.9(2)	681
[Cu(phen)(ox)(H_2O)]·H_2O (blue)	m $P2_1/c$ 4	17.407(3) 9.706(3) 8.468(3)	 103.83(3) 	CuO_3N_2 0.209	phenN_{eq} oxO_{eq} H_2O_{ap}	2.006(4,5) 1.944(3,3) 2.237(4)	N_{eq},N_{eq} O_{eq},O_{eq} N_{eq},O_{eq} O_{eq},O_{ap} O_{ap},N_{eq}	82.8(2)[d] 85.4(1)[d] 94.95(10,25) 95.75(20,95) 96.95(20,1.35)	682
[Cu($C_3H_2O_4$)(Et$_2$en)·H_2O]·H_2O (not given)	tr P–1 2	8.855(5) 9.098(4) 10.378(6)	65.92(2) 108.23(6) 110.22(4)	CuO_3N_2 0.21	enN_{eq} O_{eq} H_2O_{ap}	2.024(5,5) 1.950(4,0) 2.369(3)	N_{eq},N_{eq} O_{eq},O_{eq} N_{eq},O_{ap} O_{eq},O_{ap} N_{eq},O_{eq}	85.7(2)[d] 90.6(1)[e] 91.1(2,2) 100.6(2,3.8) 91.0(2,8)	683

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
[Cu(Me-1,3-pn)(ox)·(H_2O) (not given)	or Pbca 8	15.795(4) 11.774(3) 11.063(2)		CuO_3N_2 0.216	oxO_{eq} pnN_{eq} H_2O_{ap}	1.968(7,23) 1.988(8,10) 2.345(7)	O_{eq},O_{eq} N_{eq},N_{eq} N_{eq},O_{eq} O_{eq},O_{eq} O_{ap},N_{eq} O_{ap},O_{eq}	89.8[d] 95.7(3)[e] 89.6(3,1.2) 83.0(3) 95.9(3,1.1) 96.6(3,6.8)	684
[Cu(thyr)(phen)(H_2O)]·(NO_3)$_2$·H_2O (not given)	m $P2_1/n$ 4	11.005(2) 43.984(12) 6.775(3)	92.59(3)	CuO_3N_2 0.22	$thyrO_{eq}$ $phenN_{eq}$ H_2O_{ap}	1.92(3) 2.01(1) 2.31(1)	not given		685
[Cu(bz-L-val)$_2$(H_2O)]·$2H_2O$ (blue)	or $P2_12_12_1$ 4	21.988(8) 9.022(4) 13.975(5)		CuO_3N_2 0.23	O_{eq} N_{eq} H_2O_{ap}	1.92(2,2) 2.06(2,2) 2.21(2)	O_{eq},N_{eq} N_{eq},N_{eq} N_{eq},O_{ap} O_{eq},O_{ap}	85(1,1)[d] 89.8(1,5.8) 163(1) 100(1) 96(1)	686
[Cu(bpy)(pyx)(OH)]·H_2O (green)	or F2dd 16	5.515(1) 47.338(9) 27.791(9)		CuO_3N_2 0.236	$pyxO_{eq}$ $bpyN_{eq}$ H_2O_{ap}	1.926(6,3) 2.036(7,27) 2.216(6)	O_{eq},O_{eq} N_{eq},N_{eq} O_{eq},N_{eq} O_{ap},O_{eq} O_{ap},N_{eq}	95.7(2)[e] 80.5(3)[d] 90.7(3,3.3) 98.9(2,2.8) 95.0(3,4.9)	687
[Cu(edph)(bpy)(H_2O)]·$2H_2O$ (blue)	tr P-1 2	8.309(2) 10.362(2) 10.811(2)	91.53(1) 90.57(2) 93.43(1)	CuO_3N_2 0.24	$edphO_{eq}$ $bpyN_{eq}$ H_2O_{ap}	1.940(2,4) 2.003(2,4) 2.258(2)	O_{eq},O_{eq} N_{eq},N_{eq} O_{eq},N_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	95.7(1)[e] 80.8(1)[d] 90.7(1,0) 91.25(10,2.35) 100.6(1,7)	688
Cu[Et_2ala)$_2$(H_2O) (blue)	or $C222_1$ 4	8.249(1) 18.695(3) 11.455(2)		CuO_3N_2 0.245	N_{eq} O_{eq} H_2O_{ap}	2.075(4,0) 1.922(2,0) 2.260(4)	O_{eq},N_{eq} N_{eq},N_{eq} O_{eq},O_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	83.4(2)[d] 89.5(2,6.1) 159.9(2) 175.6(1) 92.2(1) 100.0(1)	689
[Cu(Me_2gly)$_2$(H_2O)]·$2H_2O$ (not given)	or $P2_12_12_1$ 4	7.05(1) 31.72(5) 6.51(1)		CuO_3N_2 0.27	N_{eq} O_{eq} H_2O_{ap}	2.05(2,1) 1.97(2,0) 2.27(2)	N_{eq},O_{eq} N_{eq},N_{eq} O_{eq},O_{eq} N_{eq},O_{ap} O_{eq},O_{ap}	84.7(8,4)[d] 89.0(9,4.9) 166.6(8) 162.3(8) 96.7(8,1.0) 98.9(8,7)	690
[Cu(C_3H_2O)(pmdp)·(H_2O)]·H_2O (dark blue)	m $P2_1/n$ 4	13.907(4) 11.419(3) 9.479(3)	90.15(5)	CuO_3N_2 0.279	$pmdpN_{eq}$ O_{eq} H_2O_{ap}	2.015(7,28) 1.938(6,14) 2.501(7)	N_{eq},N_{eq} O_{eq},O_{eq} N_{eq},O_{eq} N_{eq},O_{ap} O_{eq},O_{ap}	88.4(3)[d] 93.1(3)[e] 89.0(3,1.3) 111.8(3) 104.0(3)	691
Cu(thma)$_2$(H_2O) (blue)	m C2/c 4	12.955(2) 10.793(1) 10.091(2)	116.62(1)	CuO_3N_2	N_{eq} O_{eq} H_2O_{ap}	2.028(4,0) 1.958(2,0) 2.189(4)	O_{eq},N_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	84.5(1,0)[d] 94.3(1) 98.8(1)	692
Cu(dco)$_2$(H_2O) (black green)	tr P-1 2	8.338(2) 8.418(2) 11.230(2)	110.61(2) 90.11(2) 105.03(2)	CuO_3N_2	O_{eq} N_{eq} H_2O_{ap}	1.957(2,2) 1.979(1,1) 2.162(2)	O_{eq},N_{eq} O_{eq},O_{eq} N_{eq},N_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	81.5(1,3)[d] 89.6(1,8.2) 172.1(1) 169.0(1) 93.9(1,1.6) 95.6(1,4)	693
[Cu(yun)$_2$(H_2O)]·$2H_2O$ (blue)	m $P2_1$ 2	15.94(4) 6.33(3) 8.60(3)	95.6(3)	CuO_3N_2	O_{eq} N_{eq} H_2O_{ap}	1.985(10,25) 2.01(1,1) 2.24(1)	O_{eq},N_{eq}	83.0(–,5)[d] 89.3(–,9.7)	694

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$Cu(hib)_2(H_2O)$	m	17.774(2)		CuO_3N_2	N_{eq}	2.011(3,0)	N_{eq},O_{eq}	86.3(2)[d]	695
(blue green)	C2/c	16.986(1)	113.44(1)		O_{eq}	1.955(3,0)		94.6(2)	
	4	7.279(1)			H_2O_{ap}	2.135(5)	N_{eq},N_{eq}	176.5(2)	
							O_{eq},O_{eq}	148.7(2)	
							N_{eq},O_{ap}	88.3(1)	
							O_{eq},O_{ap}	105.6(1)	
$[Cu(phen)(C_3H_2O_4)\cdot(H_2O)].1.5H_2O$	tr	11.560(4)	92.12(2)	CuO_3N_2	O_{eq}	1.914(3,5)	O_{eq},O_{eq}	94.82(13)[e]	696
(blue)	P-1	11.734(5)	105.50(2)		$phenN_{eq}$	2.018(4,4)	N_{eq},N_{eq}	81.08(15)[d]	
	2	12.491(2)	109.28(3)		H_2O_{ap}	2.266(3)	O_{eq},N_{eq}	91.27(15,1.10)	
							N_{eq},O_{ap}	94.92(14,1.06)	
							O_{eq},O_{ap}	96.35(14,2.38)	
$Cu(nsnph)_2(H_2O)$	m	6.395(4)		CuO_3N_2	N_{eq}	1.983(8,5)	N_{eq},O_{eq}	82.5(1.3,2)[d]	697
(reddish brown)	$P2_1/c$	19.311(23)	98.2(1)		O_{eq}	1.974(7,5)	N_{eq},O_{ap}	91.6(1.3)	
	4	14.274(24)			H_2O_{ap}	2.195(7)	O_{eq},O_{ap}	95.9(1.3)	
$Cu(ileu)_2(H_2O)$	or	9.451(4)		CuO_3N_2	O_{eq}	1.951(7,3)	O_{eq},N_{eq}	84.4(4,2)[d]	698
(deep blue)	$P2_12_12_1$	21.67(2)			N_{eq}	1.992(7,3)	O_{eq},N_{eq}	169.1(4,6.0)	
	4	7.629(3)			H_2O_{ap}	2.475(7)	O_{ap},O_{eq}	104.6(4,7.1)	
							O_{ap},N_{eq}	86.0(4,9)	
Cu(sald)(phen)(NO_3)	tr	11.739(3)	95.74(2)	CuO_3N_2	$saldO_{eq}$	1.925(3,27)	O_{eq},O_{eq}	93.6(1)[e]	699
(dark green)	P-1	9.062(2)	112.78(2)		$phenN_{eq}$	1.998(3,7)	N_{eq},N_{eq}	82.5(1)[d]	
	2	8.773(2)	79.87(1)		O_2NO_{ap}	2.402(3)	O_{eq},O_{eq}	93.6(1)	
							N_{eq},N_{eq}	87.2(1,4.7)	
$[Cu(C_{24}H_{27}N_3O_2)\cdot(MeCN)]\cdot 2trf$	tr	12.899(5)	108.88(4)	CuO_3N_2	N_{eq}	2.02(2,0)	O_{eq},N_{eq}	91.6(8)[e]	700
(blue)	P-1	14.027(8)	102.99(4)		$MeCN_{eq}$	2.003(3)	N_{eq},N_{eq}	95.0(9)[e]	
	2	11.694(3)	100.55(4)	0.016	O_{eq}	1.93(1)	N_{eq},O_{ap}	89.2(8)[e]	
					O_{ap}	2.38(2)	N_{eq},N_{eq}	92.7(9,2.3)	
							O_{ap},O_{eq}	89.7(7)	
							O_{ap},N_{eq}	89.4(8,1.6)	
							O_{eq},N_{eq}	87.4(8,4.3)	
$[Cu(C_{25}H_{29}N_3O_2)\cdot(H_2O)]\cdot 2trf$	m	11.583(4)		CuO_3N_2	N_{eq}	2.017(4,24)	N_{eq},N_{eq}	94.8(1)[e]	700
(blue)	$P2_1/n$	17.368(6)	99.06(1)		O_{eq}	1.947(3)	N_{eq},O_{eq}	92.4(1)[e]	
	4	16.420(6)		0.045	H_2O_{eq}	2.033(3)	O_{ap},N_{eq}	90.5(1)[e]	
					O_{ap}	2.346(3)	O_{eq},N_{eq}	91.0(1,1.4)	
							N_{eq},O_{ap}	93.6(1,3.1)	
							O_{eq},O_{ap}	88.9(1,1.3)	
							O_{eq},O_{eq}	83.4(1)	
$[Cu(C_{25}H_{29}N_3O)(trf)\cdot(H_2O)]\cdot trf$	m	11.716(6)		CuO_3N_2	N_{eq}	2.011(3,22)	N_{eq},N_{eq}	95.5(1)[e]	700
(blue)	$P2_1/n$	17.400(8)	99.97(5)		O_{eq}	1.942(3)	N_{eq},O_{eq}	91.2(1)[e]	
	4	16.234(8)		0.089(1)	H_2O_{eq}	2.012(3)	O_{eq},N_{eq}	90.5(1,7)	
					$trfO_{ap}$	2.386(3)	O_{ap},N_{eq}	95.3(1,6.6)	
							O_{eq},O_{ap}	89.4(1,2)	
							O_{eq},O_{ep}	83.8(1)	
$[Cu(C_{24}H_{29}N_3O)(trf)(H_2O)]trf.H_2O$	tr	12.251(1)	107.29(5)	CuO_3N_2	O_{eq}	1.93(1)	O_{eq},N_{eq}	90.9(5)[e]	700
(blue)	P-1	12.307(1)	93.11(5)		H_2O_{eq}	2.07(1)	N_{eq},N_{eq}	95.3(5)[e]	
	2	11.795(1)	102.54(5)	0.43	N_{eq}	2.20(1,3)	O_{eq},N_{eq}	91.1(5,2)	
					$trfO_{ap}$	2.40(1)	O_{ap},N_{eq}	97.6(5,7.9)	
							O_{ap},O_{eq}	88.9(5,1)	
							O_{eq},O_{eq}	82.5(4)	
Cu(pydca)(5-Meim).(H_2O)	tr	7.575(2)	69.39(3)	CuO_3N_2	$pydN_{eq}$	1.903(5)	O_{eq},N_{eq}	79.6(3,3)[d]	701
(blue)	P-1	11.766(2)	86.41(3)		$pydO_{eq}$	2.038(6,19)		87.9(2,9.8)	
	2	16.203(3)	82.00(3)	0.05	imN_{eq}	1.926(5)	N_{eq},N_{eq}	169.3(3)	
					H_2O_{ap}	2.287(6)	O_{eq},O_{eq}	160.1(2)	
							N_{eq},O_{ap}	95.4(2,3)	
							O_{eq},O_{ap}	93.6(2)	
$[Cu(pydca)(1-Meim)\cdot(H_2O)]\cdot 2H_2O$	tr	8.908(2)	97.04(2)	CuO_3N_2	$pydO_{eq}$	2.021(4,6)	N_{eq},O_{eq}	80.8(2,1)[d]	701
(blue)	P-1	15.729(3)	91.83(2)		$pydN_{eq}$	1.895(4)		89.9(2,11.5)	
	2	5.320(4)	101.64(2)	0.10	imN_{eq}	1.925(4)	O_{eq},O_{eq}	161.4(1)	
					H_2O_{ap}	2.320(4)	N_{eq},N_{eq}	172.1(2)	
							O_{eq},O_{ap}	91.3(2,1.6)	
							N_{eq},O_{ap}	93.8(2,2.9)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
[Cu(pydca)(2–Meim).(H_2O)].H_2O	m	12.105(3)		CuO_3N_2	$pydO_{eq}$	2.041(6,4)	O_{eq},N_{eq}	79.6(3,3)[d]	701
(blue)	$P2_1/c$	13.421(3)	96.9(0)		$pydN_{eq}$	1.918(7)		89.6(3,13.2)	
	4	8.277(3)		0.10	imN_{eq}	1.929(8)	O_{eq},O_{eq}	158.2(3)	
					H_2O_{ap}	2.295(5)	N_{eq},N_{eq}	168.6(3)	
							O_{ap},O_{eq}	95.3(2,3.0)	
Cu(gly)$(H_2O)_2$	m	12.488(5)		CuO_3N_2	O_{eq}	1.974(2)	O_{eq},N_{eq}	82.7(3)[d]	702
(deep blue)	Cc_1+C2/c	9.245(6)	97.68(3)		N_{eq}	1.967(2,63)	N_{eq},N_{eq}	83.5(3)[d]	
	8	13.360(5)		0.13	H_2O_{eq}	1.946(2)	N_{eq},O_{eq}	93.0(3,10.3)	
					H_2O_{ap}	2.383(2)	O_{ap},N_{eq}	94.2(3)	
							O_{eq},O_{eq}	94.2(3)	
							O_{eq},O_{ap}	94.0(3,1.50)	
[Cu(glytyr)$(H_2O)_2$]·	or	12.498(3)		CuO_3N_2	N_{eq}	1.953(5,57)	O_{eq},N_{eq}	82.5(2)[d]	703
$2H_2O$	$P2_12_12_1$	10.429(2)			O_{eq}	1.981(5)		88.2(2,5.7)	
(not given)	4	11.978(2)		0.155	H_2O_{eq}	1.964(5)	N_{eq},N_{eq}	84.8(2)[d]	
					H_2O_{ap}	2.372(5)	O_{eq},O_{eq}	93.8(2)	
							O_{ap},O_{eq}	91.4(2,2.2)	
							O_{ap},N_{eq}	98.3(2,3.0)	
[Cu(tan)$(H_20)_2$]ClO_4	m	13.481(4)		CuO_3N_2	N_{eq}	1.96(2,1)	O_{eq},N_{eq}	83(1)[d]	704
(blue)	$P2_1/c$	8.060(4)	95.58(4)		O_{eq}	1.96(2)	N_{eq},N_{eq}	79(1)[d]	
	4	15.307(7)		0.18	H_2O_{eq}	1.98(2)	O_{eq},O_{ap}	91.7(1,1.7)	
					H_2O_{ap}	2.27(2)	N_{eq},O_{eq}	94.0(1,11)	
							N_{eq},O_{ap}	104.5(1,5)	
							O_{eq},O_{eq}	92.0(1)	
[Cu(leu–L–tyr)$(H_2O)_2$]·	or	15.545(1)		CuO_3N_2	N_{eq}	1.958(3,47)	N_{eq},N_{eq}	83.9(1)[d]	705
EtOH	$P2_12_12_1$	16.121(2)			O_{eq}	2.005(3)	N_{eq},O_{eq}	82.4(1)[d]	
(deep blue)	4	8.684(1)			H_2O_{eq}	1.966(3)		92.0(1,9.6)	
					H_2O_{ap}	2.291(3)	O_{eq},O_{eq}	90.0(1)	
							N_{eq},O_{ap}	104.1(1,4.4)	
							O_{eq},O_{ap}	88.3(1,4.6)	
$Cu(doxc)_2$	m	18.559(1)		CuO_3N_2	N_{eq}	2.024(4,0)	N_{eq},N_{eq}	161.58(18)	706
(blue)	$P2_1/c$	10.142(1)	101.60(1)		O_{eq}	1.922(4,18)	O_{eq},O_{eq}	177.66(17)	
	4	7.345(1)		0.02	O_{ap}	2.354(4)	O_{eq},N_{eq}	85.4(2,1.1)[d]	
								94.2(2,2.1)	
							N_{eq},O_{ap}	99.1(2,10.0)	
							O_{eq},O_{ap}	90.9(2,6.5)	
$Cu(C_{17}H_{17}N_2O_2)(ac)$	tr	8.157(7)	78.62(7)	CuO_3N_2	acO_{eq}	1.988(2)	O_{eq},N_{eq}	92.3(1)[e]	707
(dark green)	P–1	10.651(7)	85.81(1)		N_{eq}	1.975(3,15)		91.3(1,9)	
	2	10.900(7)	101.91(1)	0.10	O_{ap}	1.898(2)	N_{eq},N_{eq}	92.51(10)[e]	
					acO_{ap}	2.547(3)	O_{eq},O_{eq}	85.63(9)	
							O_{eq},O_{ap}	74.3(9,18.2)	
							O_{ap},N_{eq}	109.5(1,11.1)	
$Cu(L–tyr)_2$	or	13.049(7)		CuO_3N_2	O_{eq}	1.949(3,24)	N_{eq},O_{eq}	84.6(1,2)[d]	708
(not given)	$P2_12_12_1$	22.227(8)			N_{eq}	2.003((4,12)		95.9(1,9)	
	4	6.078(3)		0.11	O_{ap}	2.39(3)	N_{eq},N_{eq}	168.0(1)	
							O_{eq},O_{eq}	179.3(1)	
							O_{eq},O_{ap}	90.3(1,5)	
							N_{eq},O_{ap}	96.0(1,8.4)	
$[Cu(C_4H_8NO_3)_2]\cdot H_2O$	m	11.02(2)		CuO_3N_2	N_{eq}	1.958(5,22)	O_{eq},N_{eq}	85.0(5,5)[d]	709
(not given)	$P2_1$	4.90(1)	93.5(5)		O_{eq}	1.968(5,11)		90.3(5,5.8)	
	2	11.16(2)			O_{ap}	2.48			
$Cu(salimp)NO_3$	m	7.770(1)		CuO_3N_2	O_{eq}	1.876(3)	O_{eq},O_{eq}	90.1(1)	455
(not given)	Pn	5.978(1)	101.99(1)		N_{eq}	1.961(4,25)	N_{eq},N_{eq}	83.6(2)[d]	
	2	14.403(2)			O_2NO_{eq}	2.012(3)	O_{eq},N_{eq}	93.2(2,9)	
					O_2NO_{ap}	2.672(3)		175.6(2,8)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
Cu(ox)(1,3-pn-2-ol)	m	6.384(2)		CuO_3N_2	oxO_{eq}	1.972(5,11)	N_{eq},N_{eq}	90.9(2)[e]	710
(not given)	$P2_1/c$	9.062(2)	98.32(2)		N_{eq}	1.987(5,11)	O_{eq},O_{eq}	83.5(2)[d]	
	4	13.688(2)			O_{ap}	2.394(4)	O_{eq},N_{eq}	91.9(2,2.2)	
							O_{ap},N_{eq}	95.5(2,7.3)	
							O_{ap},O_{eq}	95.8(2,2.4)	
Cu(salalgly)(2-Meim)	m	12.484(7)		CuO_3N_2	imN_{eq}	1.982(6)	O_{eq},N_{eq}	82.5(2)[d]	711
(bluish-green)	$P2_1/c$	11.573(5)	108.91(5)		N_{eq}	1.950(5)		92.2(2)[e]	
	4	9.645(4)		0.016	O_{eq}	1.955(5,35)		90.4(2,5.2)	
					O_{ap}	2.481(4)	O_{eq},O_{eq}	172.8(2)	
							N_{eq},N_{eq}	164.5(2)	
							O_{eq},O_{ap}	93.0(2,3.0)	
							N_{eq},O_{ap}	96.9(2,0.7)	
$[Cu(cbcx)(H_2O)]\cdot(ClO_4)_2$	m	15.445(3)		CuO_3N_2	N_{eq}	1.989(5,3)	N_{eq},O_{eq}	94.0(2,2)[e]	712
(blue)	$P2_1/c$	11.412(2)	116.12(2)		O_{eq}	1.961(4,3)	N_{eq},N_{eq}	86.3(2)[d]	
	4	13.745(3)		0.08	H_2O_{ap}	2.412(5)	$O_{eq}O_{eq}$	86.0(2)	
							O_{ap},N_{eq}	94.9(2,1.9)	
							O_{ap},O_{eq}	89.8(2,3.2)	
$[Cu(carboxam)(H_2O)]\cdot NO_3\cdot H_2O$	tr	11.622(3)	90.33(2)	CuO_3N_2	N_{eq}	1.976(3,1)	O_{eq},N_{eq}	82.45(10,5)[d]	713
(blue)	P-1	11.280(3)	101.85(4)		O_{eq}	1.956(2,1)		89.8(1,7.9)	
	2	8.007(3)	115.28(3)	0.077	H_2O_{ap}	2.265(4)	O_{eq},O_{eq}	171.3(1)	
							N_{eq},N_{eq}	174.5(1)	
							O_{eq},O_{ap}	94.3(1,1.5)	
							N_{eq},O_{ap}	92.6(1,3.1)	
$[Cu(medec)(H_2O)]\cdot[Cu(medec)(ClO_4)]\cdot(ClO_4)_3\cdot H_2O$	tr	12.626(3)	114.19(2)	CuO_3N_2	O_{eq}	1.952(8,12)	O_{eq},O_{eq}	87.0(4)	714
	P-1	12.891(2)	82.79(2)		N_{eq}	1.999(10,5)	O_{eq},N_{eq}	92.2(4,1.2)[e]	
	2	13.387(3)	107.07(3)	0.12	H_2O_{ap}	2.311(2)	N_{eq},N_{eq}	88.5(4)	
(deep blue)				CuO_3N_2	O_{eq}	1.940(8,6)	O_{eq},O_{eq}	88.1(4)	
					N_{eq}	1.985(10,4)	N_{eq},N_{eq}	88.5(4)	
				0.02	O_3ClO_{ap}	2.672(4)	O_{eq},N_{eq}	92.0(4,5)[e]	
$Cu(C_{12}H_{18}N_2O_2)(H_2O)$	m	21.12(2)		CuO_3N_2	N_{eq}	1.90(–,5)	N_{eq},N_{eq}	88[d]	715
(green)	$P2_1/a$	5.62(1)	104.0		O_{eq}	1.95(–,10)	N_{eq},O_{eq}	91(–,1)[e]	
	4	11.58(2)			H_2O_{ap}	2.3	O_{eq},O_{eq}	87	
							O_{eq},O_{ap}	93.5(–,2.5)	
							N_{eq},O_{ap}	97.5(–,1.5)	
$[Cu(oxap)(NO_3)]NO_3$	tr	8.957(1)	108.59(3)	CuO_3N_2	O_{eq}	1.993(3,12)	N_{eq},O_{eq}	81.0(2,4.1)[d]	716
(not given)	P-1	10.323(4)	94.72(1)		N_{eq}	1.992(5,6)		91.4(1,8.7)	
	2	9.640(2)	101.40	0.20	O_2NO_{ap}	2.391(3)	N_{eq},N_{eq}	162.1(2)	
							O_{eq},O_{eq}	169.2(1)	
							O_{eq},O_{ap}	94.7(1,12.6)	
							N_{eq},O_{ap}	92.9(2,25.3)	
$[Cu(edip)(H_2O)]\cdot H_2O$	or	6.685(1)		CuO_3N_2	N_{eq}	2.037(6,23)	O_{eq},N_{eq}	88.4(2,1.2)[d]	717
(blue)	$Pbc2_1$	15.605(4)			O_{eq}	1.940(5,28)	N_{eq},N_{eq}	85.5(2)[d]	
	4	15.159(4)		0.24	H_2O_{ap}	2.302(5)	O_{eq},O_{ap}	99.3(2,4.0)	
							O_{eq},N_{eq}	88.4(2,1.2)	
							O_{ap},N_{eq}	94.2(2,4.5)	
							N_{eq},N_{eq}	85.5(2)	
$[Cu(cpmp)(H_2O)]\cdot 3H_2O$	m	11.5711(6)		CuO_3N_2	N_{eq}	1.952(3,1)	N_{eq},O_{eq}	84.1(1)[d]	718
(not given)	$P2_1/n$	7.7308(3)	103.92(4)		O_{eq}	1.948(2,13)	N_{eq},N_{eq}	92.1(1)[e]	
	4	21.7034(3)		0.254	H_2O_{ap}	2.244(2)	O_{ap},O_{eq}	95.3(1,9)	
							N_{eq},O_{ap}	99.8(1,3.4)	
							N_{eq},O_{eq}	84.25(10,15)	
							O_{eq},O_{eq}	4.8(1)	
							N_{eq},N_{eq}	92.9(1)	
$Cu(ebsr)(H_2O)$	m	10.516(3)		CuO_3N_2	N_{eq}	2.004(6,2)	N_{eq},N_{eq}	87.2(5)[d]	719
(not given)	$P2_1/c$	12.204(3)	143.88(2)		O_{eq}	1.962(6,1)	N_{eq},O_{eq}	84.3(2,1.0)[d]	
	4	15.631(3)		0.381	H_2O_{ap}	2.181(4)	O_{eq},O_{eq}	96.2(2)	
							O_{eq},O_{ap}	100.0(2,5.9)	
							N_{eq},O_{ap}	102.4(2,9)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$Na_2[Cu(oadp)(H_2O)]\cdot 3H_2O$ (not given)	m $P2_1/c$ 4	10.596(2) 18.459(4) 7.922(1)	 105.97(1)	CuO_3N_2	O_{eq} N_{eq} H_2O_{ap}	1.957(2,8) 1.936(2,4) 2.766(2)	N_{eq},N_{eq} O_{eq},O_{eq} O_{eq},N_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	82.6(1)[d] 87.7(1) 94.3(1,0)[e] 86.4(1,1.1) 102.3(1,4)	720
Cu(phim)[c] (not given)	tr P–1 2	12.028(3) 20.378(3) 11.387(3)	113.10(2) 84.13(2) 95.99(2)	CuO_3N_2 0.027	N_{eq} O_{eq} O_{ap}	1.950(6,3) 1.912(5,1) 2.336(6)	O_{eq},N_{eq} N_{eq},N_{eq} O_{eq},O_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	94.1(2,1.3)[e] 84.4(2)[d] 88.8(2) 91.7(2,2.0) 96.3(2,9)	721
				CuO_3N_2 0.006	N_{eq} O_{eq} O_{ap}	1.957(6,5) 1.933(5,1) 2.560(5)	O_{eq},N_{eq} N_{eq},N_{eq} O_{eq},O_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	92.6(2,5)[e] 83.7(2)[d] 91.1(2) 86.2(2,8.8) 93.7(2,10.1)	
Cu(naph) (green–brown)	m C2/c 8	34.943(6) 7.027(9) 14.797(3)	 95.14(2)	CuO_3N_2 0.13	O_{eq} N_{eq} O_{ap}	1.925(3,11) 1.942(3,6) 2.534(2)	O_{eq},N_{eq} N_{eq},N_{eq} O_{eq},O_{eq}	91.4(1,3)[e] 171.3(1,8) 84.2(1) 92.1(1)	722
Cu(mg) (blue)	or $P2_12_12_1$ 4	9.889(2) 11.548(1) 9.337(2)	 	CuO_3N_2 0.182	N_{eq} O_{eq} O_{ap}	1.959(14,7.1) 1.980(13,28) 2.226(13)	N_{eq},O_{eq} N_{eq},N_{eq} O_{eq},O_{eq} O_{ap},O_{eq} O_{ap},N_{eq}	82.5(6)[d] 93.3(6,10.8) 82.4(5)[d] 89.9(6) 96.1(7,4.5) 95.5(6,11.0)	723
Cu(thpen) (dark blue)	m $P2_1/c$ 4	9.432(10) 11.772(10) 19.382(10)	 93.46(8)	CuO_3N_2	N_{eq} O_{eq} O_{ap}	2.03(2,0) 1.98(1,3) 2.22(1)	N_{eq},N_{eq} O_{eq},N_{eq} O_{eq},O_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	86.8(6)[d] 86.6(5,1.1)[d] 159.1(5,8.2) 93.8(4) 106.2(4,6.1) 80.4(5)[d] 93.3(5,12.9)	724
$[Cu(H_2O)_2Cl_2(MeOH)]\cdot C_{10}H_{20}O_5$ (blue)	m Pn 4	8.626(6) 13.631(4) 16.155(9)	 104.99(5)	CuO_3Cl_2 CuO_3Cl_2 	H_2O_{eq} Cl_{eq} $MeHO_{ap}$ H_2O_{eq} Cl_{eq} $MeHO_{ap}$	1.99(4,0) 2.26(1,1) 2.30(2) 1.99(2,1) 2.24(1,0) 2.32(3)	Cl_{eq},Cl_{eq} O_{eq},Cl_{eq} O_{eq},O_{eq} O_{ap},Cl_{eq} O_{ap},O_{eq} Cl_{eq},Cl_{eq} O_{eq},Cl_{eq} O_{eq},O_{eq} O_{ap},Cl_{eq} O_{ap},O_{eq}	164(1) 90(1,3) 176(1) 98(1,2) 89(1,1) 163(1) 89(1,4) 171(1) 98(1,2) 94(1,2)	725
$[Cu(ura)(H_2O)Cl]_2\cdot 6H_2O$ (deep green)	m $P2_1/n$ 4	7.358(1) 20.452(4) 13.130(3)	 93.23(2) 0.215	CuO_3NCl	N_{eq} O_{eq} H_2O_{eq} Cl_{ap}	1.958(3) 1.921(3,21) 1.961(3) 2.611(2)	N_{eq},O_{eq} O_{eq},O_{eq} O_{eq},N_{eq} O_{eq},Cl_{ap} N_{eq},Cl_{ap}	91.3(1,1.1)[e] 91.3(1,1.1) 91.3(1,1.1) 95.9(1,6.9) 97.8(1)	726
Cu(salalgly)(tu) (black-green)	m C2/c 8	18.599(11) 14.275(5) 13.617(6)	 138.64(4)	CuO_3NS	O_{eq} N_{eq} tuS_{eq} O_{ap}	1.927(8,31) 1.933(7) 2.273(3) 2.771(7)	O_{eq},N_{eq} O_{eq},N_{eq} O_{eq},N_{eq} N_{eq},O_{ap} N_{eq},S_{eq} O_{eq},O_{eq} O_{eq},O_{ap} O_{eq},S_{eq} O_{ap},S_{eq}	83.3(3)[d] 93.4(4)[e] 88.4(4,5.1) 97.2(3) 160.2(3) 177.1(3) 87.3(3,2.9) 92.8(3,8.1) 97.8(2)	727
Cu(5′–imp)(bpy)·$(H_2O)]NO_3\cdot H_2O$ (deep blue)	or $P2_12_12_1$ 4	16.197(6) 23.580(7) 6.974(3)	 	CuN_3O_2 0.142	$inapN_{eq}$ $bpyN_{eq}$ H_2O_{eq} H_2O_{ap}	1.993(6) 2.006(6,3) 1.987(6) 2.287(6)	not given		728

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
Cu(bpy)(tsgly) · (EtOH) (blue-green)	m $P2_1/n$ 4	9.677(1) 10.460(1) 21.488(2)	98.27(1)	CuN_3O_2 0.077	$bpyN_{eq}$ $glyN_{eq}$ $glyO_{eq}$ $EtHO_{ap}$	1.999(5,3) 1.946(4) 1.940(4) 2.382(4)	N_{eq},N_{eq} N_{eq},O_{eq} N_{eq},O_{ap} O_{eq},O_{ap}	81.0(2)[d] 92.0(2,11.0) 84.2(2)[d] 88.5(2,4.3) 92.8(2,6.9) 91.0(2)	729
[Cu(bpy)(L–asp)(H_2O)] · $3H_2O$ (blue)	or $P2_12_12_1$ 4	21.978(2) 11.275(1) 6.841(1)		CuN_3O_2 0.126	$bpyN_{eq}$ $aspN_{eq}$ $aspO_{eq}$ H_2O_{ap}	2.001(5,12) 1.989(5) 1.937(4) 2.368(5)	N_{eq},N_{eq} O_{eq},N_{eq} O_{ap},O_{eq} O_{ap},N_{eq}	81.3(2)[d] 92.1(2,10.8) 84.5(2)[d] 88.3(2,3.8) 92.5(2) 94.2(2,8.7)	730
[Cu(bpy)(L–tyr)(H_2O)] · Cl · $3H_2O$ (blue)	hx $P6_1$ 6	9.307(2) 44.432		CuN_3O_2 0.165	$bpyN_{eq}$ $tyrN_{eq}$ $tyrO_{eq}$ H_2O_{ap}	2.006(6,12) 1.978(6) 1.939(5) 2.308(6)	N_{eq},N_{eq} O_{eq},N_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	80.8(3)[d] 92.0(3,11.2) 84.0(2)[d] 87.3(2,3.3) 93.3(3) 95.5(3,6.3)	731
[Cu(bpy)(L–ala)(H_2O)] $NO_3 \cdot H_2O$ (blue)	or $P2_12_12_1$ 4	19.113(3) 15.079(2) 5.782(1)		CuN_3O_2 0.289	$bpyN_{eq}$ $alaN_{eq}$ $alaO_{eq}$ H_2O_{ap}	2.010(4,28) 1.991(4) 1.962(4) 2.230(4)	N_{eq},N_{eq} N_{eq},O_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	81.8(2)[d] 90.3(2,8.5) 84.5(2)[d] 88.4(2,3.9) 101.8(2) 97.1(2,8.6)	731
[Cu(bpy)(topa)(H_2O)] · $BF_4 \cdot 3H_2O$ (green)	m $P2_1/a$ 4	16.259(8) 10.007(1) 16.24(4)	114.12(3)	CuN_3O_2 0.17	$bpyN_{eq}$ $topaN_{eq}$ $topaO_{eq}$ H_2O_{ap}	1.983(8,2) 2.007(8) 1.946(8) 2.317(9)	N_{eq},N_{eq} O_{eq},N_{eq} N_{eq},O_{ap} O_{eq},O_{ap}	81.3(3)[d] 91.7(4,10.0) 87.4(4,4.1) 95.1(4,2.2) 97.1(3)	732
Cu(bpy)(glyno)(H_2O) (blue)	m $P2_1/c$ 4	8.494(5) 19.950(4) 11.295(7)	110.79(4)	CuN_3O_2 0.216(1)	$bpyN_{eq}$ $glyN_{eq}$ $glyO_{ep}$ H_2O_{ap}	2.004(3,25) 1.962(3) 1.938(3) 2.355(3)	N_{eq},N_{eq} N_{eq},O_{eq} N_{eq},O_{ap} O_{eq},O_{ap}	80.8(1)[d] 103.7(1) 84.3(1)[d] 90.1(1) 88.8(1,3.0) 97.7(1) 108.9(1)	733
[Cu(bpy)(tsnO)] · H_2O (blue-violet)	m $P2_1/c$ 4	12.42(9) 10.233(4) 17.773(7)	101.65(2)	CuN_3O_2 0.064	$bpyN_{eq}$ N_{eq} O_{eq} O_{ap}	1.996(6,2) 1.974(6) 1.948(4) 2.447(4)	N_{eq},N_{eq} O_{eq},N_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	80.8(2)[d] 99.0(1)[e] 84.6(2)[d] 96.0(2) 94.4(2,11.0) 85.0(2)	661
Cu(dnsglyNO)(bpy) · (MeOH) (not given)	m $P2_1$ 2	13.980(4) 11.087(3) 8.315(3)	102.5(1)	CuN_3O_2 0.108	$bpyN_{eq}$ $glyN_{eq}$ $glyO_{eq}$ $MeOH_{ap}$	1.97(1,1) 1.96(1) 1.97(1) 2.37(1)	N_{eq},N_{eq} O_{eq},N_{eq} N_{eq},O_{ap} O_{eq},O_{ap}	80.7(5)[d] 93.9(5,13.2) 83.2(5)[d] 86.7(5,3.5) 95.4(4,8.5) 91.5(4)	664
[Cu(phen)(L–glu) · (H_2O)] · $3H_2O$[c] (blue)	m $P2_1$ 4	12.168(2) 22.222(3) 7.591(1)	106.10(2)	CuN_3O_2 0.123	$phenN_{eq}$ $gluO_{eq}$ $gluN_{eq}$ H_2O_{ap}	2.017(5,2) 1.913(4) 2.020(5) 2.294(6)	N_{eq},N_{eq} O_{eq},N_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	82.4(2)[d] 92.2(2,9.8) 84.7(2)[d] 87.5(2,2.8) 98.3(2) 92.7(2,1.9)	734
				CuN_3O_2 0.186	$phenN_{eq}$ $gluO_{eq}$ $gluN_{eq}$ H_2O_{ap}	2.015(5,15) 1.926(4) 2.003(6) 2.225(8)	N_{eq},N_{eq} N_{eq},O_{eq} O_{eq},O_{ap}	82.2(2)[d] 91.6(2,9.4) 83.7(2)[d] 96.8(3)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
[Cu(phen)(ileu)(H_2O)]· NO_3[c]	tr	12.362(2)	107.82(2)	CuN_3O_2	phenN_{eq}	1.995(7,1)	N_{eq},N_{eq}	82.3(3)[d]	735
	P1	11.593(2)	76.05(2)		ileuO_{eq}	1.919		90.1(3,5.8)	
(not given)	2	7.311(2)	93.62(2)		ileuN_{eq}	1.989(8)	O_{eq},N_{eq}	86.5(3)[d]	
					H_2O_{ap}	2.253(5)		89.3(3,2.9)	
							N_{eq},O_{ap}	95.9(3,7.9)	
							O_{eq},O_{ap}	90.1(2)	
				CuN_3O_2	phenN_{eq}	2.021(7,16)	N_{eq},N_{eq}	81.0(3)[d]	
					leuO_{eq}	1.940(5)		97.1(3,10.7)	
					leuN_{eq}	1.975(11)	O_{eq},N_{eq}	81.2(3)[d]	
					H_2O_{ap}	2.226(6)		81.7(3,5.9)	
							N_{eq},O_{ap}	97.5(3,3.4)	
							O_{eq},O_{ap}	93.7(2)	
[Cu(phen)(phalan) ·	m	5.782(2)		CuN_3O_2	phenN_{eq}	1.989(9,21)	N_{eq},N_{eq}	82.9(4)[d]	736
(H_2O)]NO_3 · H_2O	$P2_1$	20.700(6)	97.58(2)		alanN_{eq}	2.004(9)		90.6(4,7.7)	
(not given)	2	9.355(3)		0.23	alanO_{eq}	1.927(6)	N_{eq},O_{eq}	84.2(3)[d]	
					H_2O_{ap}	2.213(10)		88.0(4,3.8)	
							O_{eq},O_{ap}	103.9(3)	
							N_{eq},O_{ap}	94.3(4,2.1)	
[Cu(bampy)(H_2O)]ClO_4	tr	15.001(6)	108.3(1)	CuN_3O_2	N_{eq}	1.990(5,9)	N_{eq},N_{eq}	81.9(2)[d]	737
(green)	P-1	8.803(4)	111.8(1)		O_{eq}	1.957(4)		92.1(2,10.2)	
	2	9.099(6)	84.3(1)	0.20	N_{eq}	2.021(5)	O_{eq},N_{eq}	81.8(2)[d]	
					H_2O_{ap}	2.256(5)		88.6(2,6.8)	
							O_{eq},O_{ap}	85.4(1)	
							N_{eq},O_{ap}	99.4(2,8.2)	
[Cu(bpy)(pal)(NO_3)]NO_3	tr	8.388(2)	99.37(1)	CuN_3O_2	bpyN_{eq}	2.010(4,5)	N_{eq},N_{eq}	80.9(1)[d]	738
(bluish green)	P-1	8.727(1)	76.82(2)		palO_{eq}	1.970(4,25)	O_{eq},O_{eq}	95.5(1)[e]	
	2	15.483(2)	117.05(1)	0.105	O_2NO_{ap}	2.388(4)	O_{eq},N_{eq}	91.6(1,4.8)	
							O_{eq},O_{ap}	93.5(1,2.0)	
							N_{eq},O_{ap}	92.2(1,1.15)	
$Cu(psal)_2(py)$	m	28.79(5)		CuN_3O_2	N_{eq}	2.005(6,3)	O_{eq},N_{eq}	91.6(2,4)[e]	739
(green)	C_c2 or C_c	8.95(3)	94°50		O_{eq}	1.889(7,1)		89.4(3,2.7)	
	8	19.77(5)		0.21	pyN_{ap}	2.308(6)	O_{eq},O_{eq}	169.6(3)	
							N_{eq},N_{eq}	166.2(2)	
							O_{eq},N_{ap}	95.3(3,2.0)	
							N_{eq},N_{ap}	96.9(2,1.4)	
$Cu(Me_4rol)_2(py)$	tr	11.477(3)		CuN_3O_2	O_{eq}	1.94(1,0)	O_{eq},N_{eq}	90.1(7)[e]	740
(not given)	$P3_12_2$	27.406(5)			N_{eq}	2.03(2,0)		89.9(7,2)	
				0.12	pyN_{ap}	2.49(2)			
[Cu(carbam)(H_2O)$_2$]NO_3 ·	tr	6.811(1)	88.65(1)	CuN_3O_2	N_{eq}	1.976(1,38)	N_{eq},N_{eq}	81.93(5,6)[d]	713
$2H_2O$	P-1	10.211(1)	82.32(1)		H_2O_{eq}	1.966(1)	N_{eq},O_{eq}	97.30(5,1.44)	
(blue)	2	12.039(1)	89.79(1)	0.22	H_2O_{ap}	2.262(1)	N_{eq},O_{ap}	98.69(5,10.9)	
							O_{eq},N_{ap}	92.04(6)	
[Cu(bta)$_3$(SO_4)(H_2O)] ·	m	7.294(3)		CuN_3O_2	btaN_{eq}	2.006(5,16)	N_{eq},N_{eq}	89.95(20,65)	741
bta	$P2_1/c$	19.744(3)	82.97(3)		O_3SO_{ap}	1.980(5)	O_{eq},N_{eq}	96.0(2,4.2)	
(deep blue)	4	19.227(5)		0.157	H_2O_{ap}	2.202(5)	N_{eq},O_{ap}	89.35(20,1.95)	
							O_{eq},O_{ap}	90.0(2)	
[Cu(pcpx)(ac)(H_2O)] ·	tr	7.416(2)	74.55(3)	CuN_3O_2	pcpxN_{eq}	1.982(2,35)	N_{eq},N_{eq}	81.9(1,3)[d]	742
H_2O	P-1	8.632(4)	84.84(3)		acO_{eq}	1.942(2)	N_{eq},O_{eq}	97.4(1,1)	
(deep green)	2	13.034(3)	81.04(5)		H_2O_{ap}	2.338(2)	N_{eq},O_{ap}	95.5(1,3.0)	
							O_{eq},O_{ap}	91.5(1)	
Cu(mpid)(ac)(H_2O)[c]	tr	7.392(3)	92.03(3)	CuN_3O_2	mpidN_{eq}	1.963(6,65)	O_{eq},N_{eq}	91.25(30,65)	743
(green)	P-1	13.782(5)	104.11(5)		acO_{eq}	1.972(6)	N_{eq},N_{eq}	90.1(4,6)[e]	
	4	23.422(2)	109.98(4)		H_2O_{ap}	2.466(7)	O_{ap},N_{eq}	98.9(3,12.1)	
							O_{ap},O_{eq}	91.7(3)	
				CuN_3O_2	mpidN_{eq}	1.972(7,76)	N_{eq},N_{eq}	92.2(3,1.7)	
					acO_{eq}	1.980(7)	N_{eq},N_{eq}	90.0(3,1.0)[e]	
					H_2O_{ap}	2.426(7)	O_{ap},N_{eq}	95.9(3,10.9)	
							O_{ap},O_{eq}	97.2(3)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
Cu(tph)(benz)(H_2O)	m	18.949(9)		CuN_3O_2	$benzN_{eq}$	1.977(3,41)	N_{eq},N_{eq}	84.5(1)[d]	744
(brown)	$P2_1/c$	8.279(2)	101.60(3)		$benzO_{eq}$	1.902(2)		89.6(1,5.1)	
	4	13.499(6)		0.536	$tphN_{eq}$	2.000(3)	N_{eq},O_{eq}	91.5(1)[e]	
					H_2O_{ap}	2.740(3)		90.0(1,1.6)	
							N_{eq},O_{ap}	90.89(1,4)	
							O_{eq},O_{ap}	103.7(1)	
[Cu(ggly)(mad)(H_2O)] ·	tr	10.419(7)	96.87(4)	CuN_3O_2	$madN_{eq}$	2.021(4)	O_{eq},N_{eq}	82.6(2)[d]	745
$4H_2O$	P–1	14.146(10)	108.50(4)		$gglyN_{eq}$	1.970(4,53)		88.4(2,5.8)	
(purple blue)	2	6.844(1)	68.91(5)	0.12	$gglyO_{eq}$	1.963(4)	N_{eq},N_{eq}	82.4(2)[d]	
					H_2O_{ap}	2.347(4)		91.0(2,8.6)	
							N_{eq},O_{ap}	97.1(2,4.1)	
							O_{eq},O_{ap}	90.1(2)	
Cu(terpy)(pnp) ·	m	10.387(1)		CuN_3O_2	$terN_{eq}$	1.988(5,68)	N_{eq},N_{eq}	80.7(2,3)[d]	746
(ClO_4)	$P2_1/c$	13.103(1)	98.59(4)		$pnpO_{eq}$	1.872(3)	N_{eq},O_{eq}	99.4(2,2.2)	
(dark green)	4	16.153(2)		0.21	O_3ClO_{ap}	2.562(4)	N_{eq},O_{ap}	86.8(2,14.7)	
							O_{eq},O_{ap}	109.7(2)	
$Cu(semqu)(NO_3)_2$	tr	8.380(3)	91.5(3)	CuN_3O_2	N_{eq}	1.980(6,24)	O_{eq},N_{eq}	98.3(2,4.0)	747
(green)	P–1	11.366(4)	97.37(4)		O_2NO_{eq}	2.001(5)	N_{eq},N_{eq}	80.3(2)[d]	
	2	8.831(3)	107.80(4)	0.17	O_2NO_{ap}	2.312(5)		90.6(2)[e]	
								85.5(2,5.2)	
							O_{eq},O_{ap}	102.0(3)	
							N_{eq},O_{ap}	92.5(2,2.5)	
$Cu(nbbim)(NO_3)$	m	14.497(3)		CuN_3O_2	N_{eq}	1.984(7,84)	N_{eq},N_{eq}	82.8(3,2)[d]	748
(not given)	$P2_1/c$	14.401(3)	137.5(1)		O_2NO_{eq}	1.987(7)	N_{eq},O_{eq}	97.1(3,1.4)	
	4	15.613(4)			O_2NO_{ap}	2.631(5)	N_{eq},O_{ap}	113.2(3,17.0)	
							O_{eq},O_{ap}	53.5(3)[g]	
$[Cu(ibbim)(NO_3)]NO_3$	or	29.55(1)		CuN_3O_2	$bimN_{eq}$	1.982(6,105)	N_{eq},N_{eq}	83.2(2,2)[d]	748
(not given)	Pbca	16.366(3)			O_2NO_{eq}	2.038(6)	N_{eq},O_{eq}	97.79(2,1.8)	
	8	9.380(2)			O_2NO_{ap}	2.482(6)	N_{eq},O_{ap}	88.8(2,5.4)	
							O_{eq},O_{ap}	53.6(3)[g]	
Cu(2-C1bez)(ppzb)	m	15.887(2)		CuN_3O_2	N_{eq}	1.979(9,2)	O_{eq},O_{eq}	64.7(3)[g]	749
(not given)	$P2_1/n$	18.783(2)	96.06(2)		$ClbezO_{eq}$	2.028(8,15)			
	4	12.531(2)			N_{ap}	2.171(9)			
$[Cu(terpy)(Cla)] \cdot H_2O$	m	22.19(2)		CuN_3O_2	N_{eq}	1.992(3,61)	N_{eq},N_{eq}	80.1(1,1)[d]	750
(not given)	C2/c	13.614(5)	119.71(8)		$ClaO_{eq}$	2.059(2)	N_{eq},O_{eq}	97.7(1,1.3)	
	8	15.32(1)			$ClaO_{ap}$	2.041(2)		136.82(9)	
							O_{ap},N_{eq}	43.42(9)	
								97.7(1,1.1)	
							O_{ap},O_{eq}	79.71(8)	
[Cu(ox)(dien)] ·	m	12.287(17)		CuN_3O_2	$dienN_{eq}$	2.009(8,13)	N_{eq},N_{eq}	85.1(3,1)[d]	751
$4H_2O$	$P2_1/c$	6.559(8)	108.38(10)		O_{eq}	1.965(6)	N_{eq},O_{eq}	94.4(3,1.1)	
(royal blue)	4	17.541(23)		0.23	O_{ap}	2.230(6)	N_{eq},O_{ap}	102.8(3,1.1)	
							O_{eq},O_{ap}	78.8(2)[d]	
Cu(pydca)(Me_4pn)	m	14.970(2)		CuN_3O_2	O_{eq}	2.027(1,14)	O_{eq},N_{eq}	80.1(1,3)[d]	752
(blue)	$P2_1/c$	7.290(1)	106.64(2)		N_{eq}	1.915(2)		93.8(1,13.9)	
	4	14.822(2)		0.308	pnN_{eq}	2.011(2)	N_{eq},N_{eq}	158.0(1)	
					pnN_{ap}	2.255(2)	O_{eq},O_{eq}	157.8(1)	
							O_{eq},N_{ap}	99.7(1,3.8)	
							N_{eq},N_{ap}	95.9(1)[e]	
								100.7(1,4.8)	
Cu(dbm)(imiso)	m	20.520(4)		CuN_3O_2	$dbmN_{eq}$	1.977(5,73)	O_{eq},O_{ap}	88.1(2)[e]	753
(green)	$P2_1/n$	11.187(2)	96.83(5)		N_{eq}	2.056(5)	N_{eq},N_{eq}	89.4(2,4)[e]	
	4	12.658(3)			O_{eq}	1.954(4)	O_{ap},N_{eq}	98.4(2,11.7)	
					O_{ap}	2.178(5)	O_{eq},N_{eq}	90.9(2,7)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
[Cu(ida)(bpy)] · $6H_2O$ (not given)	tr P–1 2	11.200(7) 13.252(8) 7.975(7)	66.8(1) 115.3(1) 102.0(1)	CuN_3O_2	$bpyN_{eq}$ N_{eq} O_{eq} O_{ap}	2.008(3,19) 2.034(2) 1.952(2) 2.249(2)	N_{eq},N_{eq} N_{eq},O_{eq} N_{eq},O_{ap} O_{eq},O_{ap}	81.2(1)[d] 90.4(1,9.2) 85.6(1)[d] 90.2(1,4.6) 91.3(1,10.5) 95.3(1)	754
[Cu(tph)(benzdm)] · H_2O (deep violet)	m Pc 2	10.689(2) 6.925(3) 15.463(4)	 100.27(2) 	CuN_3O_2	N_{eq} O_{eq} $tphN_{eq}$ tpO_{ap}	2.004(3,65) 1.930(2) 1.956(3) 2.919(3)	N_{eq},N_{eq} N_{eq},O_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	84.8(1)[d] 89.1(1,4.3) 90.2(2)[e] 90.9(1,7) 87.5(1) 73.2(1)[d] 92.7(1,19.5)	755
Cu(asp)(hist)[c] (blue)	m $P2_1$ 4	10.913(3) 12.911(4) 10.206(3)	 113.83(2) 	CuN_3O_2 0.023 CuN_3O_2 0.099	$aspN_{eq}$ $aspO_{eq}$ N_{eq} O_{ap} $aspN_{eq}$ $aspO_{eq}$ N_{eq} O_{eq}	1.994(6) 1.952(6) 1.987(7,44) 2.394(6) 1.991(8) 1.957(7) 2.008(7,16) 2.285(7)	N_{eq},N_{eq} O_{eq},N_{eq} N_{eq},O_{ap} O_{eq},O_{ap} N_{eq},N_{eq} O_{eq},N_{eq} N_{eq},O_{ap} O_{eq},O_{ap}	92.7(3)[e] 92.3(3,5) 83.6(3)[d] 87.8(3,4.2) 74.2(3)[d] 85.8(3,11.6) 106.7(2) 88.9(3)[e] 92.9(3,4.0) 88.3(3)[d] 86.9(3,3.6) 74.3(3)[d] 86.9(3,12.6) 112.4(3)	756
[Cu(L–ala)(L–hist)] · $3.5H_2O$ (violet)	or $P2_12_12$ 4	10.037(7) 14.477(10) 9.735(7)		CuN_3O_2	N_{eq} $alaO_{eq}$ $alaO_{ap}$	1.955(6,34) 2.038(5) 2.527(5)	N_{eq},N_{eq} N_{eq},O_{ap} N_{eq},O_{eq} O_{eq},O_{ap}	84.5(2)[d] 93.4(2)[e] 89.0(2,4.5) 103.0(2,18.0) 91.3(2,2.5) 55.4(2)[g]	757
$Cu(dsf)_2$ (green)	m $P2_1$ 2	10.412(1) 6.656(4) 16.788(1)	 98.59(3) 	CuN_3O_2 0.154	O_{eq} N_{eq} N_{ap}	1.982(4,34) 1.958(4,33) 2.340(4)	O_{eq},N_{eq} O_{eq},O_{eq} N_{eq},N_{eq} O_{eq},N_{ap} N_{eq},N_{ap}	81.8(1)[d] 90.2(1)[e] 87.1(1,5.3) 171.1(1) 165.0(2) 93.7(1,6.4) 75.0(1)[d] 96.3(2,21.3)	758
$Cu\{Me_2N(CH_2)_2 \cdot MeN(CH_2)_2O\}_2$ (not given)	m Cc 2	16.405(12) 10.192(6) 12.038(10)	 113.60(7) 	CuN_3O_2	N_{eq} O_{eq} N_{ap}	2.107(14,5) 1.890(17,3) 2.598(12)	not given		357
$[Cu(amsal)(H_2O)]PF_6$ (dark violet)	m $P2_1/c$ 4	10.182(2) 14.863(3) 11.188(2)	 98.6(1) 	CuN_3O_2 0.174	O_{eq} N_{eq} H_2O_{ap}	1.89(1) 1.98(17) 2.38(1)	O_{eq},N_{eq} N_{eq},N_{eq} N_{eq},O_{ap} O_{eq},O_{ap}	94.7(5)[e] 95.0(5,3) 84.1(5,1)[d] 94.9(5,6.7) 95.6(4)	759
$[Cu(monsal)(ClO_4)] \cdot ClO_4$ (dark violet)	tr P–1 2	8.787(2) 9.907(1) 12.393(3)	93.05(6) 109.51(6) 97.93(6)	CuN_3O_2 0.078	O_{eq} N_{eq} O_3ClO_{ap}	1.894(3) 1.984(5,53) 2.634(5)	N_{eq},O_{eq} N_{eq},N_{eq} O_{eq},O_{ap} N_{eq},O_{ap}	95.1(2)[c] 95.0(2,1) 85.3(2,6)[d] 89.1(2) 93.6(2,7.3)	760
$[Cu(C_9H_{11}N_3OS)(py)] \cdot NO_3$ (not given)	m C2/c 8	19.835(9) 15.069(8) 13.701(7)	 119.65(8) 	CuN_3O_2 0.03	pyN_{eq} N_{eq} O_{eq} O_{ap}	1.999(9) 1.960(8,2) 1.916(7) 2.81	N_{eq},N_{eq} N_{eq},O_{eq} 	80.6(3)[d] 88.8(3,8.2) 91.9(3)[e] 91.2(3.7)	761

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
[Cu(btos)(py)]·EtOH	tr	10.525(2)	95.25(1)	CuN_3O_2	pyN_{eq}	1.998(3)	N_{eq},N_{eq}	89.0(1)[e]	762
(not given)	P–1	12.072(2)	113.00(1)		N_{eq}	1.946(3,5)		94.3(1,5.3)	
	2	12.624(2)	110.15(1)		O_{eq}	1.937(2)	O_{eq},N_{eq}	80.03(9)	
					O_{ap}	2.846(2)	O_{eq},N_{ap}	80.03(9)[d]	
								87.38(9,7.35)	
							O_{eq},O_{ap}	116.53(8)	
							N_{eq},O_{ap}	56.87(8)[g]	
								84.47(814.41)	
[Cu(edms)(im)]·$2H_2O$	m	8.663(3)		CuN_3O_2	imN_{eq}	1.968(4)	O_{eq},O_{ap}	87.7(1)[d]	763
(not given)	$P2_1/c$	10.792(6)	100.82(2)		N_{eq}	2.005(4,15)	O_{eq},N_{eq}	91.7(2)[e]	
	4	14.658(9)			O_{eq}	1.996(3)		90.6(2,1.1)	
					O_{ap}	2.320(3)	N_{eq},N_{eq}	85.2(2)[d]	
								89.6(2,4.4)	
							O_{ap},N_{eq}	95.6(2,17.7)	
[Cu(pyala)].$2H_2O$	or	5.877(2)		CuN_3O_2	N_{eq}	2.00(1,11)	O_{eq},O_{eq}	96.5(5)	764
(blue)	$P2_12_12_1$	11.535(2)			O_{eq}	1.93(1,4)	O_{eq},N_{eq}	83.7(6,2.4)d	
	4	28.09(1)			N_{ap}	2.38(1)	O_{eq},N_{ap}	94.7(5,2.6)	
							N_{eq},N_{ap}	85.7(5)e	
								96.5(5,10.8)	
							N_{eq},N_{eq}	95.3(6,6)	
Cu(acpn)	m	11.65(4)		CuN_3O_2	O_{eq}	1.942(1,0)	N_{eq},O_{eq}	87.85(6,0)[e]	765
(green)	C2/c	18.481(6)	93.53(3)		N_{eq}	2.006(2)		89.68(6,1.83)	
	4	14.019(3)			N_{ap}	2.291(4)	O_{eq},O_{eq}	73.68(8)	
							N_{eq},N_{eq}	168.48(9)	
							N_{eq},N_{ap}	104.9(1)[h]	
								95.8(1,9.2)	
							O_{eq},N_{ap}	93.15(20,2.55)	
[Cu(ghl)]·$15H_2O$	tg	14.937(4)		CuN_3O_2	O_{eq}	1.96	N_{eq},N_{eq}	91.7(–,2.0)[d]	766
(dark blue)	$P4_12_12$	25.903(9)			N_{eq}	1.97(–,9)	N_{eq},O_{ap}	92.1(–,11.0)	
	($P4_32_12$)				O_{ap}	2.49	N_{eq},O_{eq}	96.5(–,3.9)	
Cu(mbp)	tr	10.073(2)	73.89(2)	CuN_3O_2	O_{eq}	1.938(5,13)	O_{eq},O_{eq}	152.3(3)	767
(dark green)	P–1	12.438(3)	67.54(1)		N_{eq}	1.967(5,16)	O_{eq},N_{eq}	89.6(2,0)[e]	
	2	13.080(3)	86.99(2)	0.159	N_{ap}	2.374(10)		90.0(2,2.6)	
							O_{eq},N_{ap}	103.8(3,2.8)	
							N_{eq},N_{ap}	87.6(3,1.4)	
Cu(dpthn)	m	6.753(2)		CuN_3O_2	N_{eq}	2.043(2,5)	O_{eq},N_{eq}	89.41(9,25)[d]	768
(blue)	$P2_1/c$	13.229(6)	95.22(3)		O_{eq}	1.937(2,1)	N_{eq},N_{eq}	87.58(9)[d]	
(at 150K)	4	19.702(8)		0.228	N_{ap}	2.282(2)	O_{eq},O_{eq}	90.65(9)	
							N_{eq},N_{ap}	82.28(9.75)[d]	
							O_{eq},N_{ap}	110.06(8,50)	
Na[Cu(tes)]·$3H_2O$	tr	7.473(3)	81.13(5)	CuN_3O_2	O_{eq}	1.978(5,4)	O_{eq},O_{eq}	87.9(2)	769
(blue)	P–1	10.826(5)	84.75(4)		N_{eq}	2.064(6,26)	N_{eq},O_{eq}	93.4(2)[e]	
	2	14.593(9)	79.39(3)		N_{ap}	2.197(7)		93.1(2,3)	
							N_{eq},N_{eq}	86.0(2)[d]	
							O_{eq},N_{ap}	100.4(3,6.0)	
							N_{eq},N_{ap}	84.8(3)[d]	
							N_{eq},N_{ap}	85.4(3,6)	
$Cu(4\text{–}Methz)_3Cl_2$	m	14.147(6)		CuN_3Cl_2	N_{eq}	2.058(3,15)	N_{eq},N_{eq}	88.37(12,25)	770
(green)	$P2_1/a$	8.621(6)	115.36(3)		Cl_{eq}	2.319(1)	Cl_{eq},N_{eq}	89.22(9,2.70)	
	4	16.035(7)		0.35	Cl_{ap}	2.461(1)	N_{eq},Cl_{ap}	97.42(10,5.67)	
							Cl_{eq},Cl_{ap}	104.71(4)	
$Cu(terpy)Cl_2$	m	16.088(8)		CuN_3Cl_2	N_{eq}	2.020(5,68)	N_{eq},N_{eq}	78.9(4,4)[d]	771
(light green)	$P2_1/a$	8.249(5)	94.66(3)		Cl_{eq}	2.252(5)	N_{eq},Cl_{eq}	98.5(4,1.3)	
	4	10.680(4)		0.26	Cl_{ap}	2.469(5)	Cl_{eq},Cl_{ap}	104.5(4)	
							Cl_{ap},N_{eq}	96.9(4,4.5)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(terpy)Cl_2]\cdot H_2O$ (dark green)	m C2/c 8	17.18(1) 9.54(1) 18.76(1)	 96.8(1) 	CuN_3Cl_2 0.33	N_{eq} Cl_{eq} Cl_{ap}	2.009(3,65) 2.221(1) 2.554(1)	N_{eq},N_{eq} Cl_{eq},N_{eq} Cl_{eq},Cl_{ap} N_{eq},Cl_{ap}	79.5(1,0)[d] 98.7(1,3) 100.9(1) 95.9(1,1.5)	771
$Cu(bpno)Cl_2$ (green)	m $P2_1/c$ 4	11.737(4) 11.744(4) 15.326(4)	 94.03(2) 	CuN_3Cl_2 0.35	N_{eq} Cl_{eq} Cl_{ap}	2.039(4,156) 2.231(1) 2.495(1)	N_{eq},N_{eq} Cl_{eq},N_{eq} N_{eq},Cl_{ap} Cl_{eq},Cl_{ap}	80.1(1,4)[d] 97.6(1,1) 93.8(1,2.4) 113.3(1)	772
$[Cu(pyh)Cl_2\cdot 0.5H_2O$ (dark green)	m C2/c 8	15.698(3) 9.135(2) 19.378(4)	 90.91(1) 	CuN_3Cl_2 0.232	N_{eq} Cl_{eq} Cl_{ap}	2.008(4,37) 2.280(1) 2.587(1)	N_{eq},N_{eq} Cl_{eq},N_{eq} N_{eq},Cl_{ap} Cl_{eq},Cl_{ap}	79.7(1)[d] 91.0(2)[e] 93.3(1,4) 94.7(1,1.6) 100.7(1)	773
$[Cu(bzimp)Cl_2]\cdot dmf$ (green)	m $P2_1/n$ 4	9.150(1) 12.908(3) 18.964(4)	 93.33(1) 	CuN_3Cl_2 0.260	N_{eq} Cl_{eq} Cl_{ap}	2.029(7,29) 2.215(3) 2.559(3)	N_{eq},N_{eq} N_{eq},Cl_{eq} N_{eq},Cl_{ap} Cl_{eq},Cl_{ap}	78.5(3,2)[d] 99.7(2,1) 94.2(2,5.1) 103.53(9)	774
$[Cu(dapd)Cl_2]\cdot 2H_2O$ (not given)	tr P–1 2	7.992(2) 10.282(3) 10.462(3)	105.15(2) 107.05(2) 106.43(2)	CuN_3Cl_2	N_{eq} Cl_{eq} Cl_{ap}	2.010(3,78) 2.220(1) 2.463(1)	N_{eq},N_{eq} Cl_{eq},N_{eq} N_{eq},Cl_{ap} Cl_{eq},Cl_{ap}	77.6(1,1)[d] 99.5(1,5.6) 98.2(1,2.6) 101.73(2)	775
α–$[Cu(tioim)_3](BF_4)_2$ (blue)	m $P2_1/n$ 4	12.796(6) 12.742(3) 19.788(3)	 95.38(3) 	CuN_3S_2	S_{eq} N_{eq} S_{ap}	2.398(2) 1.985(5,45) 2.616(2)	N_{eq},N_{eq} N_{eq},S_{eq} N_{eq},S_{ap} S_{eq},S_{ap}	90.6(2,2.4) 91.5(2)[e] 89.0(2,2.0) 91.4(2,9) 92.5(2)[e] 100.66(9)	776
$Cu(9\text{–}aneN_3)Br_2$ (green)	tr P–1 2	7.031(1) 7.623(1) 10.241(2)	86.61(1) 76.37(1) 77.27(1)	CuN_3Br_2	N_{eq} Br_{eq} N_{ap}	2.047(1,1) 2.433(1,12) 2.230(4)	N_{eq},N_{eq} Br_{eq},Br_{eq} Br_{eq},N_{eq} Br_{eq},N_{ap} N_{eq},N_{ap}	82.32(17)[d] 93.26(3) 91.08(12,84) 107.16(12,1.11) 82.90(17,57)[d]	777
$Cu(paphy)Br_2$ (green)	m $P2_1/n$ 4	12.86(2) 11.944(5) 8.770(7)	 97.17(6) 	CuN_3Br_2	N_{eq} Br_{eq} Br_{ap}	2.01(5,3) 2.37(5) 2.62(6)	N_{eq},N_{eq} N_{eq},Br_{eq} N_{eq},Br_{ap} Br_{eq},Br_{ap}	78.6(5,6)[d] 99.6(3,9) 94.8(3,1.9) 103.2(9)	778
$Cu(imaz)Br_2$ (green)	m Cc 4	7.540(1) 13.613(2) 13.537(3)	 95.69(2) 	CuN_3Br_2	N_{eq} Br_{eq} Br_{ap}	2.015(10,24) 2.436(2) 2.609(2)	N_{eq},N_{eq} Br_{eq},N_{eq} N_{eq},Br_{ap} Br_{eq},Br_{ap}	87.6(4)[e] 80.1(4)[d] 83.9(4,3.9) 92.9(3,1.1) 98.8(3,2.3) 107.2(1)	779
$Cu(bpac)Br_2$ (green)	m $P2_1/c$ 4	9.500(5) 11.142(4) 13.897(8)	 93.58(8) 	CuN_3Br_2 0.1	N_{eq} Br_{eq} Br_{ap}	2.029(2,162) 2.384(5) 2.672(5)	N_{eq},N_{eq} N_{eq},Br_{eq} Br_{eq},Br_{ap} N_{eq},Br_{ap}	79.98(9,27)[d] 97.07(7,1.01) 112.5(2) 93.5(8,2.0)	780
$[Cu(daph)I_2]I$ (brown)	m $P2_1/c$ 4	10.705(2) 7.936(1) 19.472(3)	 97.23(2) 	CuN_3I_2	N_{eq} I_{eq} I_{ap}	2.02(4,11) 2.536(7) 2.974(8)	N_{eq},N_{eq} I_{eq},N_{eq} N_{eq},I_{ap} I_{eq},I_{ap}	78.2(12,12)[d] 101.0(10,15) 93.4(10,17) 99.1(2)	781
$[Cu(pymep)Cl(H_2O)]PF_6$ (blue)	or Pbca 8	7.922(1) 15.763(1) 29.623(1)	 	CuN_3OCl	N_{eq} Cl_{eq} H_2O_{ap}	2.007(6,43) 2.240(2) 2.439(7)	N_{eq},N_{eq} N_{eq},Cl_{eq} N_{eq},O_{ap} Cl_{eq},O_{ap}	81.5(2)[d] 92.3(3)[e] 86.9(3,5.4) 95.7(2,3.5) 85.3(2,9) 100.2(3) 116.3(2)	782

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$Cu(Me_5dien)(ClO_4)Cl$	or	13.123(8)		CuN_3OCl	N_{eq}	2.048(13,18)	N_{eq},N_{eq}	85.5(5,3)[d]	783
(blue)	$P2_12_12_1$	7.730(5)			Cl_{eq}	2.226(5)	N_{eq},Cl_{eq},	94.4(4,1)	
	4	15.646(4)			O_3ClO_{ap}	2.681(21)	N_{eq},O_{ap}	93.1(6,1.8)	
								107.7(6)	
							Cl_{eq},O_{ap}	85.7(5)	
Cu(bquan)(2–pyc)Cl	or	11.876(5)		CuN_3OCl	N_{eq}	1.958(11,6)	N_{eq},N_{eq}	92.4(5)[e]	784
(not given)	Pbca	9.778(5)			$pycN_{eq}$	2.033(10)		94.6(5,2.2)	
	8	20.489(12)		0.15	$pycO_{eq}$	1.968(9)	N_{eq},O_{eq}	82.6(4)[d]	
					Cl_{ap}	2.794(4)	Cl_{ap},O_{eq}	90.4(3)	
							N_{eq},Cl_{ap}	92.6(3,5.7)	
Cu(bpnp)Cl	tr	6.938(1)	114.56(3)	CuN_3OCl	N_{eq}	2.014(5,46)	N_{eq},N_{eq}	82.6(1,3)[d]	785
(green)	P–1	11.782(6)	92.70(2)		Cl_{eq}	2.256(13)	Cl_{eq},N_{eq}	95.2(1,8)	
	2	12.678(3)	95.36(2)	0.223	O_{ap}	2.268(25)	N_{eq},O_{ap}	91.7(1)[e]	
								95.1(1,5.0)	
							Cl_{eq},O_{ap}	98.7(1)	
$[Cu(gly)(phen)Cl]\cdot H_2O$	or	6.795(3)		CuN_3OCl	O_{eq}	1.945(6)	N_{eq},O_{eq}	84.5(3)[d]	736
(not given)	$P2_12_12_1$	12.496(4)			N_{eq}	2.007(7)		87.2(3,2.7)	
	4	17.273(5)		0.334	$phenN_{eq}$	2.019(7,12)	N_{eq},N_{eq}	81.8(3)[d]	
					Cl_{ap}	2.546(2)		89.8(3,8.0)	
							N_{eq},Cl_{ap}	98.1(2,5.3)	
$Cu(sttp)(HCO_3)$	m	9.484(2)		CuN_3OS	S_{eq}	2.277(3)	S_{eq},N_{eq}	85.1(2,1.1)[e]	786
(dark blue)	$P2_1/n$	9.305(2)	100.04(2)		N_{eq}	2.013(10,54)	S_{eq},O_{ap}	88.3(3)	
(at 130K)	2	21.370(5)			HO_2CO_{ap}	2.246(12)	N_{eq},N_{eq}	91.8(4,9)[e]	
							N_{eq},O_{ap}	110.0(7,13.8)	
$[Cu(13–aneN_3O)Br]Br$	m	7.753(7)		CuN_3OBr	N_{eq}	2.02(2,1)	O_{eq},N_{eq}	82.0(9,1.1)[d]	787
(pale blue)	$P2_1/c$	14.78(2)	104.4(2)		O_{eq}	2.06(2)	N_{eq},N_{eq}	88.9(12)[d]	
	4	13.83(2)		0.47	Br_{ap}	2.515(5)	N_{eq},N_{eq}	96.3(11)[e]	
							N_{eq},N_{eq}	92.6(12,3.7)	
							N_{eq},O_{eq}	82.0(9,1.1)	
Cu(stpp)Cl	tr	10.061(6)	102.12(4)	CuN_3SCl	N_{eq}	2.025(8,63)	N_{eq},N_{eq}	163.7(2)	788a
(dark green)	P–1	13.646(7)	104.02(4)		S_{eq}	2.335(2)	S_{eq},N_{eq}	144.4(2)	
	2	14.930(8)	108.20(4)	0.274	Cl_{ap}	2.373(3)	N_{eq},Cl_{ap}	107.3(2,11.1)	
							S_{eq},Cl_{ap}	97.3(1)	
$[Cu(bdma)Cl]Cl\cdot 2H_2O$	m	17.243(8)		CuN_3SCl	N_{eq}	2.080(6,64)	Cl_{eq},N_{eq}	90.1(2)	788b
(green)	$P2_1/c$	10.001(5)	109.52(6)		S_{eq}	2.332(3)	N_{eq},S_{eq}	86.6(2)[d]	
	4	14.763(7)		0.38	Cl_{eq}	2.266(2)	N_{eq},N_{eq}	89.2(2)[e]	
					N_{ap}	2.150(6)	N_{eq},N_{ap}	93.4(2)[e]	
								95.4(2,2.0)	
							S_{eq},Cl_{eq}	88.2(2)	
							Cl_{eq},N_{ap}	114.6(2)	
							S_{eq},N_{ap}	94.5(2)	
Cu(tioam)(bpy)Br	tr	13.928(7)	77.07(5)	CuN_3SBr	$bpyN_{eq}$	2.045(10,5)	N_{eq},N_{eq}	79.1(4)[d]	789
(green)	P–1	10.331(5)	89.49(4)		N_{eq}	2.04(1)		89.2(4,10.1)	
	2	7.285(4)	96.83(5)		S_{eq}	2.338(4)	N_{eq},S_{eq}	83.6(3)[d]	
					Br_{ap}	2.527(2)		90.3(3,2.0)	
							N_{eq},Br_{ap}	96.7(3,1.2)	
							S_{eq},Br_{ap}	107.3(1)	
$[Cu(pms)Br]ClO_4$	m	14.600(7)		CuN_3SBr	N_{eq}	2.010(8,41)	N_{eq},N_{eq}	82.2(3,1.0)[d]	634
(not given)	$P2_1/a$	17.155(8)	94.89(2)		Br_{eq}	2.375(2)	N_{eq},S_{ap}	84.5(2)[d]	
	4	7.686(1)			S_{ap}	2.762(3)	Br_{eq},N_{eq}	92.5(2,4.2)	
							S_{ap},N_{eq}	90.0(2,10.7)	
							N_{eq},N_{eq}	82.2(3,1.0)	
							S_{ap},Br_{eq}	101.3(1)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(teaz)Cl_3]\cdot H_2O$	tr	8.188(7)	93.0(1)	$CuCl_3NS$	N_{eq}	2.052(10)	N_{eq},S_{eq}	85.7(3)[d]	790
(green)	P–1	8.778(7)	96.5(1)		S_{eq}	2.263(4)	N_{eq},Cl_{eq}	88.9(3)	
	2	7.219(7)	117.3(1)		Cl_{eq}	2.230(4,43)	Cl_{eq},Cl_{eq}	95.9(1)	
					Cl_{ap}	2.628(5)	S_{eq},Cl_{eq}	88.3(1)	
							Cl_{eq},Cl_{ap}	91.7(1,3.0)	
							Cl_{ap},S_{eq}	105.5(1)	
							Cl_{ap},N_{eq}	95.4(3)	
$Cu(tcyc)Cl_2$	or	7.444(5)		CuS_3Cl_2	S_{eq}	2.334(2,2)	S_{eq},S_{eq}	87.8(1)[d]	791
(green)	$P2_12_12$	10.892(7)			Cl_{eq}	2.264(3,7)	Cl_{eq},S_{eq}	88.0(1,7)	
	4	13.509(1)			S_{ap}	2.682(2)	Cl_{eq},Cl_{eq}	96.0(1)	
							S_{eq},S_{ap}	85.2(1,1.0)[d]	
							Cl_{eq},S_{ap}	100.2(1,3.9)	
$Cu(tse)_2$	m	9.575(6)		$CuSe_3S_2$	Se_{eq}	2.500(4,9)	Se_{eq},Se_{eq}	77.95(2,35)	792
(not given)	$P2_1/c$	11.245(6)	112.89(8)		S_{eq}	2.347(5,8)			
	4	16.791(8)		0.27	Se_{ap}	2.884(5)			
$[Cu(bpy)F_2(H_2O)]\cdot 2H_2O$	m	10.697(2)		CuF_2N_2O	F_{eq}	1.887(4,3)	F_{eq},F_{eq}	92.6(2,–)	793
(turboquoise blue)	$P2_1/n$	16.968(2)	90.47(1)		N_{eq}	2.008(5,4)	O_{ap},F_{eq}	95.9(2,2)	
	4	6.918(1)			H_2O_{ap}	2.214(5)	N_{eq},O_{ap}	98.0(2,3.2)	
							N_{eq},F_{eq}	92.0(2,6)	
							N_{eq},N_{eq}	80.3(2)[d]	
$[Cu(phen)F_2(H_2O)]\cdot$	m	6.985(2)		CuF_2N_2O	F_{eq}	1.891(4,1)	F_{eq},F_{eq}	92.9(2)	794
$2H_2O$	$P2_1/n$	17.406(2)	92.41(2)		N_{eq}	2.0334(5,6)	O_{ap},F_{eq}	94.8(2,8)	
(sky blue)	4	10.581(2)			H_2O_{ap}	2.216(5)	N_{eq},F_{eq}	91.8(2,5)	
							O_{ap},N_{eq}	97.8(2,3.0)	
							N_{eq},N_{eq}	81.0(2)[d]	
$[Cu(bipyam)(H_2O)_2F]F\cdot$	m	12.879(4)		CuO_2N_2F	pyN_{eq}	1.986(4,0)	O_{eq},O_{eq}	89.6(2)	795
$3H_2O$	$P2_1/n$	6.954(4)	98.06(5)		H_2O_{eq}	1.984(4)	O_{ap},F_{eq}	93.1(1)	
(not given)	4	17.360(7)		0.194	F_{eq}	1.934(3)	O_{ap},N_{eq}	99.9(2,2.9)	
					H_2O_{ap}	2.218(4)	F_{eq},O_{eq}	87.1(1)	
							F_{eq},N_{eq}	90.6(2)	
							N_{eq},N_{eq}	89.9(1)[e]	
							N_{eq},O_{eq}	90.6(2)	
$(Cu(dmpo)_2C1]_2[CuCl_4]$	tg	15.330(2)		CuO_2N_2Cl	N_{eq}	2.010(6,0)	N_{eq},N_{eq}	167.4(3)	796
(not given)	$P-42_1c$	13.992(4)			O_{eq}	2.064(5,0)	O_{eq},O_{eq}	143.9(2)	
	2			0.476	Cl_{ap}	2.367(4)	O_{eq},N_{eq}	88.1(3,8)[d]	
							O_{eq},Cl_{ap}	108.1(2)	
							N_{eq},Cl_{ap}	96.3(2)	
				$CuCl_4$	Cl	2.250(3,0)	Cl,Cl	115.1(0,1)	
(Cu(bpy) (4–pxa)Cl]·	m	14.342(2)		CuO_2N_2Cl	O_{eq}	1.901(4,8)	N_{eq},N_{eq}	80.7(1)[d]	738
2H20	$P2_1/n$	8.374(1)	112.31(1)		$bpyN_{eq}$	2.004(4,8)	O_{eq},O_{eq}	91.6(6)[e]	
(deep green)	4	17.331(2)		0.214	Cl_{ap}	2.659(1)	O_{eq},N_{eq}	92.3(1,2)	
							O_{eq},Cl_{eq}	97.3(1,4.1)	
							N_{eq},Cl_{ap}	95.3(1,3.6)	
$(Cu(pyx)(bpy)Cl]ClO_4\cdot$	tr	12.136(5)	96.91(2)	CuO_2N_2Cl	N_{eq}	1.993(4,9)	N_{eq},N_{eq}	81.3(2)[d]	797
H_2O	P–1	13.283(4)	91.25(3)		$pyxO_{eq}$	1.953(4,25)	O_{eq},O_{eq}	91.4(2)[d]	
(not given)	2	7.195(2)	71.63(3)		Cl_{ap}	2.559(2)	O_{eq},N_{eq}	92.1(2,1)	
							O_{eq},Cl_{ap}	98.3(1,5.1)	
							N_{eq},Cl_{ap}	96.7(1,1.7)	
$[Cu(Me_3pcx)Cl]_2SO_4\cdot$	m	14.679(2)		CuO_2N_2Cl	O_{eq}	1.982(6,9)	O_{eq},N_{eq}	82.2(2,1)[d]	591
$8H_2O$[c]	$P2_1/c$	13.070(2)	111.56(2)		N_{eq}	1.966(6,1)		95.3(4,1.1)	
(blue)	4	23.958(6)		0.324	Cl_{ap}	2.500	O_{eq},Cl_{ap}	102.2(2,9.8)	
							N_{eq},Cl_{ap}	95.9(2,1.8)	
				CuO_2N_2Cl	O_{eq}	1.979(6,3)	O_{eq},N_{eq}	82.2(1,1)[d]	
					N_{eq}	1.970(6,5)		95.1(1,4)	
				0.308	Cl_{ap}	2.496	$O_{eq}Cl_{ap}$	99.8(2,4.6)	
							N_{eq},Cl_{ap}	98.1(2,1.0)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(benox)Cl]ClO_4$	m	11.757(2)		CuO_2N_2Cl	N_{eq}	1.979(6,19)	N_{eq},N_{eq}	93.7(3)[e]	798
(green)	$P2_1/n$	18.325(3)	108.16(2)		O_{eq}	2.098(5,50)	O_{eq},O_{eq}	79.8(2)[d]	
	4	10.396(2)		0.29	Cl_{ap}	2.411(2)	N_{eq},O_{eq}	92.2(2,2)[e]	
							O_{eq},Cl_{ap}	94.2(2,2.8)	
							N_{eq},Cl_{ap}	101.7(2,9.5)	
$Cu(imth)(NO_3)_2]\cdot MeOH$	m	16.299(1)		CuO_2N_2S	N_{eq}	1.981(2,20)	N_{eq},S_{eq}	90.2(1,3.4)[e]	799
(not given)	Cc	9.573(1)	119.068(5)		S_{eq}	2.366(1)	N_{eq},N_{eq}	177.0(1)	
	4	16.162(2)			O_2NO_{eq}	2.040(2)	N_{eq},O_{eq}	89.5(1,4)	
					O_2NO_{ap}	2.282(2)	S_{eq},O_{eq}	162.8(1)	
							N_{eq},O_{ap}	91.5(1,4.0)	
							S_{eq},O_{ap}	98.4(1)	
							O_{eq},O_{ap}	98.3(1)	
$Cu(Meimth)(NO_3)_2$	m	18.060(5)		CuO_2N_2S	S_{eq}	2.369(1)	S_{eq},N_{eq}	84.03(9,17)[d]	800
(green)	$P2_1/n$	7.063(4)	104.13(3)		N_{eq}	1.941(3,2)	S_{eq},O_{eq}	171.53(8)	
	4	13.229(3)		0.13	O_2NO_{eq}	1.987(2)	N_{eq},N_{eq}	157.0(1)	
					O_2NO_{ap}	2.405(2)	N_{eq},O_{ap}	99.9(1,1.5)	
							N_{eq},O_{eq}	97.3(1,1.8)	
							O_{eq},O_{ap}	81.0(1)	
$[Cu(karbaz)(NO_3)\cdot$	m	8.20(3)		CuO_2N_2S	N_{eq}	2.00	not given		801
$(H_2O)]NO_3\cdot H_2O$	$P2_1/c$	15.95(5)	120.5(5)		S_{eq}	2.35			
(not given)	4	14.41(5)		0.3	H_2O_{eq}	2.03			
					O_2NO_{ap}	2.35			
$[Cu(dbenzd)(H_2O)\cdot$	tr	7.909(6)	103.10(6)	CuO_2N_2S	S_{eq}	2.322(2)	N_{eq},N_{eq}	176.6(3)	802
$(ClO_4)]ClO_4$	P-1	10.972(7)	95.56(6)		N_{eq}	1.973(6,13)	N_{eq},S_{eq}	90.6(2,2.3)[e]	
(not given)	2	16.65(1)	103.98(5)		H_2O_{eq}	2.045(5)	N_{eq},O_{eq}	88.6(2,0.8)	
					O_3ClO_{ap}	2.346(6)	N_{eq},O_{ap}	91.4(3,2.9)	
							S_{eq},O_{ap}	100.5(2)	
							O_{eq},O_{ap}	102.8(23)	
$[Cu(bbes)(MeOH)(H_2O)]\cdot$	tr	9.306(3)	92.23(2)	CuO_2N_2S	N_{eq}	1.981(3,3)	S_{eq},O_{eq}	158.6(1)	803
$(ClO_4)_2$	P-1	10.072(5)	96.63(4)		S_{eq}	2.297(1)	S_{eq},N_{eq}	90.8(1,4.5)[e]	
(dark green)	2	14.194(5)	108.56(3)		H_2O_{eq}	1.995(2)	N_{eq},O_{eq}	88.4(1,2.3)	
					$MeHO_{ap}$	2.261(3)	N_{eq},N_{eq}	174.6(1)	
							S_{eq},O_{ap}	94.8(1)	
							O_{eq},O_{ap}	106.6(1)	
							N_{eq},O_{ap}	92.6(1,5)	
$[Cu(bbes)(acac)]PF_6\cdot$	tr	13.961(3)	101.57(4)	CuO_2N_2S	acO_{eq}	1.918(8,0)	O_{eq},O_{eq}	91.8(4)[e]	803
Etac	P-1	12.892(3)	104.99(4)		N_{eq}	2.006(13,0)	O_{eq},N_{eq}	87.7(5,4)	
(blue green)	2	10.154(3)	104.34(4)	0.15	S_{ap}	2.696(5)	N_{eq},S_{ap}	90.1(4,7)[e]	
							O_{eq},S_{ap}	98.2(3)	
$[Cu(tsc)(H_2O)]\cdot H_2O$	m	9.476(6)		CuO_2N_2S	N_{eq}	2.008(5,12)	O_{eq},S_{eq}	92.2(2)	804
(green)	$P2_1/n$	6.446(2)			O_{eq}	1.996(5)	O_{eq},N_{eq}	81.6(2)[d]	
	4	13.187(5)	99.33(4)	0.172	S_{eq}	2.23(2)		89.0(2,7.4)	
					H_2O_{ap}	2.32(5)	S_{eq},N_{eq}	84.2(2)[d]	
							N_{eq},N_{eq}	169.4(2)	
							N_{eq},O_{ap}	95.2(2,4.4)	
							O_{eq},O_{ap}	90.9(2)	
							S_{eq},O_{ap}	96.8(1)	
$[Cu(ttda)(Me_4en)]\cdot$	m	15.35(1)		CuO_2N_2S	O_{eq}	1.945(6)	S_{eq},O_{eq}	84.3(2)[d]	805
$(ClO_4)_2$	$P2_1/n$	15.04(1)	98.74(2)		S_{eq}	2.386(3)	S_{eq},N_{eq}	99.3(2)	
(not given)	4	10.91(1)		0.155	$diaetN_{eq}$	2.020(7,6)	N_{eq},O_{eq}	88.9(3)	
					O_{ap}	2.180(6)	S_{eq},O_{ap}	81.9(2)[d]	
							N_{eq},O_{ap}	99.9(3,0)	
							O_{eq},O_{ap}	96.1(3)	
Cu(cbps)	m	18.689(4)		CuO_2N_2S	O_{eq}	1.922(2,20)	O_{eq},O_{eq}	160.91(9)	806
(black)	C2/c	13.735(5)	100.61(2)		N_{eq}	1.999(3,6)	N_{eq},N_{eq}	176.1(1)	
	8	22.669(9)			S_{ap}	2.686(1)	O_{eq},N_{eq}	90.3(1,4.4)[e]	
							O_{eq},S_{ap}	99.0(7,1.6)	
							N_{eq},S_{ap}	88.0(8,3)[e]	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$Cu(NH_3)(ac)_2Br$	or	9.01(1)		CuO_2N_2Br	acO_{eq}	1.998(6,3)	N_{eq},O_{eq}	90.0(1,4)	807
(blue)	$Pna2_1$	7.60(1)			H_3N_{eq}	1.984(6,0)	N_{eq},Br_{ap}	96.5(1)	
	4	10.38(1)			Br_{ap}	2.865(3)	O_{eq},Br_{ap}	90.2(2,1.6)	
[Cu(xyhist)(H_2O)Br]·	tr	8.161(2)	105.18(1)	CuO_2N_2Br	O_{eq}	1.902(7)	O_{eq},O_{eq}	85.6(3)	808
NO_3	P–1	10.368(2)	102.12(1)		N_{eq}	1.974(8,3)	N_{eq},N_{eq}	93.8(3)[e]	
(green)	2	11.110(2)	72.10(1)		H_2O_{eq}	2.011(7)	O_{eq},N_{eq}	91.4(3)[e]	
					Br_{ap}	2.813(2)		90.5(3,9)	
							O_{eq},Br_{ap}	96.3(2,5.4)	
							N_{eq},Br_{ap}	94.8(2,6.6)	
[Cu(dtic)Cl_2(MeOH)]·	tr	8.493(3)	90.5(2)	CuO_2Cl_2N	O_{eq}	2.035(2)	N_{eq},O_{eq}	79.4(1)[d]	809
MeOH	P–1	9.054(3)	105.66(2)		N_{eq}	1.970(2)	N_{eq},Cl_{eq}	94.1(9)	
(green)	2	10.969(2)	104.68(2)	0.16	Cl_{eq}	2.232(1,6)	O_{eq},Cl_{eq}	89.3(1)	
					$MeHO_{ap}$	2.477(1)	Cl_{eq},Cl_{eq}	95.8(3)	
							N_{eq},O_{ap}	94.5(1)	
							O_{eq},O_{ap}	92.9(1)	
							Cl_{eq},O_{ap}	95.9(1,4)	
$Cu(sglyc)Cl_2$	or	10.036(3)		CuO_2Cl_2S	S_{eq}	2.322(2)	Cl_{eq},Cl_{eq}	95.3(4)	810
(pale green)	$P2_12_12_1$	12.882(3)			O_{eq}	2.024(4)	Cl_{eq},S_{eq}	92.2(1)	
	4	6.696(2)			Cl_{eq}	2.259(2.6)	Cl_{eq},O_{eq}	90.0(1)	
					O_{ap}	2.429(4)	S_{eq},O_{eq}	83.8(1)[d]	
							Cl_{eq},O_{ap}	97.0(1,2.4)	
							S_{eq},O_{ap}	79.5(1)[d]	
							O_{eq},O_{ap}	93.2(2)	
$Cu(2\text{–}Mepy)_2Cl_2(H_2O)$	tr	8.464(4)	93.45(2)	CuN_2Cl_2O	N_{eq}	2.015(1,2)	Cl_{eq},Cl_{eq}	173.66(2)	432b
(blue)	P–1	12.552(4)	113.56(3)		Cl_{eq}	2.305(1,9)	Cl_{eq},N_{eq}	89.85(4,2.31)	
	2	7.345(2)	99.52(3)	0.11	H_2O_{ap}	2.500(1)	N_{eq},N_{eq}	173.98(5)	
							Cl_{eq},O_{ap}	93.17(5,8.7)	
							N_{eq},O_{ap}	92.91(5,3.49)	
$Cu(damet)Cl_2$	tg	12.040(4)		CuN_2Cl_2O	N_{eq}	2.061(10,7)	Cl_{eq},N_{eq}	90.5(3,4.9)	811
(blue green)	$P4_12_12$	18.198(9)			O_{eq}	2.040(8)	Cl_{eq},O_{eq}	160.9(3)	
	8				Cl_{eq}	2.255(4)	N_{eq},O_{eq}	81.0(3.6)[e]	
					Cl_{ap}	2.436(3)	N_{eq},N_{eq}	153.7(4)	
							Cl_{eq},Cl_{ap}	107.81(12)	
							N_{eq},Cl_{ap}	99.65(30,1.15)	
							O_{eq},Cl_{ap}	91.22(24)	
$Cu(mpyx)Cl_2$	tr	8.221(3)	99.89(3)	CuN_2Cl_2O	N_{eq}	2.075(2,61)	N_{eq},N_{eq}	81.94(7)[e]	812
(dark green)	P–1	9.265(4)	100.21(3)		Cl_{eq}	2.227(1,23)	N_{eq},Cl_{eq}	94.57(6)	
	2	11.351(3)	100.08(3)		O_{ap}	2.400(2)		169.92(6,2.68)	
							Cl_{eq},Cl_{eq}	92.26(6,2.17)	
$Cu(xyhist)Cl_2$	m	16.667(3)		CuN_2Cl_2O	O_{eq}	1.922(5)	not given		813
(not given)	$P2_1/n$	10.293(4)	91.16(9)		N_{eq}	2.003(5,28)			
	4	8.966(1)			Cl_{eq}	2.369(2)			
					Cl_{ap}	2.635(2)			
$Cu(thdam)Cl_2$	m	9.450(4)		CuN_2Cl_2O	O_{eq}	1.97	N_{eq},N_{eq}	78.3	814
(not given)	$P2_1/c$	10.571(5)	102.6(3)		N_{eq}	1.98(–,3)	N_{eq},O_{eq}	82.1	
	4	15.857(10)			Cl_{eq}	2.271	Cl_{eq},N_{eq}	90.3	
					Cl_{ap}	2.61	O_{eq},Cl_{eq}	100.2	
							N_{eq},Cl_{ap}	94.2	
							O_{eq},Cl_{ap}	100.2	
							Cl_{eq},Cl_{ap}	95	
$[Cu(thcbh)_2(SO_4)]\cdot$	m	13.430(5)		CuN_2S_2O	N_{eq}	2.013(5,3)	S_{eq},N_{eq}	87.2(2,1)[d]	815
$4H_2O$	$P2_1/c$	8.340(3)	122.8(1)		S_{eq}	2.262(3,2)	S_{eq},S_{eq}	95.0(1)	
(violet)	4	17.070(9)			O_3SO_{ap}	2.794(5)	N_{eq},N_{eq}	90.7(2)	
							N_{eq},O_{ap}	83.1(2,5.5)	
							S_{eq},O_{ap}	98.2(1,8.5)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(pmed)(H_2O)]\cdot(ClO_4)_2$ (brown)	m $P2_1/c$ 4	20.222(1) 7.882(1) 22.708(2)	 114.98(1) 	CuN_2S_2O 0.2	N_{eq} S_{eq} H_2O_{ap}	1.97(2,3) 2.321(6,3) 2.29(1)	S_{eq},S_{eq} S_{eq},N_{eq} N_{eq},N_{eq} N_{eq},O_{ap} S_{eq},O_{ap}	88.8(2) 94.4(6,3)[c] 85.4(7)[d] 95.9(6,4) 94.9(3,3.0)	816
$[Cu(peas)(NO_3)]PF_6$ (dark blue)	m $P2_1/c$ 4	11.922(2) 11.186(2) 17.298(2)	 93.04(1) 	CuN_2S_2O 	N_{eq} S_{eq} O_2NO_{eq} S_{ap} 	2.055(5,24) 2.334(2) 1.991(4) 2.564(2) 	S_{eq},N_{eq} S_{eq},O_{eq} N_{eq},N_{eq} N_{eq},O_{eq} S_{eq},S_{ap} N_{eq},S_{ap} O_{eq},S_{ap}	87.8(2)[d] 87.7(1) 94.7(2)[e] 88.4(2) 99.2(1) 87.9(1)[d] 90.5(1,2.6) 98.9(1)	817
$[Cu(pdto)(ClO_4)]ClO_4$ (not given)	m $P2_1/c$ 4	8.902(1) 21.343(2) 11.879(1)	 108.03(1) 	CuN_2S_2O 0.25	N_{eq} S_{eq} O_3ClO_{ap}	2.010(5,2) 2.314(2,3) 2.264(5)	S_{eq},S_{eq} N_{eq},N_{eq} N_{eq},S_{eq} S_{eq},O_{ap} N_{eq},O_{ap}	88.1(1)[d] 91.7(2) 88.3(1,1)[e] 97.4(1,4) 96.2(2,3.4)	818
$Cu(9\text{-}aneN_2S)Br_2$ (green)	m $P2_1/n$ 4	7.603(1) 13.167(2) 10.873(2)	 91.94(1) 	CuN_2Br_2S 	N_{eq} Br_{eq} S_{ap} 	2.025(20,5) 2.426(2,23) 2.567(3) 	N_{eq},N_{eq} Br_{eq},Br_{eq} Br_{eq},N_{eq} N_{eq},S_{ap} Br_{eq},S_{ap}	83.8(4)[d] 94.9(1) 90.0(3,1) 84.6(3,1.7)[d] 104.4(1,3.6)	819
$Cu(thiapy)Cl_2$ (dark green)	tr P–1 2	7.912(4) 8.793(5) 15.082(7)	92.79(9) 101.75(8) 66.56(9)	$CuCl_2S_2N$ 	S_{eq} N_{eq} Cl_{eq} Cl_{ap}	2.368(2,2) 2.036(8) 2.274(4) 2.385(3)	not given		820
$Cu(dipen)Cl_2$ (green)	m $P2_1/n$ 4	7.381(1) 13.916(3) 14.336(6)	 100.10(2) 	$CuCl_2S_2N$ 0.317	N_{eq} S_{eq} Cl_{eq} Cl_{ap}	2.024(3) 2.360(1,10) 2.255(1) 2.495(1)	S_{eq},Cl_{eq} S_{eq},S_{eq} N_{eq},Cl_{eq} N_{eq},S_{eq} N_{eq},Cl_{ap} S_{eq},Cl_{ap} Cl_{eq},Cl_{ap}	93.35(10,5) 155.6(1) 171.0(1) 84.9(1,2) 87.4(1) 100.9(1,5) 101.6(1)	821
$Cu(thiocarb)Cl_2$ (blue green)	m $P2_1/n$ 4	9.163(2) 8.925(5) 17.590(9)	 102.08(1) 	$CuCl_2S_2N$ 	Cl_{eq} N_{eq} S_{eq} Cl_{ap} 	2.246(4) 2.002(2) 2.294(4,3) 2.590(4) 	Cl_{eq},N_{eq} S_{eq},S_{eq} Cl_{eq},Cl_{ap} Cl_{ap},S_{eq} Cl_{ap},N_{eq}	168.5(1.5) 161.5(1.5) 103.5(1.5) 98.3(1.5,5) 88.1(1.5)	822
$Cu(etspy)Cl_2$ (green)	m I2/c 8	14.669(6) 7.418(4) 29.412(8)	 103.03(4) 	$CuCl_2S_2N$ 0.367 	Cl_{eq} S_{eq} N_{eq} Cl_{ap} 	2.242(4) 2.351(4,7) 2.016(10) 2.428(3) 	Cl_{eq},Cl_{ap} S_{eq},Cl_{ap} S_{eq},Cl_{eq} S_{eq},S_{eq} N_{eq},Cl_{ap} N_{eq},Cl_{eq} N_{eq},S_{eq}	106.3(1) 98.3(1,1.1) 91.8(1,4) 161.3(1)[f] 93.59(3) 160.2(3) 85.3(3,6)[d]	823
$Cu(dzbx)Cl_2$[c] (green)	m P2/a 8	14.677(9) 7.555(1) 29.696(4)	 101.00(2) 	$CuCl_2S_2N$ 0.381 $CuCl_2S_2N$ 0.375 	Cl_{eq} S_{eq} N_{eq} Cl_{ap} Cl_{eq} S_{eq} N_{eq} Cl_{ap}	2.247(3) 2.347(4,4) 2.000(7) 2.4229(4) 2.260(4) 2.348(3,10) 2.00(10) 2.410(4)	Cl_{eq},Cl_{ap} S_{eq},Cl_{eq} S_{eq},S_{eq} S_{eq},Cl_{ap} S_{eq},N_{eq} N_{eq},Cl_{ap} N_{eq},S_{eq} Cl_{eq},Cl_{eq} S_{eq},Cl_{eq} S_{eq},Cl_{ap} S_{eq},S_{eq} N_{eq},Cl_{eq} N_{eq},Cl_{ap} N_{eq},S_{eq}	102.1(2,6) 92.0(1,4) 154.0(1) 102.1(2,6) 166.1(3) 91.8(3) 85.0(2,1.1)[d] 101.3(1) 91.8(1) 101.2(1,1.6) 156.2(1) 164.5(3) 94.2(3) 85.1(3,2)[d]	823

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(pdta)Br_2]\cdot H_2O$	m	9.292(2)		CuS_2Br_2N	S_{eq}	2.286(2,2)	S_{eq},S_{eq}	161.9(3)	504
(not given)	$P2_1/n$	9.153(2)	102.08(1)		N_{eq}	2.000(5)	S_{eq},Br_{eq}	97.7(3,3)	
	4	17.929(6)			Br_{eq}	2.388(2)	S_{eq},N_{eq}	85.7(3,1)	
					Br_{ap}	2.732(2)	Br_{eq},Br_{ap}	103.5(3)	
							Br_{eq},N_{eq}	87.1(3)	
$[Cu(pdta)I_2]\cdot C_3H_7NO$	m	8.257(3)		CuS_2I_2N	S_{eq}	2.279(2,0)	S_{eq},S_{eq}	162.9(3)	504
(not given)	$P2_1/a$	25.664(11)	101.93(2)		N_{eq}	2.017(5)	S_{eq},I_{eq}	97.6(3,2.0)	
	4	9.432(4)			I_{eq}	2.590(2)	S_{eq},N_{eq}	85.8(3,2)	
					I_{ap}	2.958(2)	I_{eq},I_{ap}	103.7(3)	
							I_{eq},N_{eq}	91.9(3)	
B: TRIGONAL-BIPYRAMIDAL									
$K[Cu(hex)_2(NCS)_3]\cdot$	m	11.425(3)		CuN_5	SCN_{eq}	2.016(7,70)	N_{eq},N_{eq}	122.5(–,14.5)	824
$2H_2O$	$P2_1/n$	12.514(3)	109.25(5)		N_{ap}	2.097(5,5)			
(green)	4	19.347(4)							
$[Cu(bpy)_2(NH_3)](BF_4)_2$	m	9.051(12)		CuN_5	H_3N_{eq}	2.045(7)	N_{eq},N_{eq}	120.0(3,11.8)	825
(not given)	$P2_1/c$	13.493(22)	103°20′		N_{eq}	2.091(7,21)	N_{eq},N_{ap}	79.6(3,1)[d]	
	4	19.278(26)			N_{ap}	1.970(7,12)		89.9(3,10.4)	
							N_{ap},N_{ap}	175.7(3)	
$[Cu(C_7H_{18}N_2)_2(NO_2)]\cdot$	m	9.212(4)		CuN_5	O_2N_{eq}	2.052(20)	N_{eq},N_{eq}	120.0(15,20.9)	826
NO_2	Ic	23.531(7)	95.98(3)		N_{eq}	2.122(10,39)	N_{eq},N_{ap}	83.5(4,1.1)[d]	
(not given)	4	9.979(3)			N_{ap}	2.060(8,69)		90.1(1.4,7.9)	
							N_{ap},N_{ap}	179.2(4)	
$[Cu(bpy)_2(NCS)]NCS$[e]	tr	10.815(4)	110.74(4)	CuN_5	SCN_{eq}	1.969(9)	N_{eq},N_{eq}	120.0(4,11.4)	827
(dark green)	P–1	14.457(5)	90.90(4)		N_{eq}	2.092(9,16)	N_{eq},N_{ap}	79.7(4,2)[d]	
	4	16.291(10)	110.48(3)		N_{ap}	1.975(10,8)		89.9(4,10.4)	
							N_{ap},N_{ap}	175.3(4)	
				CuN_5	SCN_{eq}	1.951(14)	N_{eq},N_{eq}	120.0(4,26.8)	
					N_{eq}	2.037(10,6)	N_{eq},N_{ap}	79.8(4,1.0)[d]	
					N_{ap}	2.065(9,5)		90.0(4,11.2)	
							N_{ap},N_{ap}	173.5(4)	
$[Cu(bpy)_2(NCS)]NO_3\cdot$	tr	12.098(4)	102.80(3)	CuN_5	SCN_{eq}	2.010(3)	N_{eq},N_{eq}	120.0(1,3.5)	828
H_2O	P–1	12.810(5)	107.56(2)		N_{eq}	2.079(3,2)	N_{eq},N_{ap}	80.0(1,0)[d]	
(green)	2	7.777(2)	76.03(3)		N_{ap}	1.992(2,3)		89.2(1,10.2)	
							N_{ap},N_{ap}	176.4(4)	
$[Cu(bpy)_2(NCS)]BF_4$	m	12.791(3)		CuN_5	SCN_{eq}	1.967(9)	N_{eq},N_{eq}	120.0(3,17.9)	829
(green)	C2/c	24.641(4)	107.4(1)		N_{eq}	2.095(7,26)	N_{eq},N_{ap}	79.9(3,2)[d]	
	8	15.456(3)			N_{ap}	1.987(7,7)		89.8(3,10.1)	
							N_{ap},N_{ap}	174.7(2)	
$[Cu(1,3\text{-}pn)_2(NCS)]\cdot$	hx	13.75(2)		CuN_5	SCN_{eq}	2.11(12)	N_{eq},N_{eq}	120.0(14.2)	830
ClO_4	$P6_3$	14.55(2)			N_{eq}	2.095(120,5)	N_{eq},N_{ap}	90.2(3,3)[e]	
(blue)	6				N_{ap}	2.015(120,15)		90.0(3,1.0)	
							N_{ap},N_{ap}	178.7(3)	
$[Cu(bpy)_2(NCO)]ClO_4$	tr	10.20(2)	90.7(2)	CuN_5	OCN_{eq}	1.961(8)	N_{eq},N_{eq}	120.0(3,14.7)	831
(green)	P–1	13.55(4)	99.7(2)		N_{eq}	2.103(8,8)	N_{eq},N_{ap}	79.5(3,0)[d]	
	2	7.98(1)	105.1(2)		N_{ap}	1.994(9,13)	N_{ap},N_{ap}	173.7(3)	
$[Cu(bpy)_2(sach)]sach\cdot$	or	15.546(2)		CuN_5	$sachN_{eq}$	1.963(6)	N_{eq},N_{eq}	120.0(3,15.4)	832
$3H_2O$	$C222_1$	26.223(4)			N_{eq}	2.084(8,12)	N_{eq},N_{ap}	79.9(3,1)[d]	
(blue)	8	16.878(3)			N_{ap}	1.968(7,5)	N_{ap},N_{ap}	174.5(3)	
$[Cu(phen)_2(NCS)]\cdot$	tr	7.930(4)	96.01(3)	CuN_5	SCN_{eq}	1.981(4)	N_{eq},N_{eq}	120.0(1,6.8)	833
cnmet	P–1	11.018(4)	98.93(3)		N_{eq}	2.096(3,18)	N_{eq},N_{ap}	80.6(1,2)[d]	
(dark green)	2	15.512(6)	108.00(3)		N_{ap}	1.993(3,5)		90.0(1,9.6)	
							N_{ap},N_{ap}	173.92(13)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(phen)_2(NCS)]\cdot ndcm$ (dark green)	tr P–1 2	7.937(4) 11.249(6) 15.144(6)	99.59(4) 98.00(4) 110.59(4)	CuN_5	SCN_{eq} N_{eq} N_{ap}	1.963(3) 2.091(3,11) 1.987(3,7)	N_{eq},N_{eq} N_{eq},N_{ap} N_{ap},N_{ap}	120.0(1,8.0) 80.7(1,2)[d] 90.0(1,4.4) 172.24(11)	834
$Cu(pymep)(NCS)_2$ (green)	m $P2_1/a$ 4	17.22(4) 8.594(2) 12.206(3)	 103.25(3) 	CuN_5	SCN_{eq} N_{eq} N_{ap}	2.003(3,26) 1.999(3) 2.048(4,17)	N_{eq},N_{eq} N_{eq},N_{ap} N_{ap},N_{ap}	119.9(2,5.1) 80.3(1)[d] 92.2(1)[e] 90.0(2,9.7) 172.5(1)	835
$[Cu(pymep)(N_3)_2]\cdot 2H_2O$ (green)	m $P2_1/n$ 4	10.543(2) 9.653(1) 16.638(3)	 97.90(2) 	CuN_5	$(N_3)_{eq}$ N_{eq} N_{ap}	2.013(8,27) 2.080(6) 2.039(7,1)	N_{eq},N_{eq} N_{eq},N_{ap} 	120.0(3,12.1) 78.8(3)[d] 91.3(2)[e] 89.8(3,11.0)	836
$Cu(pyhis)(N_3)_2$ (brown green)	tr P–1 2	10.262(8) 9.177(6) 7.688(5)	104.42(4) 94.09(4) 92.64(4)	CuN_5	$(N_3)_{eq}$ N_{eq} N_{ap}	2.096(3,81) 2.065(2) 1.993(2,25)	N_{eq},N_{eq} N_{eq},N_{ap} N_{ap},N_{ap}	119.7(8,26.3) 79.80(8)[d] 91.17(8)[e] 90.3(8,10.5) 170.46(8)	837
fac–$[Cu(ade)_2(dien)]\cdot H_2O$ (blue)	m $P2_1/n$ 4	16.015(2) 14.577(2) 7.959(1)	 90.11(1) 	CuN_5	$adeN_{eq}$ N_{eq} $adeN_{ap}$ N_{ap}	2.036(6) 2.085(7,55) 1.998(9) 2.043(6)	N_{eq},N_{eq} N_{eq},N_{ap} N_{ap},N_{ap}	119.2(3,22.9) 82.3(3,3)[d] 90.2(3,10.4) 175.7(3)	838
$[Cu(dien)(bipyam)]\cdot (NO_3)_2$ (not given)	m $P2_1/c$ 4	12.201(5) 16.052(6) 9.851(4)	 90.76(2) 	CuN_5 0.44	$dienN_{eq}$ N_{eq} N_{ap} $dienN_{ap}$	2.049(5,14) 2.142(5) 2.009(5) 2.050(5)	N_{eq},N_{eq} N_{eq},N_{ap} N_{ap},N_{ap}	100.7(,3.6) 137.2(1) 83.9(2,1)[d] 88.9(2)[e] 99.8(2) 170.7(1)	533
$[Cu(trea)(NH_3)](ClO_4)_2$ (not given)	cc $P2_13$ 4	11.626(3)		CuN_5	N_{eq} N_{ap} H_3N_{ap}	2.082(6,0) 2.041(8) 2.023(11)	N_{eq},N_{eq} N_{eq},N_{ap} N_{eq},N_{eq}	119.2(3) 90.0(2,5.1) 84.9(2,0)[d] 180.0	517a
[Cu(pmd)(NCS)]NCS (green)	m $P2_1/c$ 4	13.93(1) 9.78(1) 15.06(1)	 96.8(1) 	CuN_5	SCN_{eq} N_{eq} N_{ap}	1.986(8) 2.138(8,109) 1.99(8,8)	N_{eq},N_{eq} N_{eq},N_{ap}	108.1(3,1.4) 143.8(3) 80.03(3,8)[d] 94.2(3)	630
[Cu(tren)(NCS)]NCS (dark blue)	or $P2_12_12_1$ 4	9.158(1) 14.000(2) 11.285(1)	 	CuN_5	SCN_{ap} N_{eq} N_{ap}	1.939(8) 2.085(4,59) 2.033(4)	N_{eq},N_{ap} N_{ap},N_{ap}	84.1(2,2)[d] 177.9(2)	839
α–[Cu(bpdz)NCS)]NCS (blue)	tr P–1 2	16.66(4) 7.88(2) 9.11(3)	124.4(1) 83.0(1) 91.6(1)	CuN_5 N_{ap}	SCN_{eq} N_{eq} 	2.119(12) 2.034(11,5) 1.988(10,1)	N_{eq},N_{eq} N_{eq},N_{ap} N_{ap},N_{ap}	119.9(5,25.2) 81.6(4,1.9) 93.3(4)[e] 90.4(5,10.7) 174.5(4)	840
[Cu(bpdz)NCS)]NCS (blue-green)	m $B2_1/c$ 8	26.75(7) 7.62(2) 19.08(5)	 90.36(5) 	CuN_5	SCN_{eq} N_{eq} N_{ap}	2.162(14) 2.053(11,8) 1.988(11,4)	N_{eq},N_{eq} N_{eq},N_{ap} N_{ap},N_{ap}	119.9(5,25.2) 82.8(5,9)[d] 93.6(4)[e] 90.4(5,10.9) 176.7(5)	840
$[Cu(doct)(NCS)]ClO_4$[c] (not given)	or $Pca2_1$,Pcam 8	23.90(4) 8.56(2) 14.71(3)	 	CuN_5 N_{ap} CuN_5 N_{eq} N_{ap}	SCN_{eq} N_{eq} 1.98(3,0) SCN_{eq} 2.02(3,4) 2.06(2,2)	2.12(3) 2.09(2,1) 2.19(3)	N_{eq},N_{eq} N_{eq},N_{ap} N_{ap},N_{ap} N_{eq},N_{eq} N_{eq},N_{ap} N_{ap},N_{ap}	120(1,24) 86(1,3)[d] 91(1,11) 165(1) 120(1,27) 85(1,3)[d] 91(1,8) 167(1)	841

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
[Cu(tren)(NCS)]BPh_4 (green)	m $P2_1/c$ 2	14.977(5) 9.764(2) 21.226(6)	98.79(3)	CuN_5	N_{eq} N_{ap} SCN_{ap}	2.074(6,14) 2.047(6) 1.946(7)	N_{eq},N_{eq} N_{eq},N_{ap} N_{ap},N_{ap}	118.8(2,6.5) 83.9(2,1)[d] 179.0(2)	842
[Cu(tren)(NCO)]BPh_4 (blue)	m $P2_1/c$ 2	14.003(6) 10.399(5) 20.436(9)	94.00(3)	CuN_5	N_{eq} N_{ap} OCN_{ap}	2.09(1,1) 2.06(1) 1.87(1)	N_{eq},N_{eq} N_{eq},N_{ap} N_{ap},N_{ap}	118.9(5,7.3) 83.8(5,1.0)[d] 90.1(5,9.5) 176.7(6)	842
[Cu(tpea)(NCS)]·[$Cu(NCS)_2$] (green)	m $P2_1/c$ 4	18.026(9) 8.847(4) 16.302(7)	113.18(5)	CuN_5	N_{eq} N_{ap} SCN_{ap}	2.090(4,61) 2.037(4) 1.959(4)	N_{eq},N_{eq} N_{eq},N_{ap}	120(2,23.3) 89.6(2)[d] 90.2(2,2.3) 91.6(2,7)[e]	788b
[Cu(trenen)]Br_2 (blue)	or $P2_12_12_1$ 4	8.75(1) 13.19(2) 12.90(2)		CuN_5	N_{eq} N_{ap}	2.06(2,3) 2.025(20,15)	N_{eq},N_{eq} N_{eq},N_{ap} N_{ap},N_{ap}	119.4(7,8.8) 85.0(6,1.8)[d] 90.2(7,14.8) 169.6(6)	843
[Cu(imep)]$(ClO_4)_2$ (green)	m C2/c 8	19.065(9) 11.370(4) 23.802(12)	108.17(4)	CuN_5	N_{eq} N_{ap}	1.999(6,82) 2.051(6,15)	N_{eq},N_{eq} N_{eq},N_{ap} N_{ap},N_{ap}	120.0(2,19.2) 78.6(2)[d] 79.0(2,4) 157.9(2)	844
[Cu(tridec)]$(ClO_4)_2$ (not given)	m $P2_1/n$ 4	17.786(8) 8.035(5) 19.400(9)	111.49(5)	CuN_5	N_{eq} N_{ap}	2.06(2,9) 1.99(2,0)	N_{eq},N_{eq} N_{eq},N_{ap} N_{ap},N_{ap}	120.0(8,24.4) 79.3(7.8)[d] 93.0(8,0)[e] 89.8(8,11.3) 174.0(7)	845
[$Cu(C_{21}H_{27}N_7)$]$(BF_4)_2$·0.5MeOH (not given) (at 118K)	tr P–1 2	11.983(3) 10.360(4) 12.906(6)	68.51(3) 73.63(3) 67.06(3)	CuN_5	N_{eq} N_{ap}	2.009(8,8.5) 2.036(4,23)	N_{eq},N_{eq} N_{eq},N_{ap} N_{ap},N_{ap}	120.0(3,18.5) 79.1(2,4)[d] 86.9(3,2)[e] 91.0(3,16.7) 158.1(2)	546b
[Cu(picdien)]·[$CuCl_4$] (blue)	m $P2_1/n$ 4	11.822(2) 13.845(2) 13.619(2)	93.17(2)	CuN_5	N_{eq} N_{ap}	2.051(4,22) 2.243(4) 2.042(4,7)	N_{eq},N_{eq} N_{eq},N_{ap} N_{ap},N_{ap}	82.8(2,1.1)[d] 115.5(1) 159.9(1) 80.5(1,1.2)[d] 99.3(1,4.0) 176.2(2)	203
				$CuCl_4$	Cl	2.270(1,23)	Cl,Cl	109.4(1,4.9)	
[$Co(NH_3)_6$]($CuCl_5$] (not given)	c Fd–3c 32	22.085(2)		$CuCl_5$	Cl_{eq} Cl_{ap}	2.3937(3) 2.3005(3)	Cl_{eq},Cl_{eq} Cl_{eq},Cl_{ap} Cl_{ap},Cl_{ap}	120.0(1) 90.0(1) 180.0(1)	846
[$Cr(NH_3)_5(H_2O)$]·[$CuCl_5$] (not given)	c Fd3c 32	22.208(3)		$CuCl_5$	Cl_{eq} Cl_{ap}	2.388(3) 2.309(3)	not given		847
[Cu(bheg)]ClO_4·H_2O (pale blue)	m $P2_1/n$ 4	22.646(2) 9.369(1) 10.619(2)	108.69(1)	CuO_4N	O_{eq} O_{ap} N_{ap}	2.006(3,11) 2.181(4) 1.916(3) 2.003(3)	O_{eq},O_{eq} O_{eq},N_{ap} O_{ap},N_{ap}	118.7(1,22.8) 83.7(1,1.3)[d] 171.4(1)	848
$(PPh_4)_2$[$CuCl(NO_3)_2$]·CH_2Cl_2 (green) (at 130K)	tr P–1 2	11.13(1) 11.56(1) 19.65(2)	101.02(1) 93.74(1) 104.05(2)	CuO_4Cl	O_{eq} O_{eq} O_{ap} Clap	1.992(6) 2.292(6,20) 1.995(5) 2.273(2)	O_{eq},O_{eq} O_{eq},O_{ap} O_{eq},Cl_{ap} Cl_{ap},O_{ap}	54.1(2)[g] 119.7(2,44.0) 88.9(2,5.6) 91.8(2,1.1) 170.5(2)	849
[Cu(tmpa)F]PF_6·CH_2Cl_2 (blue)	or Pbab,Pcab 8	11.869(2) 15.891(3) 26.116(6)		CuN_4F	N_{eq} N_{ap} F_{ap}	2.024(10,20) 2.069(10) 1.853(8)	N_{eq},N_{eq} N_{eq},N_{ap} N_{eq},F_{ap} N_{ap},F_{ap}	117.7(4,7.1) 81.5(3)[d] 81.2(4,7) 98.8(3,7) 179.5(4)	850

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(bpy)_2(H_2O)]S_2O_6$ (blue)	m C2/c 4	8.03(5) 16.99(5) 15.73(5)	103.5(5)	CuN_4O	H_2O_{eq} N_{eq} N_{ap}	2.158(15) 2.013(9,0) 1.977(9,0)	N_{eq},N_{eq} N_{eq},O_{eq} O_{eq},N_{ap} N_{eq},N_{ap} N_{ap},N_{ap}	129.8(5) 115.1(3.0) 87.3(3) 81.4(4,0)[d] 91.2(5,9.8) 177.6(5)	851
$[Cu(bpy)_2(H_2O)]S_5O_6$ (turquoise blue)	m $P2_1/c$ 4	7.651(2) 12.980(3) 26.140(5)	95.50(5)	CuN_4O	H_2O_{eq} N_{eq} N_{ap}	2.057(5) 2.074(6,50) 1.978(6,5)	N_{eq},N_{eq} N_{eq},O_{eq} N_{eq},N_{ap} O_{eq},N_{ap} N_{ap},N_{ap}	114.4(3) 124.3(2,19.4) 80.3(2,1.0)[d] 90.0(3,11.4) 90.2(2,1.2) 179.1(2)	852
$[Cu(bpy)_2(S_2O_8)]\cdot H_2O$ (turquoise)	tr P-1 2	7.612(2) 9.684(2) 15.557(4)	100.64(5) 82.03(5) 96.81(5)	CuN_4O	$O_7S_2O_{eq}$ N_{eq} N_{ap}	2.367(4) 2.036(4,4) 1.966(5,7)	N_{eq},N_{eq} O_{eq},N_{eq} N_{eq},N_{ap} O_{eq},N_{ap} N_{ap},N_{ap}	141.0(1) 109.5(2,16.5) 81.6(2,2)[d] 91.4(2,10.3) 86.3(2,1.5) 172.2(1)	853
$[Cu(bpy)_2(acasp)]\cdot$ $EtOH\cdot(H_2O)$ (blue)	tr P-1 2	12.947(4) 12.462(4) 11.152(3)	115.44(6) 106.53(5) 74.32(5)	CuN_4O	$aspO_{eq}$ N_{eq} N_{ap}	1.977(6) 2.103(9,9) 1.960(7,2)	N_{eq},N_{eq} O_{eq},N_{eq} N_{eq},N_{ap} O_{eq},N_{ap} N_{ap},N_{ap}	96.7(3) 131.6(3,6.6) 80.1(3,1)[d] 87.7(3,9.5) 93.3(3,1.0) 172.5(3)	854
$[Cu(Me_4bpy)_2(ClO_4)]\cdot$ ClO_4 (not given)	m $P2_1/c$ 4	17.775(2) 12.785(3) 14.514(2)	110.51(3)	CuN_4O	O_3ClO_{eq} N_{eq} N_{ap}	2.491(6) 2.046(6,6) 1.969(5,10)	N_{eq},N_{eq} N_{eq},O_{eq} N_{eq},N_{ap} O_{eq},N_{ap} N_{ap},N_{ap}	120.6(3) 119.7(2,4.1) 82.3(2,3)[d] 95.0(2,13.7) 80.2(2,3.9) 160.2(3)	855
$[Cu(Me_4bpy)_2(H_2O)]\cdot$ $(ClO_4)_2\cdot H_2O$[c] (not given)	m $P2_1/c$ 8	14.594(2) 16.192(3) 28.934(2)	103.50(4)	CuN_4O	H_2O_{eq} N_{eq} N_{ap}	2.004 2.159(18,53) 1.977(16,3)	N_{eq},N_{eq} N_{eq},O_{eq} N_{eq},N_{ap} O_{eq},N_{ap} N_{ap},N_{ap}	108(1) 120(1,9) 80(1,1)[d] 94(1,15) 85(1,3) 170(1)	855
				CuN_4O	H_2O_{eq} N_{eq} N_{eq}	2.100(18) 2.146(17,4) 2.016(17,13)	N_{eq},N_{eq} N_{eq},O_{eq} N_{eq},N_{ap} O_{eq},N_{ap} N_{ap},N_{ap}	108(1) 126(1,5) 79.5(10,5)[d] 92(1,15) 87(1,1) 172(1)	
$[Cu(phen)_2(H_2O)]\cdot$ $(BF_4)_2$ (green)	m C2/c 4	19.099(6) 8.100(3) 16.177(5)	100.54(5)	CuN_4O	H_2O_{eq} N_{eq} N_{ap}	2.238(8) 2.041(7,0) 1.985(6,0)	N_{eq},N_{ap} N_{eq},O_{eq} O_{eq},N_{ap}	91.4(3,8.8)[d] 111.7(3) 86.4(3)	856
$[Cu(phen)_2(H_2O)]\cdot$ $(NO_3)_2$ (green)	m C2/c 4	22.58(2) 7.23(1) 16.58(2)	123.6(1)	CuN_4O	H_2O_{eq} N_{eq} N_{ap}	2.18(1) 2.03(1,0) 1.99(1,0)	N_{eq},N_{eq} N_{eq},O_{eq} N_{eq},N_{ap} O_{eq},N_{ap} N_{ap},N_{ap}	139.6(4) 110.0(4) 91.6(4,8.6)[d] 85.5(1) 171.0(4)	857
$[Cu(2,9\text{-}Me_2phen)_2\cdot$ $(NO_3)]\cdot Cl_3ac\cdot Cl_3acH$ (green)	m Cc 4	24.301(9) 8.075(2) 18.13(6)	91.44(3)	CuN_4O	O_2NO_{eq} N_{eq} N_{ap}	2.15(4) 2.11(1,4) 2.05(1,1)	N_{eq},N_{eq} N_{eq},O_{eq} O_{eq},N_{ap} N_{eq},N_{ap} N_{ap},N_{ap}	110(1) 125(1,19) 85(1,3) 82(1,1)[d] 93.3(1,12.3) 169(1)	858

TABLE II *(Continued)*

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(6\text{-}Mebpy)_2(BF_3OH)]\cdot BF$ (green)	m $P2_1/c$ 4	9.005(2) 17.868(2) 15.298(3)	104.13(1)	CuN_4O	O_{eq} $bpyN_{eq}$ $bpyN_{ap}$	2.034(3) 2.071(4,12) 1.994(4,4)	N_{eq},N_{eq} N_{eq},O_{eq} O_{eq},N_{ap} N_{eq},N_{ap} N_{ap},N_{ap}	110.6(1) 124.7(1,4.1) 90.8(1,3) 80.8(2,1)[d] 89.6(2,9.8) 178.0(2)	859
$[Cu(bpym)_2(H_2O)]ClO_4\cdot 2H_2O$ (blue green)	m C2/c 4	18.232(3) 7.613(1) 16.842(4)	96.27(2)	CuN_4O	H_2O_{eq} N_{eq} N_{ap}	1.993(4) 2.094(4,0) 1.993(4,0)	N_{eq},N_{eq} O_{eq},N_{ap} N_{eq},N_{ap} O_{eq},N_{eq} N_{ap},N_{ap}	99.8(1) 90.5(1) 79.8(1,0)[d] 89.7(1,9.9) 130.1(1) 179.0(1)	860
$[Cu(phenet)(H_2O)]\cdot(ClO_4)_2$ (green)	m $P2_1/c$ 4	12.075(2) 14.340(2) 16.201(2)	103.27(1)	CuN_4O	H_2O_{eq} N_{eq} N_{ap}	2.198(4) 2.092(5,3) 1.976(5,9)	N_{eq},N_{eq} N_{eq},O_{eq} O_{eq},N_{ap} N_{eq},N_{ap} N_{ap},N_{ap}	132.6(2) 113.7(2,6.0) 86.5(2,2.8) 82.2(2,2)[d] 91.5(2,11.0) 172.2(2)	861
$[Cu(tetb)(NO_3)]ClO_4$ (blue)	m $P2_1/c$ 4	8.769(5) 17.809(5) 14.344(5)	not given	CuN_4O	O_2NO_{eq} N_{eq} N_{ap}	2.106(8) 2.104(9,24) 1.982(9.11)	N_{eq},N_{ap}	85.8(4)[d] 93.0(4)[e]	862
$[Cu(btma)(NO_3)]NO_3\cdot 0.5H_2O$ (green)	m $P2_1/c$ 4	24.254(2) 14.107(2) 16.329(2)	105.94(1)	CuN_4O	N_{eq} N_{ap} O_2NO_{ap}	2.084(3.64) 2.059(3) 1.938(3)	N_{eq},N_{eq} N_{eq},N_{ap} N_{eq},O_{ap} N_{ap},O_{ap}	117.9(2,19.1) 81.9(1,1.3)[d] 97.8(1,2.3) 177.2(1)	863
$[Cu(bpy)_2(CN)]NO_3\cdot 2H_2O$ (dark blue)	m $P2_1/n$ 4	9.263(3) 24.678(4) 10.123(3)	109.83(8)	CuN_4C	NC_{eq} N_{eq} N_{ap}	1.974(5) 2.125(5,37) 2.002(4,6)	N_{eq},N_{eq} N_{eq},C_{eq} N_{eq},N_{ap} C_{eq},N_{ap} N_{ap},N_{ap}	95.4(2) 132.3(2,5.8) 79.4(2.8)[d] 86.9(2,8.3) 94.5(3,3) 170.9(1)	864
$[Cu(phen)_2(CN)]NO_3\cdot H_2O$ (dark blue)	tr P–1 2	10.816(2) 12.098(2) 10.118(2)	105.62(2) 110.10(2) 66.68(2)	CuN_4C	NC_{eq} N_{eq} N_{ap}	1.935(10) 2.113(6,11) 2.008(10,7)	N_{eq},N_{eq} N_{eq},C_{eq} N_{eq},N_{ap} C_{eq},N_{ap} N_{ap},N_{ap}	98.6(2) 130.7(3,(1.7) 80.3(3,4)[d] 88.1(3,8.2) 92.9(5,11) 174.3(3)	865
$[Cu(phen)_2(CN)]$cnment$\cdot 2H_2O$ (dark green)	tr P–1 2	10.262(3) 10.595(2) 11.950(4)	88.36(2) 84.28(2) 83.07(2)	CuN_4C	NC_{eq} N_{eq} N_{ap}	1.970(5) 2.106(3,10) 2.002(3,1)	C_{eq},N_{eq} N_{eq},N_{eq} C_{eq},N_{ap} N_{eq},N_{ap} N_{ap},N_{ap}	128.33(14,3.53) 103.34(11) 95.02(14,9) 80.21(12,29)[d] 86.86(12,6.94) 169.92(12)	866
$[Cu(phen)_2(CN)]_2\cdot(phen)_2(NCS)]_2\cdot 5\cdot 5H_2O$[c] (not given)	or $P2_1P2_1P2_1$ 4	10.175(5) 14.146(5) 39.575(5)		CuN_4C	NC_{eq} N_{eq} N_{ap}	1.948(8) 2.107(6,22) 2.080(6,3)	N_{eq},N_{eq} C_{eq},N_{eq} C_{eq},N_{ap} N_{ap},N_{ap}	97.4(2) 131.3(3,4.6) 94.6(3,1.6) 80.6(2.4)[d] 87.0(2,6.8)	867
				CuN_4C	NC_{eq} N_{eq} N_{ap}	1.947(8) 2.119(7,3) 2.006(6,4)	N_{eq},N_{ap} N_{eq},N_{eq} C_{eq},N_{eq} C_{eq},N_{ap} N_{eq},N_{ap} N_{ap},N_{ap}	170.8(3) 97.5(2) 131.2(3,4.6) 95.2(3,3.0) 80.9(3.1)[d] 86.6(3,6.0) 169.7(3)	

TABLE II (*Continued*)

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(bpy)_2Cl]_2S_5S_6 \cdot 6H_2O$ (torquoise blue)	tr C–1 2	20.577(4) 14.777(3) 8.726(2)	94.72(5) 101.91(5) 92.03(5)	CuN_4Cl	Cl_{eq} N_{eq} N_{ap}	2.292(4) 2.009(6,7) 1.990(6,2)	N_{eq},N_{eq} N_{eq},Cl_{eq} N_{eq},N_{ap} Cl_{eq},N_{ap} N_{ap},N_{ap}	107.3(2) 126.4(2,4.4) 79.8(3,1)[d] 88.5(3,9.0) 92.7(2,7) 177.8(2)	852
$[Cu(bpy)_2Cl]PF_6H_2O$ (blue)	m $P2_1/b$ 4	21.403(5) 12.235(3) 8.599(2)	 92.68(2) 	CuN_4Cl	Cl_{eq} N_{eq} N_{ap}	2.108(6) 2.107(6,2) 2.001(6,5)	N_{eq},N_{eq} N_{eq},Cl_{eq} Cl_{eq},N_{ap} N_{eq},N_{ap} N_{ap},N_{ap}	123.8(2) 118.1(2,2.4) 92.2(2,1) 79.9(2,3)[d] 89.0(2,7.4) 175.5(2)	868
$[Cu(phen)_2Cl]Cl_2 \cdot 3H_2O \cdot (Me_2CO)_2$ (green)	m $P2_1/b$ 4	19.345(4) 22.1(9) 13.660(4)	 64.28(2)	CuN_4Cl	Cl_{eq} N_{eq} N_{ap}	2.257(2) 2.130(4,22) 1.992(4,2)	N_{eq},N_{eq} Cl_{eq},N_{eq} N_{eq},N_{ap} N_{ap},N_{ap} Cl_{eq},N_{ap}	106.4(1) 126.8(1,6.2) 80.9(2,3)[d] 86.6(2,7.2) 168.8(2) 95.5(1,1.3)	869
				CuN_4Cl	Cl_{eq} N_{eq} N_{ap}	2.281(1) 2.132(3,6) 1.997(4,2)	N_{eq},N_{eq} Cl_{eq},N_{eq} Cl_{eq},N_{ap} N_{eq},N_{ap} N_{ap},N_{ap}	100.0(1) 130.0(1,4) 94.3(2,2) 80.3(2,2)[d] 87.1(2,8.0) 170.8(1)	
$[Cu(phen)_2Cl]ClO_4$ (deep green)	m $P2_1/c$ 4	12.668(1) 11.247(1) 17.222(1)	 111.50(1) 	CuN_4Cl	Cl_{eq} N_{eq} N_{ap}	2.298(2) 2.107(6,30) 1.995(6,9)	N_{eq},N_{eq} Cl_{eq},N_{ap} N_{ap},N_{ap}	81.1(2,5)[d] 89.1(2,9.1) 91.6(2,7) 176.2(3)	870
$[Cu(bpy)_2Cl]ClO_4$ (blue)	m $P2_1/c$ 4	10.761(5) 12.253(5) 16.990(5)	 112.18(5) 	CuN_4Cl	Cl_{eq} N_{eq} N_{ap}	2.263(3) 2.106(5,30) 1.992(4,1)	N_{eq},N_{eq} N_{eq},Cl_{eq} N_{eq},N_{ap} Cl_{eq},N_{ap} N_{ap},N_{ap}	96.3(2) 131.9(2,5.2) 79.7(2,5)[d] 85.6(2,11.8) 92.8(2,7) 174.5(1)	871
$[Cu(bpy)_2Cl]NO_3 \cdot 3H_2O$ (blue)	m $P2_1/a$ 4	14.305(5) 21.213(5) 8.234(5)	 114.90(4) 	CuN_4Cl	Cl_{eq} N_{eq} N_{ap}	2.308(3) 2.101(6,12) 1.989(6,0)	N_{eq},N_{eq} N_{eq},Cl_{eq} N_{eq},N_{ap} Cl_{eq},N_{ap} N_{ap},N_{ap}	102.7(2,6.1) 126.5(2,2.2) 85.5(3,12.1) 80.0(2,1)[d] 92.6(2,6) 174.9(2)	871
$[Cu(phen)_2Cl]NO_3 \cdot H_2O$ (turboquoise)	tr P–1 2	11.128(1) 12.026(4) 9.738(2)	108.84(2) 108.54(2) 67.83(2)	CuN_4Cl	Cl_{eq} N_{eq} N_{ap}	2.292(1) 2.040(2,51) 1.988(4,1)	N_{eq},N_{eq} Cl_{eq},N_{eq} Cl_{eq},N_{ap} N_{eq},N_{ap} N_{ap},N_{ap}	105.0(1) 127.5(1,8.3) 92.3(1,5) 81.1(1.3)[d] 88.6(4,7.9) 175.6(1)	872
$[Cu(bpy)_2Cl]BF_4$ (green)	m $P2_1/n$ 4	16.187(7) 12.177(3) 10.793(3)	 104.41(3) 	CuN_4Cl	Cl_{eq} N_{eq} N_{ap}	2.285(3) 2.111(8,3 2) 1.995(7,12)	N_{eq},N_{eq} N_{eq},Cl_{eq} N_{eq},N_{ap} Cl_{eq},N_{ap} N_{ap},N_{ap}	97.6(3) 131.2(3,3.6) 79.6(3.1)[d] 88.4(3,9.4) 92.4(3,7) 175.2(4)	873
$[Cu(bpy)_2Cl]pcp$ (light green)	tr P–1 2	12.278(3) 15.769(4) 7.331(2)	97.73(2) 100.01(2) 106.53(2)	CuN_4Cl	Cl_{eq} N_{eq} N_{ap}	2.277(3) 2.090(9,28) 1.984(8,15)	N_{eq},N_{eq} Cl_{eq},N_{eq} Cl_{eq},N_{ap} N_{eq},N_{ap} N_{ap},N_{ap}	107.3(3) 126.4(2,12.2) 92.8(2,8) 79.5(3,9)[d] 88.3(3,9.7) 174.3(3)	874
$[Cu(bipyam)_2Cl]Cl$ (green)	m $P2_1/n$ 4	9.704(3) 14.493(4) 14.704(16)	 97.88(5) 	CuN_4Cl	Cl_{eq} N_{eq} N_{ap}	2.290(3) 2.111(6,23) 1.997(6,3)	N_{eq},N_{eq} N_{eq},Cl_{eq} N_{eq},N_{ap} Cl_{eq},N_{ap} N_{ap},N_{ap}	99.9(2) 130.0(2,12.7) 87.9(3,4.2)[d] 92.1(3,4.2) 88.4(2,1.3) 176.6(2)	875

TABLE II *(Continued)*

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(bipyam)_2Cl]\cdot 4H_2O$	m	12.556(6)		CuN_4Cl	Cl_{eq}	2.334(4)	N_{eq},N_{eq}	97.5(2)	876
(green)	$P2_1/a$	28.002(7)	99.98(6)		N_{eq}	2.100(6,72)	Cl_{eq},N_{eq}	131.2(2,26.8)	
	4	6.997(4)			N_{ap}	2.003(6,2)	N_{eq},N_{ap}	86.9(2,3)[d]	
								91.3(2,8.4)	
							Cl_{eq},N_{ap}	89.5(2,1.0)	
							N_{ap},N_{ap}	173.0(2)	
$[Cu(tbaz)_2Cl]Cl\cdot H_2O$	m	14.778(3)		CuN_4Cl	Cl_{eq}	2.313(2)	N_{eq},N_{eq}	103.4(2)	877
(pale green)	$P2_1/c$	11.713(2)	101.61(2)		N_{eq}	2.088(6)	Cl_{eq},N_{eq}	128.4(2,14.8)	
	4	14.100(3)				2.235(6)	Cl_{eq},N_{ap}	94.7(2,2.1)	
					N_{ap}	1.963(6,5)	N_{eq},N_{ap}	79.6(2,1.0)[d]	
								86.9(2,8.3)	
							N_{ap},N_{ap}	170.1(3)	
$[Cu(pyox)_2Cl]\cdot 0{\cdot}5H_2O$	m	18.071(3)		CuN_4Cl	Cl_{eq}	2.268(1)	N_{eq},N_{eq}	98.6(1)	878
(not given)	C2/c	16.690(2)	114.62(4)		N_{eq}	2.152(2,64)	Cl_{eq},N_{eq}	130.7(1,16.2)	
	8	16.974(2)			N_{ap}	2.006(2,4)	Cl_{eq},N_{ap}	92.2(1,8)	
							N_{eq},N_{ap}	80.3(1,9)[d]	
								88.5(1,9.1)	
							N_{ap},N_{ap}	175.4(1)	
$[Cu(tmpa)Cl]PF_6$	or	14.924(3)		CuN_4Cl	Cl_{eq}	2.233(2)	N_{eq},N_{eq}	117.7(3,1.7)	879
(not given)	I2ab	16.632(4)			N_{eq}	2.065(9,47)	N_{eq},N_{ap}	81.1(4,4)[d]	
	8	17.346(3)			N_{ap}	2.050(6)	N_{eq},Cl_{ap}	98.9(3,1.3)	
							N_{ap},Cl_{ap}	179.1(4)	
$[Cu(tepa)Cl]PF_6$	m	12.483(2)		CuN_4Cl	Cl_{eq}	2.289(1)	N_{eq},N_{eq}	95.7(1)[e]	879
(not given)	$P2_1/c$	12.939(2)	90.20(1)		N_{eq}	2.164(3,64)	N_{eq},Cl_{eq}	131.6(1,28.2)	
	4	16.268(2)			N_{ap}	2.050(3,12)	N_{eq},N_{ap}	90.3(1,4.0)[e]	
								92.3(1,6.0)	
							Cl_{eq},N_{ap}	88.4(1,2.9)	
							N_{ap},N_{ap}	171.1(1)	
$[Cu(tet)Cl]Cl0_4\cdot Me_3CN$	m	12.860(2)		CuN_4Cl	Cl_{eq}	2.305(5)	N_{eq},N_{eq}	106.6(3)	880
(green)	$P2_1/c$	17.036(3)	96.33(2)		N_{eq}	2.133(8,73)	Cl_{eq},N_{eq}	126.3(2,6)	
	4	14.585(2)			N_{ap}	2.009(9,28)	N_{eq},N_{ap}	78.7(3,1.2)[d]	
$[Cu(bpycp)Cl]_2\cdot$	tr	9.570(2)	92.66(2)	CuN_4Cl	Cl_{eq}	2.343(1)	N_{eq},N_{eq}	114.2(1)	881
$[Cu_2Cl_6]$	P-1	14.017(2)	96.81(2)		N_{eq}	2.121(4,26)	Cl_{eq},N_{eq}	122.9(1,18.8)	
(green)	1	14.567(2)	103.61(2)		N_{ap}	2.004(3,1)	N_{eq},N_{ap}	80.0(1,5)[d]	
								96.0(1,5)[e]	
								91.7(1,18.9)	
							Cl_{eq},N_{ap}	88.7(1,1.1)	
							N_{ap},N_{ap}	168.9(1)	
$[Cu(tren)Cl]BPh_4$	m	13.678(5)		CuN_4Cl	N_{eq}	2.091(3,25)	N_{eq},N_{eq}	118.7(1,5.1)	842
(blue)	$P2_1/c$	10.288(3)	94.84(3)		N_{ap}	2.081(3)	N_{eq},N_{ap}	83.4(1,4)[d]	
	2	20.432(6)			Cl_{ap}	2.253(1)	$N_{eq}Cl_{ap}$	96.7(1,2.7)	
							N_{ap},Cl_{ap}	177.8(1)	
$[Cu(ptr)Cl]PF_6\cdot$	m	15.30(3)		CuN_4Cl	Cl_{eq}	2.296(3)	N_{eq},N_{eq}	78.8(3)[d]	882
$NaPF_6\cdot 3Me_3CN$	$P2_1/n$	12.520(4)	95.15(2)		N_{eq}	2.23(1,10)	N_{eq},Cl_{eq}	140.2(2,11.5)	
(blue)	4	22.781(4)			N_{ap}	2.002(8,17)	N_{eq},N_{ap}	94.7(3)[e]	
								91.3(3,4.0)	
							Cl_{eq},N_{ap}	88.5(2,1.8)	
							N_{ap},N_{ap}	176.4(3)	
$[Cu(bpy)_2(tu)](Cl0_4)_2$	or	11.05(1)		CuN_4S	tuS_{eq}	2.369(4)	N_{eq},N_{eq}	110.5(3)	883
(green)	$P2_12_12_1$	20.16(2)			N_{eq}	2.098(7,1)	N_{eq},S_{eq}	124.4(2,0)	
	4	12.13(1)			N_{ap}	1.980(7,1)	S_{eq},N_{ap}	92.9(2,6)	
							N_{eq},N_{ap}	80.2(3,6)[d]	
								88.4(3,10.5)	
							N_{ap},N_{ap}	173.9(2)	

TABLE II *(Continued)*

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(phen)_2(tu)]\cdot(ClO_4)_2\cdot H_2O$	m	10.38(2)		CuN_4S	tuS_{eq}	2.405(4)	N_{eq},N_{eq}	123.2(1)	884
(not given)	$P2_1/c$	37.27(3)	95.3(1)		N_{eq}	2.084(4,4)	N_{eq},S_{eq}	118.3(1,1.9)	
	4	7.60(1)			N_{ap}	2.035(5,22)	S_{eq},N_{ap}	90.6(1,3.1)	
							N_{eq},N_{ap}	81.2(1,4)[d]	
								89.7(1,8.9)	
							N_{ap},N_{ap}	178.7(1)	
$[Cu(fpsem)(bpy)]ClO_4$	tr	8.560(3)	106.35(3)	CuN_4S	N_{eq}	2.050(4)	N_{eq},N_{eq}	90.7(2)	885
(green)	P–1	9.452(4)	94.66(3)		S_{eq}	2.275(2)	N_{eq},S_{eq}	133.3(1,23.7)	
	2	13.078(4)	95.27(3)		$bpyN_{eq}$	2.179(1)	N_{eq},N_{ap}	79.3(2,1.1)[d]	
					N_{ap}	1.950(4)		89.4(2,14.6)	
					$bpyN_{ap}$	1.986(4)	S_{eq},N_{ap}	84.1(1)d	
								91.8(1,7.7)	
							N_{ap},N_{ap}	174.9(2)	
$[Cu(Me_4pyal)(tu)]\cdot(ClO_4)_2$	m	9.91(1)		CuN_4S	tuS_{eq}	2.344(3)	N_{eq},N_{eq}	108.9(1.1)	883
(not given)	$P2_1/c$	11.42(1)	98.5(2)		N_{eq}	2.099(16,49)	N_{eq},S_{eq}	125.1(5,6.1)	
	4	21.72(1)			N_{ap}	1.986(7,9)	S_{eq},N_{ap}	95.2(4,8)	
							N_{eq},N_{ap}	80.7(6,5)[d]	
								91.7(9)[h]	
								87.0(9,7.4)	
							N_{ap},N_{ap}	169.6(5.0)	
$[Cu(tetb)(mbn)]\cdot H_2O$	m	8.387(3)		CuN_4S	$mbnS_{eq}$	2.359(4)	N_{eq},N_{eq}	103.5(1)	886
(green)	$P2_1/n$	21.1(1)	90.92(3)		N_{eq}	2.163(10,31)	N_{eq},N_{ap}	84.4(4,1)[d]	
	4	14.677(5)			N_{ap}	1.999(10,2)		90.0(4,8)[e]	
								87.2 (4,3.5)	
							S_{eq},N_{eq}	128.1(3,7.3)	
							S_{eq},N_{ap}	94.5(3,3.6)	
							N_{ap},N_{ap}	170.8(4)	
[Cu(tetb)(mac)]·3MeOH	m	13.920(6)		CuN_4S	$macS_{eq}$	2.328(5)	S_{eq},N_{eq}	127.0(4,1.9)	887
(green)	$P2_1/n$	13.753(2)	92.25(3)		N_{eq}	2.127(13,2)	S_{eq},N_{ap}	93.7(4,4.7)	
	4	14.472(6)			N_{ap}	2.005(13,5)	N_{ap},N_{ap}	172.5(6)	
$[Cu(tetb)(spp)]\cdot(MeOH)_2$	m	14.003(2)		CuN_4S	$sppS_{eq}$	2.314(2)	N_{eq},N_{eq}	104.0(2)	888
(green)	$P2_1/n$	13.683(2)	91.85(2)		$tetN_{eq}$	2.161(4,8)	S_{eq},N_{eq}	127.8(1,1.8)	
	4	14.548(4)		0.074	$tetN_{ap}$	2.016(4,15)	S_{eq},N_{ap}	94.1(1,4.1)	
							N_{eq},N_{ap}	84.2(2,0)[d]	
								90.3(2,5)[e]	
								87.3(2,3.5)	
							N_{ap},N_{ap}	171.1(2)	
$[Cu(bpy)_2Br]Br$	m	11.463(3)		$CuN_4Br.$	Br_{eq}	2.429(2)	N_{eq},N_{eq}	106.7(3)	889
(not given)	$P2_1/c$	11.246(2)	121.50(2)		N_{eq}	2.080(8,5)	N_{eq},Br_{eq}	126.7(2,2.0)	
	4	17.785(4)			N_{ap}	1.978(6,1)	N_{eq},N_{ap}	80.4(3,1)[d]	
								92.5(3,12.1)	
							Br_{eq},N_{ap}	90.9(2,5)	
							N_{ap},N_{ap}	177.3(3)	
$[Cu(bpy)_2Br]BF_4$	m	10.862(2)		CuN_4Br	Br_{eq}	2.419(3)	N_{eq},N_{eq}	99.4(3)	890
(not given)	$P2_1/c$	12.240(2)	113.87(5)		N_{eq}	2.091(9,23)	Br_{eq},N_{eq}	130.4(3,4.2)	
	4	17.304(2)			N_{ap}	1.996(7,1)	Br_{eq},N_{ap}	92.1(3,9)	
							N_{eq},N_{ap}	79.9(3,3)[d]	
								88.6(3,9.0)	
							N_{ap},N_{ap}	175.6(2)	
$[Cu(aepy)_2Br)Br$	m	8.883(6)		CuN_4Br	Br_{eg}	2.702(2)	N_{eq},N_{eq}	149.4(3)	891
(blue)	C2/c	11.853(13)	67.57(3)		N_{eq}	2.027(4,0)	Br_{eq},N_{eq}	105.3(1,0)	
	4	16.940(14)			N_{ap}	2.065(3,0)	Br_{eq},N_{ap}	89.01(9,0)	
							N_{eq},N_{ap}	90.3(2,2.6)	
								92.8(2.0)[d]	
							N_{ap},N_{ap}	178.0(2)	

TABLE II *(Continued)*

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$Cu(Et_4dien)(N_3)Br$	tr	7.683(2)	111.67(2)	CuN_4Br	Br_{eq}	2.586(1)	N_{eq},N_{eq}	128.8(2)	892
(dark green)	P–1	12.848(1)	99.54(2)		$dienN_{eq}$	2.193(4,32)	Br_{eq},N_{eq}	114.6(1,9.3)	
	2	9.916(1)	93.14(3)		$dienN_{ap}$	2.015(5)	Br_{eq},N_{ap}	94.3(2,4.5)	
					$(N_3)_{ap}$	1.927(6)	N_{eq},N_{ap}	83.8(2)[d]	
								88.2(2,6.0)	
							N_{ap},N_{ap}	171.4(2)	
$[Cu(bpy)_2I]I$	tr	10.66(5)	93.3(5)	CuN_4I	I_{eq}	2.70	N_{eq},N_{eq}	107	893
(brown)	P–1	14.37(5)	101.1(5)		N_{eq}	2.03(–,7)	N_{eq},I_{eq}	124	
	2	7.44(5)	107.6(5)		N_{ap}	2.015(–,15)	N_{eq},N_{ap}	82(–,1)[d]	
								89	
							N_{ap},I_{eq}	92	
$[Cu(bpy)_2I]ClO_4$	tr	7.420(2)	108.41(2)	CuN_4I	I_{eq}	2.675(4)	N_{eq},N_{eq}	114.3(3)	890
(not given)	P–1	10.944(2)	95.09(2)		N_{eq}	2.095(8,5)	N_{eq},I_{eq}	122.9(3,1)	
	2	14.270(2)	99.27(2)		N_{ap}	1.988(6,1)	N_{eq},N_{ap}	80.2(3,1)[d]	
								88.7(3,10.8)	
							I_{eq},N_{ap}	92.4(2,1.4)	
							N_{ap},N_{ap}	174.4(2)	
$[Cu(phen)_2I]]\cdot S_8$	or	7.984(5)		CuN_4I	I_{eq}	2.672(3)	I_{eq},N_{eq}	125.3(3,0)	894
(not given)	Pbcb	16.690(4)			N_{eq}	2.10(1,0)	I_{eq},N_{ap}	92.3(3,0)	
	4	22.986(12)			N_{ap}	2.00(1,0)	N_{eq},N_{ap}	80.4(4,0)	
								88.7(4,8.7)	
							N_{ap},N_{ap}	175.5(4)	
$[Cu(bipyam)_2I]\cdot ClO_4$[c]	m	19.21(1)		CuN_4I	I_{eq}	2.697(3)	N_{eq},N_{eq}	102.3(10)	895
(dark green)	$P2_1/c$	13.47(1)	111.88(15)		N_{eq}	2.075(16,19)	I_{eq},N_{eq}	128.9(8,9.1)	
	4	19.50(5)			N_{ap}	1.992(15,0)	I_{eq},N_{ap}	88.2(8,2)	
							N_{eq},N_{ap}	91.3(11,6.5)[e]	
								85.9(10,4)	
							N_{ap},N_{ap}	175.6(10)	
				CuN_4I	I_{eq}	2.717(3)	N_{eq},N_{eq}	88.4(11)	
					N_{eq}	2.048(18,12)	N_{eq},I_{eq}	130.2(8,5.5)	
					N_{ap}	2.012(13,13)	I_{eq},N_{ap}	87.6(8,3)	
							N_{eq},N_{ap}	84.0(11,3)	
								91.7(11,3.3)[e]	
							N_{ap},N_{ap}	174.7(10)	
[Cu(pya–dpt)I]I·MeOH	m	9.670(4)		CuN_4I	I_{eq}	2.766(2)	N_{eq},N_{eq}	92.5(3,1.0)[e]	641
(green)	$P2_1/c$	12.351(6)	95.60(3)		N_{eq}	2.133(7,10)	N_{eq},N_{eq}	79.0(3)[d]	
	4	17.074(5)		0.1	N_{ap}	1.991(7,5)	I_{eq},N_{ap}	94.3(2,3)	
							I_{eq},N_{eq}	108.4(2,2.1)	
							N_{eq},N_{ap}	88.7(3,9.7)	
							N_{eq},N_{eq}	142.4(3)	
							N_{ap},N_{ap}	168.6(3)	
[Cu(iqa–dpt)I]I	m	11.210(3)		CuN_4I	I_{eq}	2.761(1)	N_{eq},N_{eq}	92.1(2,3.2)[e]	641
(green)	$P2_1/n$	10.920(4)	96.11(2)		N_{eq}	2.118(6,3)	N_{eq},N_{eq}	79.6(2)[d]	
	4	17.323(5)		0.1	N_{ap}	1.981(6,2)	I_{eq},N_{eq}	113.4(2,1.3)	
							I_{eq},N_{ap}	93.6(2,9)	
							N_{eq},N_{ap}	88.6(2,9.0)	
							N_{eq},N_{eq}	132.5(2)	
							N_{ap},N_{ap}	169.7(2)	
$[Cu(Me_4pyal)I]I$	m	12.68(1)		CuN_4I	I_{eq}	2.639(3)	N_{eq},N_{eq}	115.1(5)	896
(not given)	$P2_1/c$	18.45(1)	111.9(1)		N_{eq}	2.08(1,5)	N_{eq},I_{eq}	122.4(5,17.6)	
	4	8.92(1)			N_{ap}	2.015(10,15)	N_{eq},N_{ap}	81.7(5,9)[d]	
								87.7(5,8.8)	
							I_{eq},N_{ap}	94.5(4,1.1)	
							N_{ap},N_{ap}	171.1(5)	
$[Cu(qxa)_2(H_2O)_3]\cdot(ClO_4)_2$	m	8.263(2)		CuO_3N_2	H_2O_{eq}	2.036(6,158)	O_{eq},O_{eq}	120.0(2,37.6)	897
(dark green)	$P2_1/c$	17.259(7)	90.07(2)		N_{ap}	2.046(6,10)	O_{eq},N_{ap}	91.8(3,4.6)	
	4	15.307(5)							

TABLE II *(Continued)*

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(picl)_2(H_2O)]\cdot 2H_2O$	m	15.593(6)		CuO_3N_2	H_2O_{eq}	2.080(5)	O_{eq},O_{eq}	120.0(6,3)	898
(not given)	C2/c	7.940(6)	107.58(3)		O_{eq}	1.995(5,0)	O_{eq},N_{ap}	80.1(5,0)[d]	
	4	16.983(6)			N_{ap}	2.021(5,0)		90.1(6,14.5)	
							N_{ap},N_{ap}	168.9(6)	
$Cu(qcarb)_2(H_2O)$	m	7.756(1)		CuO_3N_2	H_2O_{eq}	2.143(3)	O_{eq},O_{eq}	120.0(1,20.3)	899
(not given)	$P2_1/c$	7.628(2)	95.31(1)		O_{eq}	1.958(3,1)	O_{eq},N_{ap}	82.3(1,2)[d]	
	4	29.573(5)			N_{ap}	2.013(3,1)		94.8(1,3.1)	
							N_{ap},N_{ap}	168.2(1)	
$[Cu(ted)(NO_3)]NO_3$	or	14.104(2)		CuO_3N_2	N_{eq}	2.011(8,0)	N_{eq},N_{eq}	138.6(5)	900
(dark blue)	Pnma	8.882(3)			O_2NO_{eq}	2.291(8)	$N_{eq}O_{eq}$	110.6(3)	
	4	12.054(1)			N_{ap}	1.982(12)	N_{eq},N_{ap}	86.3(5,0)[d]	
					O_2NO_{ap}	2.026(7)	O_{eq},N_{ap}	95.6(4)	
							O_{eq},O_{ap}	58.9(2)[g]	
							N_{eq},O_{ap}	102.0(3)	
							N_{ap},O_{ap}	154.5(4)	
Cu(2,9-Me_2phen)·$(dmc)_2$	m	18.213(1)		CuO_3N_2	N_{eq}	2.045(3)	O_{eq},N_{eq}	131.4(1,5.4)	901
	$P2_1/c$	8.649(1)	105.32(1)		$dmcO_{eq}$	2.126(6,116)	O_{eq},O_{eq}	95.8(1)	
(yellow)	4	20.728(1)			N_{ap}	1.988(4)	O_{eq},N_{ap}	101.7(1,3.7)	
					$dmcO_{ap}$	1.979(3)	O_{eq},O_{ap}	61.9(1)[g]	
								77.9(1,16.0)	
							N_{eq},O_{ap}	100.5(1)	
							N_{eq},N_{ap}	82.5(1)[d]	
							O_{ap},N_{ap}	153.8(4)	
$Cu(pco)_2Br_2$	tr	7.431(7)	91.04(7)	CuO_3Br_2	Br_{eq}	2.465(1,33)	Br_{eq},Br_{eq}	112.8(1)	902
(not given)	P-1	7.869(10)	90.83(7)		O_{eq}	2.036(5)	Br_{eq},O_{eq}	123.6(2,6.7)	
	2	13.739(13)	93.56(6)		O_{ap}	1.962(5,25)	Br_{eq},O_{ap}	93.0(2,3.1)	
							O_{eq},O_{ap}	84.5(2)[e]	
								84.6(2,1)	
							O_{ap},O_{ap}	169.1(2)	
$(Bu_4N)_2[Cu(Clqo)_2\cdot$	m	14.706(4)		CuN_3O_2	OCN_{eq}	1.85(1)	O_{eq},O_{eq}	109.9(4)	903
$(NCO)]OCN$	$P2_1/n$	23.859(4)	96.79(2)		O_{eq}	2.085(1,55)	O_{eq},N_{eq}	125.1(7,9.8)	
(red)	4	15.661(5)			N_{ap}	2.00(2,0)	O_{eq},N_{ap}	86.2(4,7.0)	
								80.2(4,7)[d]	
							N_{eq},N_{ap}	96.6(5,5)	
							N_{ap},N_{ap}	166.6(5)	
$Cu(Clqo)_2$(2-Meim)	not given			CuN_3O_2	imN_{eq}	1.963(5)	N_{eq},N_{eq}	138.3(2)	904
(not given)					O_{eq}	2.138(3)	N_{eq},O_{eq}	110.8(2,17.4)	
					N_{eq}	2.038(6)	N_{eq},N_{ap}	97.2(2)	
					N_{ap}	1.989(6)	O_{eq},N_{ap}	80.2(2)[d]	
					O_{ap}	1.978(5)	N_{eq},O_{ap}	81.6(3)[d]	
								87.3(3,5.7)	
							O_{eq},O_{ap}	91.7(2)	
							N_{ap},O_{ap}	169.6(2)	
$Cu(pmk)(NO_3)_2$	m	11.356(1)		CuN_3O_2	O_2NO_{eq}	2.154(3,0)	O_{eq},O_{eq}	80.4(2)	905
(green)	C2/c	17.325(5)	91.61(3)		N_{eq}	2.03	N_{eq},O_{eq}	139.5(–,5)	
	4	8.829(2)			N_{ap}	1.964(4,0)	N_{eq},N_{ap}	91[c]	
								81[d]	
								86(–,5)	
							O_{eq},N_{ap}	93.2(2,1.3)	
							N_{ap},N_{ap}	171.2(2)	
$Cu\{HB(Bu^tpz)_3\}NO_2$	or	15.987(7)		CuN_3O_2	N_{eq}	1.954(5)	N_{eq},N_{eq}	90.1(2)[e]	241
(not given)	Pnma	17.178(4)				2.100(4)		102.0(2)	
	4	9.233(5)			O_{ap}	1.976(5)	O_{ap},O_{ap}	58.7(2)[g]	
						2.169(6)	N_{eq},O_{ap}	111.1(2,14.9)	
								169.5(2)	

TABLE II *(Continued)*

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
[Cu(terpy)(croc)]·	tr	15.204(3)	84.18(2)	CuN_3O_2	$terN_{eq}$	2.020(8,8)	N_{eq},O_{eq}	97.7(3,8.6)	906
[Cu(terpy)(croc)·	P–1	12.825(2)	110.18(2)		O_{eq}	2.318(7)	O_{eq},O_{ap}	81.9(2)[d]	
$(H_2O)]\cdot 4H_2O$	2	11.006(2)	105.22(2)		$terN_{ap}$	1.946(8)	O_{eq},N_{ap}	105.6(3)	
(not given)					O_{ap}	1.940(7)	N_{eq},O_{ap}	99.1(3,2)	
							N_{eq},N_{ap}	80.1(3,2)[d]	
							N_{ap},O_{ap}	172.4(4)	
Cu(urac)	tr	11.296(4)	71.83(6)	CuN_3O_2	O_{eq}	2.11(1,11)	O_{eq},O_{eq}	110(1)	907
(blue)	P–1	11.469(4)	113.77(7)		N_{eq}	2.07(1)	O_{eq},N_{eq}	126(1,25)	
	2	13.589(5)	113.38(7)		N_{ap}	2.00(1,1)	O_{eq},N_{ap}	92(1)[e]	
								87(1,5)	
							N_{eq},N_{ap}	96(1,3)[e]	
								95.5(10,3.5)	
							N_{ap},N_{ap}	169(10)	
Cu(barb)	or	15.635(6)		CuN_3O_2	O_{eq}	2.070(4,47)	O_{eq},O_{eq}	103.3(2)	908
(blue)	Pbca	16.801(6)			N_{eq}	2.072(8)	O_{eq},N_{eq}	127.8(3,18.8)	
	8	17.33(7)			N_{ap}	1.933(5,2)	O_{eq},N_{ap}	90.8(3,8)[e]	
								90.0(8,4.2)	
							N_{eq},N_{ap}	90.6(3,4.8)[e]	
$[Cu(hsal)]\cdot C_6H_6$	m	13.095(3)		CuN_3O_2	O_{eq}	1.946(7,5)	O_{eq},O_{eq}	145.6(3)	909
(dark green)	$P2_1/a$	16.671(4)	93.78(4)		N_{eq}	2.337(9)	O_{eq},N_{eq}	107.2(3,2.7)	
	4	11.532(3)			N_{ap}	1.954(8,3)	N_{eq},N_{ap}	87.6(3)[d]	
								87.4(4,2)	
							O_{eq},N_{ap}	91.6(3,1)[e]	
								90.8(3,1.7)	
							N_{ap},N_{ap}	177.7(4)	
Cu(ipnp)	m	22.234(5)		CuN_3O_2	N_{eq}	2.292(2)	O_{eq},O_{eq}	141.72(7)	910
(green)	C2/c	11.753(5)	135.57(2)		O_{eq}	1.985(2,9)	N_{eq},O_{eq}	109.08(8,6.53)	
	8	19.005(4)			N_{ap}	1.955(2,1)	O_{eq},N_{ap}	90.86(8,2.44)	
							N_{eq},N_{ap}	87.46(8,7.2)[e]	
							N_{ap},N_{ap}	174.71(9)	
$Cu(mmbp)]\cdot 2H_2O$	m	29.128(6)		CuN_3O_2	N_{eq}	2.077(4)	O_{eq},O_{eq}	121.7(1)	911
(green)	C2/c	8.503(2)	106.63(2)		O_{eq}	2.015(2,0)	O_{eq},N_{eq}	119.1(1,13.0)	
	4	13.921(5)			N_{ap}	1.973(2,0)	O_{eq},N_{ap}	90.8(1,1.7)[e]	
							N_{eq},N_{ap}	88.9(1,3.6)[d]	
							N_{ap},N_{ap}	177.3(1)	
$[Cu(pcam)]ClO_4$	tg	8.071(5)		CuN_3O_2	O_{eq}	2.129(7,87)	O_{eq},O_{eq}	84.1(3)[d]	912
(dark blue)	$P4_1$	8.071(5)			N_{eq}	1.944(7)	O_{eq},N_{eq}	138.0(3,12.1)	
	4	21.291(8)		0.006	N_{ap}	2.004(9,6)	O_{eq},N_{ap}	95.5(3,4.3)	
							N_{eq},N_{ap}	82.5(3,0)[d]	
							N_{ap},N_{ap}	165.0(3)	
$Cu(igu)_3Cl_2$	m	19.097(5)		CuN_3Cl_2	Cl_{eq}	2.334(1,0)	Cl_{eq},Cl_{eq}	136.79(9)	913
(green)	C2/c	11.512(2)	107.26(3)		N_{eq}	2.154(7)	N_{eq},Cl_{eq}	97.2(4,14.4)	
	4	12.049(3)			N_{ap}	2.038(2,0)	N_{eq},N_{ap}	90.1(1)	
							N_{ap},Cl_{eq}	89.95(10,55)	
							N_{ap},N_{ap}	179.7(8)	
$Cu\{(3,5\text{–}Me_2pz)_6P_3N_3\}\cdot$	m	21.338(4)		CuN_3Cl_2	Cl_{eq}	2.555(2,12)	Cl_{eq},Cl_{eq}	142.28(10)	914
Cl_2	$P2_1/n$	11.43(3)	104.37(2)		N_{eq}	2.360(5)	Cl_{eq},N_{eq}	108.86(13,54)	
(green)	4	18.285(3)			N_{ap}	1.981(5,7)	Cl_{eq},N_{ap}	92.94(16,4.10)	
							N_{eq},N_{ap}	80.84(19,16)[d]	
							N_{ap},N_{ap}	160.74(21)	

TABLE II *(Continued)*

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$Cu(1,2\text{-}Me_2im)_3Cl_2$[c]	or	15.205		CuN_3Cl_2	Cl_{eq}	2.391(2,15)	Cl_{eq},Cl_{eq}	137.6(1)	915
(green)	$Pca2_1$	8.791			N_{eq}	2.144(5)	Cl_{eq},N_{eq}	111.2(2,7.3)	
	8	29.81			N_{ap}	2.001(5,3)	Cl_{eq},N_{ap}	89.5(2,2.2)	
							N_{eq},N_{ap}	91.4(2,4)	
							N_{ap},N_{ap}	177.2(2)	
				CuN_3Cl_2	Cl_{eq}	2.393(2,29)	Cl_{eq},Cl_{eq}	138.5(1)	
					N_{eq}	2.145(5)	Cl_{eq},N_{eq}	110.8(3,6.5)	
					N_{ap}	2.009(5,5)	Cl_{eq},N_{ap}	89.3(2,2.3)	
							N_{eq},N_{ap}	92.2(2,5)	
							N_{ap},N_{ap}	175.6(2)	
$[Cu(pium)Cl_2]ClO_4$	or	15.220(2)		CuN_3Cl_2	Cl_{eq}	2.402(2,32)	Cl_{eq},Cl_{eq}	103.3(1)	916
(not given)	Pcam	7.946(4)			N_{eq}	2.094(5)	Cl_{eq},N_{eq}	128.4(1,3.3)	
	4	14.953(5)			N_{ap}	1.968(4,0)	N_{eq},N_{ap}	81.3(1,0)[d]	
							Cl_{eq},N_{ap}	95.5(1,1.5)	
							N_{ap},N_{ap}	161.9(2)	
β-$[Cu(tioim)_3](BF_4)_2$	or	14.424(3)		CuN_3S_2	N_{eq}	2.119(7)	N_{ap},N_{ap}	178.9(3)	776
(green)	$Pna2_1$	10.790(2)			S_{eq}	2.436(3,42)	N_{eq},S_{eq}	101.6(2)	
	4	20.127(3)			N_{ap}	1.991(7,6)		127.1(2)	
							N_{ap},N_{eq}	90.0(3,2)	
							N_{ap},S_{eq}	92.0(2,1.0)[e]	
								90.1(2,3.4)	
							S_{eq},S_{eq}	131.2(1)	
$[Cu(bddh)(3,5\text{-}Me_2pz)](BF_4)_2$	m	18.360(3)		CuN_3S_2	S_{eq}	2.441(3,37)	S_{eq},S_{eq}	91.67(9)	917
	$P2_1/c$	9.419(3)	100.29(1)		pzN_{eq}	1.977(6)	S_{eq},N_{eq}	134.1(2,6.2)	
(blue)	4	16.068(2)			N_{ap}	1.970(6.8)	S_{eq},N_{ap}	86.6(2,6.0)[d]	
							N_{eq},N_{ap}	95.6(2)	
							N_{ap},N_{ap}	171.7(3)	
$[Cu(ppm)Br_2]\cdot H_2O$	m	8.38(1)		CuN_3Br_2	Br_{eq}	2.517(3,81)	Br_{eq},Br_{eq}	111.9(1)	918
(green)	$P2_1/c$	27.60(3)	114.6(1)		N_{eq}	2.067(13)	Br_{eq},N_{eq}	124.1(4,8.2)	
	4	7.69(1)			N_{ap}	1.986(14,3)	Br_{eq},N_{ap}	94.7(4,2.5)	
							N_{eq},N_{ap}	81.3(5,1.7)[d]	
							N_{ap},N_{ap}	162.2(5)	
$Cu(mpab)Br_2$	m	8.742(3)		CuN_3Br_2	Br_{eq}	2.434(1,20)	Br_{eq},Br_{eq}	131.32(4)	919
(not given)	$P2_1/n$	29.408(5)	107.77(2)		N_{eq}	2.423(1)	Br_{eq},N_{eq}	114.4(1,5.2)	
	4	8.522(1)			N_{ap}	1.985(5,4)	$Br_{eq}N_{ap}$	95.03(10,1.43)	
							N_{eq},N_{ap}	77.4(2,2)[d]	
							N_{ap},N_{ap}	155.3(2)	
$Cu(terpy)I_2$	m	13.689(3)		CuN_3I_2	I_{eq}	2.647(1,0)	I_{eq},I_{eq}	108.41(3)	920
(not given)	I2/c	9.510(2)	97.59(4)		N_{eq}	1.942(8)	I_{eq},N_{eq}	125.8(2,0)	
	4	11.605(3)			N_{ap}	2.014(8,0)	I_{eq},N_{ap}	96.3(2,1.2)	
							N_{eq},N_{ap}	79.2(2,0)[d]	
							N_{ap},N_{ap}	158.3(4)	
$Cu(dien)I_2$	m	15.140(4)		CuN_3I_2	I_{eq}	2.834(2,215)	I_{eq},I_{eq}	109.2(1)	921
(green)	$P2_1/a$	9.960(4)	105.95(1)		N_{eq}	2.034(9)	I_{eq},N_{eq}	125.5(2,23.2)	
	4	7.526(2)			N_{ap}	1.993(7,7)	I_{eq},N_{ap}	92.0(3,5.6)	
							N_{eq},N_{ap}	84.5(3,3)[d]	
							N_{ap},N_{ap}	166.0(4)	
$H[Cu(dibyo)_2Cl_3]$	or	10.674(1)		$CuCl_3N_2$	Cl_{eq}	2.375(2,0)	not given		922
(not given)	R32				N_{ap}	2.118(6,0)			
	3	12.042(2)							

TABLE II *(Continued)*

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(zoct)_2Cl_3]ClO_4$	or	13.157(8)		$CuCl_3N_2$	Cl_{eq}	2.349(6,5)	Cl_{eq},Cl_{eq}	120(1,2.3)	923
(not given)	$Pbc2_1$	12.379(8)			N_{ap}	2.141(14,14)	Cl_{eq},N_{ap}	90.0(2,2.5)	
	4	13.114(8)					N_{ap},N_{ap}	176.4(5)	
$[Cu(bapur)Cl_3]Cl{\cdot}H_2O$	m	13.508(3)		$CuCl_3N_2$	Cl_{eq}	2.364(4,156)	Cl_{eq},Cl_{eq}	120.0(1,29.4)	924
(blue)	$P2_1/a$	21.181(4)	110.644(2)		N_{ap}	2.013(7,18)	Cl_{eq},N_{ap}	90.5(3,4.5)	
	4	10.661(2)					N_{ap},N_{ap}	173.4(3,4)	
$Cu(dmsO)_2Br_2$	or	8.257(2)		$CuBr_3O_2$	Br_{eq}	2.552(4,225)	Br_{eq},Br_{eq}	120.0(2,26.1)	925
(dark brown)	Pnma	11.772(2)			O_{ap}	1.962(9,0)	Br_{eq},O_{ap}	89.8(3,3.1)	
	4	11.749(2)					O_{ap},O_{ap}	173.9(6)	
Cu(bheg)Cl	or	14.18(1)		CuO_3NCl	O_{eq}	2.060(4,97)	O_{eq},O_{eq}	118.6(1,14.8)	926
(green)	Pbca	15.835(7)			N_{ap}	2.007(3)	O_{eq},N_{ap}	83.1(1,1.4)[d]	
	8	8.188(3)			Cl_{ap}	2.203(1)	O_{eq},Cl_{ap}	96.83(9,6.8)	
							Cl_{ap},N_{ap}	179.29(9)	
Cu(bheg)Br	m	12.910(2)		CuO_3NBr	O_{eq}	2.067(7,107)	O_{eq},O_{eq}	120.0(3,19.3)	927
(green)	$P2_1/n$	8.748(1)	105.11(1)		N_{ap}	2.024(6)	O_{eq},Br_{ap}	96.7(2,3.5)	
	4	8.894(2)			Br_{ap}	2.359(1)	O_{eq},N_{ap}	83.4(2,2.6)[d]	
							Br_{ap},N_{ap}	178.8(2)	
[Cu(acaz)Cl]Cl	m	14.695(9)		CuN_3OCl	N_{eq}	2.125(20,5)	O_{eq},N_{eq}	69.2(7)[d]	928
(green)	$P2_1/n$	12.955(6)	91.84(4)		O_{eq}	2.59(2)		102.7(7,33.5)	
	4	13.831(6)			N_{ap}	1.95(2)	N_{eq},N_{eq}	146.6(8)	
					Cl_{ap}	2.20(1)	O_{eq},Cl_{ap}	90.5(5)	
							N_{eq},Cl_{ap}	98.6(6,1.6)	
							O_{eq},N_{ap}	90.0(7)	
							N_{eq},N_{ap}	81.1(8,2.2)[d]	
							Cl_{ap},N_{ap}	178.6(6)	
$Cu(dthp)(NO_3)_2$	m	18.492(5)		CuO_2S_2N	S_{eq}	2.373(2,29)	S_{eq},S_{eq}	144.8(1)	635b
(green)	$P2_1/c$	14.375(3)	101.19(2)		O_2NO_{eq}	2.244(6)	S_{eq},O_{eq}	107.2(2,20.1)	
	4	8.554(2)			N_{ap}	1.982(6)	S_{eq},O_{ap}	95.7(2,7)	
					O_2NO_{ap}	1.927(5)	S_{eq},N_{ap}	85.0(2,4)[d]	
							O_{eq},N_{ap}	93.9(2)	
							O_{eq},O_{ap}	84.3(2)	
							N_{ap},O_{ap}	177.9(2)	
$[Cu(2,9\text{-}Me_2phen)Cl_2{\cdot}$	m	9.886(6)		CuN_2Cl_2O	Cl_{eq}	2.304(4,10)	Cl_{eq},Cl_{eq}	155.6(2)	929
$(H_2O)]$	$P2_1$	8.159(8)	105.55(10)		N_{eq}	2.236(11)	Cl_{eq},N_{eq}	102.1(3,1.6)	
(green)	2	9.517(6)			N_{ap}	1.982(9)	Cl_{eq},N_{ap}	90.8(4,4.2)	
					H_2O_{ap}	1.975(9)	Cl_{eq},O_{ap}	87.7(4,7)	
							N_{eq},N_{ap}	79.7(4)δ	
							N_{eq},O_{ap}	107.6(4)	
							N_{ap},O_{ap}	171.1(5)	
$Cu(nphyr)Cl_2(H_2O)$	m	8.934(3)		CuN_2Cl_2O	Cl_{eq}	2.289(2,2)	Cl_{eq},Cl_{eq}	151.9(1)	930
(black)	$P2_1/n$	11.427(4)	103.65(3)		N_{eq}	2.243(7)	Cl_{eq},N_{eq}	104.0(2,5)	
	4	17.382(5)			N_{ap}	2.005(7)	Cl_{eq},O_{ap}	88.3(2,7)	
					H_2O_{ap}	2.019(6)	Cl_{eq},N_{ap}	93.8(2,1.4)	
							N_{eq},O_{ap}	94.3(2)	
							N_{eq},N_{ap}	77.1(3)[d]	
							N_{eq},O_{ap}	171.2(2)	
$Cu(bzph)_2Cl_2$	tr	13.397(3)	72.26(1)	CuN_2Cl_2O	Cl_{eq}	2.288(1,10)	Cl_{eq},Cl_{eq}	141.7(1)	931
(brown)	P-1	10.752( )	91.58(1)		O_{eq}	2.256(3)	Cl_{eq},O_{eq}	109.0(1,1.3)	
	2	9.205(2)	106.86(1)		N_{ap}	2.024(4,4)	Cl_{eq},N_{ap}	91.8(1,6.0)	
							O_{eq},N_{ap}	79.3(1)[e]	
								84.6(1,5.1)	
							N_{eq},N_{ap}	168.2(1)	

TABLE II *(Continued)*

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$Cu(thdec)Cl_2$ (green)	or Pbca 8	17.960(4) 14.104(9) 10.400(12)		CuN_2Cl_2S	Cl_{eq} S_{eq} N_{ap}	2.343(3,31) 2.493(3) 1.998(8,13)	Cl_{eq},Cl_{eq} Cl_{eq},S_{eq} Cl_{eq},N_{ap} S_{eq},N_{ap} N_{ap},N_{ap}	132.19(12) 113.9(1,10.3) 90.3(3,2.0) 88.9(2,1.2)[e] 176.31(32)	932
$Cu(memia)Cl_2$ (green)	m $P2_1/n$ 4	7.025(2) 8.486(2) 19.484(6)	98.07(3)	CuN_2Cl_2S	Cl_{eq} S_{eq} N_{ap}	2.414(2,139) 2.428(2) 1.973(4,15)	Cl_{eq},Cl_{eq} S_{eq},Cl_{eq} Cl_{eq},N_{ap} S_{eq},N_{ap} N_{ap},N_{ap}	118.1(2) 121.0(2,17.8) 92.8(2,5.3) 83.7(2,2.1)[d] 166.4(3)	933
$[Cu((bmdhp)(H_2O)]\cdot(ClO_4)_2$ (deep green)	m $P2_1/n$ 4	18.459(3) 10.362(2) 16.365(3)	117.14(1)	CuN_2S_2O	H_2O_{eq} S_{eq} N_{eq} S_{ap} N_{ap}	2.225(4) 2.337(1) 1.997(4) 2.328(1) 1.950(4)	S_{eq},N_{eq} O_{eq},S_{eq} S_{eq},O_{eq} S_{ap},S_{eq} S_{ap},O_{eq} S_{ap},N_{eq} N_{ap},S_{eq} N_{ap},O_{eq} N_{ap},N_{eq} S_{ap},N_{ap}	143.9(1) 106.3(1) 108.2(1) 88.69(5)[e] 84.2(1) 84.5(1)[d] 85.0(1)[d] 94.4(1) 102.7(2) 172.7(1)	934
$[Cu(bbtt)(H_2O)]\cdot(ClO_4)_2\cdot 5EtOH$ (at 221K) (not given)	m $P2_1/n$ 4	18.865(3) 12.652(2) 17.902(7)	101.99(2)	CuN_2S_2O	H_2O_{eq} S_{eq} N_{ap}	1.968(8) 2.464(4,14) 1.948(9,3)	S_{eq},S_{eq} O_{eq},S_{eq} S_{eq},N_{ap} O_{eq},N_{ap} N_{ap},N_{ap}	88.18(9)[d] 135.9(4,9) 83.1(3,5)[d] 88.3(3,5.9) 92.7(5,3) 175.2(3)	935
$Cu(bddn)(H_2O)](BF_4)_2$ (green)	m $P2_1/c$ 4	18.508(5) 9.253(3) 15.743(5)	107.9(3)	CuN_2S_2O	H_2O_{eq} N_{eq} S_{eq} N_{ap} S_{ap}	2.17(1) 2.00(1) 2.363(5) 1.99(1) 2.366(6)	N_{eq},O_{eq} S_{eq},N_{eq} S_{eq},O_{eq} N_{ap},N_{eq} N_{ap},O_{eq} N_{ap},S_{eq} S_{ap},S_{eq} S_{ap},N_{eq} S_{ap},O_{eq}	120.3(5) 135.8(5) 102.0(3) 95.5(5) 90.4(5) 96.4(4)[e] 79.9(2)[d] 89.7(4)[e] 87.0(4)	936
$Cu(pma)(SO_4)$ (blue)	tr P–1 2	11.415(1) 12.673(1) 9.806(1)	101.18(1) 94.28(1) 71.00(1)	CuN_2S_2O	Seq Neq Nap O_3SO_{ap}	2.423(2,38) 2.021(5) 2.033(4) 1.909(4)	S_{eq},S_{eq} S_{eq},N_{eq} S_{eq},N_{ap} N_{eq},N_{ap} N_{eq},O_{ap} S_{eq},O_{ap}	108.2(7) 124.8(1,4.6) 87.6(1,0)[d] 82.3(2)[d] 88.9(2) 98.2(2,2.2)	937
$[Cu(bhdhx)Cl]BF_4$ (not given)	tr P–1 2	10.066(3) 8.253(2) 11.864(3)	104.85(2) 100.46(3) 114.72(2)	CuN_2S_2Cl	Cl_{eq} S_{eq} N_{ap}	2.266(1) 2.511(1,23) 1.950(3,6)	Cl_{eq},S_{eq} S_{eq},S_{eq} Cl_{eq},N_{ap} S_{eq},N_{ap} N_{ap},N_{ap}	135.7(5,10.3) 88.55(4)[d] 94.1(1,1.2) 82.2(1,2)[d] 87.0(1,1.5) 171.7(1)	938
$(Cu(Mebhdhx)Cl]Cl\cdot 2H_2O$ (dark green)	tr P–1 2	8.270(5) 10.890(5) 11.478(5)	87.52(4) 76.93(5) 71.52(4)	CuN_2S_2Cl	Cl_{eq} S_{eq} N_{ap}	2.2864(7) 2.495(1,33) 1.942(2,3)	S_{eq},S_{eq} Cl_{eq},S_{eq} S_{eq},N_{ap} Cl_{eq},N_{ap} N_{ap},N_{ap}	89.35(2)[d] 148.07(3) 87.97(6,4.62)[d] 89.73(6,6.38) 93.93(6,13) 172.13(8)	939
$[Cu(bbdh)Cl]Cl\cdot 2EtOH$ (green)	m $P2_1/c$ 4	14.930(2) 17.109(4) 10.774(2)	97.23(2)	CuN_2S_2Cl	Cl_{eq} S_{eq} N_{ap}	2.241(2) 2.498(2,64) 1.965(6,4)	S_{eq},S_{eq} S_{eq},Cl_{eq} S_{eq},N_{ap} Cl_{eq},N_{ap} N_{ap},N_{ap}	90.39(6)[d] 134.74(8,7.45) 82.8(2,8)[d] 85.05(20,3.15) 97.0(2,2) 165.9(2)	940

TABLE II *(Continued)*

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromophore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
$[Cu(bddh)Cl]_2[CuCl_4]$	m	19.018(4)		CuN_2S_2Cl	Cl_{eq}	2.249(4)	S_{eq},S_{eq}	91.1(1)[d]	917
(blue)	Cc	14.840(3)	100.24(3)		S_{eq}	2.451(3,29)	Cl_{eq},S_{eq}	136.0(1,14.0)	
	4	14.963(3)			N_{ap}	1.986(10,6)	S_{eq},N_{ap}	86.3(3,6.9)[d]	
							Cl_{eq},N_{ap}	95.5(3,3)	
							N_{ap},N_{ap}	168.8(4)	
				$CuCl_4$	Cl	2.17(2,5)	Cl,Cl	109.5(7,19.0)	
						2.53(2)			
$[Cu(bbidh)Br]Br{\cdot}H_2O$	tr	8.397(2)	103.74(1)	CuN_2S_2Br	Br_{eq}	2.417(3)	S_{eq},S_{eq}	87.9(2)[d]	941
(green)	P–1	11.415(2)	94.49(2)		S_{eq}	2.518(6,48)	S_{eq},Br_{eq}	136.1(2,13.6)	
	2	18.016(2)	100.48(2)		N_{ap}	1.935(20,5)	S_{eq},N_{ap}	82.5(6,6)[d]	
								87.3(6,6.7)	
							Br_{eq},N_{ap}	94.2(5,6)	
							N_{ap},N_{ap}	171.8(8,6)	
$Cu(thdec)Br_2$	or	18.440(15)		CuN_2Br_2S	Br_{eq}	2.501(4,40)	Br_{eq},Br_{eq}	130.5(2)	932
(green)	Pbca	14.214(9)			S_{eq}	2.478(10)	Br_{eq},S_{eq}	114.7(3,11.2)	
	8	10.587(12)			N_{ap}	2.035(23,4)	Br_{eq},N_{ap}	90.2(7,3.2)	
							S_{eq},N_{ap}	89.0(7,1.7)[e]	
							N_{ap},N_{ap}	174.2(8)	
$[Cu(bbes)Br_2]CHCl_3$	or	11.554(5)		CuN_2Br_2S	Br_{eq}	2.573(2,103)	Br_{eq},Br_{eq}	149.2(1)	799
(not given)	Pnma	14.397(7)			S_{eq}	2.458(3)	Br_{eq},S_{eq}	105.4(1,3.7)	
	4	14.861(7)			N_{ap}	1.965(6,0)	Br_{eq},N_{ap}	89.2(2,1)	
							S_{eq},N_{ap}	93.1(2)	
$[Cu(nsp)I]ClO_4$	m	17.292(3)		CuN_2S_2I	N_{eq}	2.052(9)	N_{ap},N_{eq}	87.1(3,1.2)[d]	634
(not given)	$P2_1/n$	14.441(2)	100.29(1)		S_{eq}	2.396(4,56)	N_{ap},S_{eq}	88.2(3)[d]	
	4	7.820(7)			N_{ap}	2.053(8)	I_{ap},N_{eq}	99.9(2)	
					I_{ap}	2.604(1)	I_{ap},S_{eq}	91.95(90,75)	
							S_{eq},S_{eq}	110.4(1)	
							S_{eq},N_{eq}	115.1(3)	
								132.2(3)	
							I_{ap},N_{ap}	177.1(3)	
$Cu(methio)Cl_2$	m	20.138(1)		$CuCl_2S_2N$	Cl_{eq}	2.242(1,4)	Cl_{eq},Cl_{eq}	146.09(6)	942
(red)	$P2_1/c$	8.173(1)	111.20(2)		N_{eq}	2.164(4)	Cl_{eq},N_{eq}	106.95(10,95)	
	4	15.533(3)			S_{ap}	2.420(1,11)	S_{ap},N_{eq}	81.79(9,1)[d]	
							S_{ap},Cl_{eq}	92.41(5,78)	
							S_{ap},S_{ap}	163.57(5)	
C: SQUARE-PYRAMIDAL—TRIGONAL-BIPYRAMIDAL									
$Cu(terpy)(NCS)_2$	m	13.724(3)		CuN_5	SCN	2.020(7,0)	N,N	79.5(1)[d]	943
(green)	C2/c	9.501(1)	110.54(2)		N	2.021(5,0)		98.5(3,4)	
	4	14.187(3)			N	1.937(7)		158.9(2)	
								130.9(2)	
Cu(imiso)(dbm)	m	20.520(4)		CuN_3O_2	O	2.178(5)	O,N	98.4(2,11.7)	944
(not given)	$P2_1/n$	11.187(2)	96.83(5)		N	1.904(5)		178.3(2)	
	4	12.658(3)				2.053(5,2)	N,N	89.4(2,4)[e]	
								155.6(2)	
							O,O	88.1(2)[e]	
Cu(mazoc)	or	9.758(1)		CuN_3O_2	N	1.958(2,4)	O,N	90.3(2,1.8)	945
(green)	Pbca	35.922(2)			O	1.965(4,12)		102.6(2,1.8)	
	8	17.899(2)			N	2.326(5)	O,O	154.9(2)	
							N,N	177.8(2)	
								89.0(2,1)[e]	
Cu(azoc)	m	17.746(3)		CuN_3O_2	O	1.963(2,0)	O,O	146.3(1)	945
(green)	C2/c	7.108(1)	121.68(1)		N	2.389(3)	O,N	106.9(1,0)	
	4	17.278(2)			N	1.962(2,0)		92.1(1,8)[e]	
							N,N	86.0(1,0)[e]	
								171.9(1)	

TABLE II *(Continued)*

Compound (colour)	*Cr.cl. Sp.gr. Z*	*a[Å] b[Å] c[Å]*	*α[°] β[°] γ[°]*	*Chromo-phore Cu-out of plane [Å]*	*Cu-L [Å]*		*L-Cu-L [°]*		*Ref.*
Cu(pcnoc)	tr	11.437(1)	101.02(1)	CuN_3O_2	N	1.961(3,1)	O,N	90.5(1,3.8)	945
(green)	P-1	13.374(1)	116.73(1)		O	1.950(3,20)		102.01(1,5.5)	
	2	13.611(1)	101.14(1)		N	2.415(3)	O,O	155.7(1)	
						N,N		87.8(1,1)[e]	
								175.3(1)	
Cu(terpy(Br_2)	m	16.618(3)		CuN_3Br_2	Br	2.493(1,0)	N,N	79.1[d]	943
(green)	C2/c	9.280(10)	125.61(4)		N	2.037(7,0)		158.2(2,–)	
	4	11.396(7)			N	2.493(1,0)	N,Br	96.5(1,–)	
								125.5	
							Br,Br	96.5(1,–)	

a Where more than one chemically equivalent distance or angle are present the mean values are tabulated. The first number in paranthesis is e.s.d. and the second is a maximum deviation from the mean.
b The chemical identity of coordinated atom/ligand is specified in these columns.
c There are two crystallografically independent molecules are present.
d Five - membered metallocyclic ring.
e Six - membered metallocyclic ring.
f There are square - pyramidal and trigonal - bipyramidal units.
g Four - membered metallocyclic ring.
i Eight - membered metallocyclic ring.
j Another neutral molecule contain CuO_3N_2 chromophore.

Both electronic and steric effects of the ligands can be seen in the opening of the L-Cu-L bond angles of the respective metallocyclic rings. For the four-membered rings the mean L-Cu-L angles are 57° (O donor) and 62° (N donor). For the five-membered rings the mean angles are: 84.5° (O donor), 80° (unsaturated N donor), 85° (saturated N donor) and 88° (S donor). The metallocyclic intraligand L-Cu-L ring angle opens with increasing size of the ring, for example: 57° (four-membered) < 84.5° (five-membered) < 93° (six-membered) when L is an oxygen donor; 62° (four-membered) < 84° (five-membered) < 97° (six-membered) < 104° (seven-membered) when L is a nitrogen donor ligand.

There are examples $[Cu(17\text{-}aneN_5)][CuBr_4]$[232] $[Cu(acac)Cl]_2 \cdot [Cu(bgH)_2]$,[363] $[Cu(Me_2tu)_2(H_2O)][Cu(pba)] \cdot 3H_2O$[385] and $[Cu(dmpo)_2Cl]_2 \cdot [CuCl_4]$[796] which contain two inequivalent monomeric species. In $[Cu(17\text{-}aneN_5)][CuBr_4]$[232] and $[Cu(dmpo)_2Cl]_2[CuCl_4]$,[796] the complex cations are square-pyramidal and the complex anions are tetrahedral. In the remaining two species[363, 385] square-pyramidal and square-planar configurations about the copper(II) atoms take place.

Crystallographic and structural data for almost one hundred and fifty trigonal-bipyramidal copper(II) compounds are summarized in Table IIB. From Table IIB one can see examples of uni-, bi-, tri-, tetra- and even pentadentate ligands, creating varying amounts of distortion about the Cu(II) center.

In general, the mean Cu-L equatorial bond distances are somewhat longer than the apical Cu-L bond distances. The Cu-L bond distances found for penta-coordinate copper(II) derivatives in Table III are summarized. The mean Cu-L(equatorial) bond

distances in the series of square-pyramidal derivatives are somewhat shorter than those of trigonal-bipyramidal complexes, while for the mean Cu-L(apical) bond distaces are longer.

The metallocyclic intra-ligand O-Cu-O ring angle opens with increasing size of the ring, for example: 58.4(4.0,3.5)° (four-membered) < 83.5(1.6,1.0)° (five-membered) < 91.0(1.5,1.5)° (six-membered).

TABLE III Summary of the mean Cu-L bond distances [Å] in penta - coordinate derivatives[a]

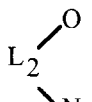
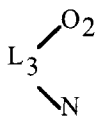
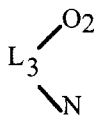
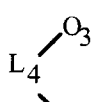
Donor atom	*Coval. radius [Å]*	*SQUARE – PYRAMIDAL*		*TRIGONAL – BIPYRAMIDAL*	
		L(eguatorial)	*L(apical)*	*L(equatorial)*	*L(apical)*
F	0.72	1.90(2,3)	2.52	1.85	
L – O	0.73	1.98(7,9)	2.33(31.65)	2.13(8,13)	1.96(5,6)
$L-O_2$		2.01(12,12)	2.32(28,5)	2.23(23,9)	2.01(12,13)
L – N	0.75	1.97(7,29)	2.26(22,41)	2.04(19,14)	2.00(13,14)
$L-N_1$		2.01(6,7)	2.22(10,25)	2.12(13,12)	1.99(3,14)
$L-N_3^2$		2.00(9,19)	2.25(8,14)	2.06(7,13)	2.01(7,4)
$L-N_4$		2.00(18,11)	2.20(7,5)	2.10(12,13)	2.02(2,6)
$L-N^5$		2.02(6,10)	2.18(10,13)	2.08(14,16)	2.02(4,4)
Cl	0.99	2.28(7,9)	2.51(14,26)	2.32(21,25)	2.25(5,5)
L – S	1.02	2.27	2.65(23,23)	2.35(4,5)	
Br	1.14	2.41(2,32)	2.63(18,23)	2.50	2.43(7,11)
I	1.33	2.56(2, 3)	2.88(14,15)	2.71	2.60
		1.95(6,11)		2.04	1.98
		2.00(4,8)		2.03	2.00
		1.99(7,5)	2.34(16,14)		
		1.96(6,10)			
		1.95(8,8)	2.36(5,4)	2.25	
			1.99(9,18)		2.02
		1.93(2,2)	2.49(19,28)	2.06	
		1.95(2,2)			2.01

TABLE III *(Continued)*

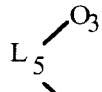
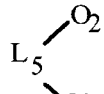
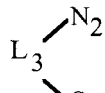
Donor atom	*Coval. radius [Å]*	*SQUARE – PYRAMIDAL*		*TRIGONAL – BIPYRAMIDAL*	
		L(eguatorial)	*L(apical)*	*L(equatorial)*	*L(apical)*
		1.94(5,12)	2.27	2.59	
		2.01(10,12)	2.16	2.12	1.95
		1.96(4,14)	2.53(19,29)		
		1.96(6,10)			
				2.09	1.92
					2.00
		1.95(4, 6)	2.37(15,20)		
		1.97(3, 6)			
		1.96(5, 3)	2.49	2.04	
		2.01(6, 8)	2.30(10, 8)	2.13	1.97
			2.29(14,19)		
		2.03(15, 6)			
		2.02(4, 3)		2.12	1.99
		2.31(5, 9)	2.62	2.24	
		1.99(5, 6)			1.99
		2.34(4, 3)	2.74(17,21)	2.43	
		2.01(1, 3)		2.16	1.98
		2.33(5, 4)		2.37	2.42

TABLE III *(Continued)*

Donor atom	*Coval. radius [Å]*	*SQUARE – PYRAMIDAL* *L(eguatorial)*	*L(apical)*	*TRIGONAL – BIPYRAMIDAL* *L(equatorial)*	*L(apical)*
$L_4(N_3)S$		2.03(8,11)	2.15		
		2.30(6,4)	2.66		
$L_4(N_2)S_2$		2.01(11,7)	1.98	1.97	
		2.32(2,3)	2.56	2.43	2.35
$L_2(S)Se$		2.35			
		2.50	2.88		
$L_3(O_2)S$		1.98(3,4)			
			2.35(3,3)		
$L_4(O)N_2S$		2.00			
		2.01			
		2.23			
$L_5(O_4)N$				2.09	1.92
					2.00
$L_5(O_2)N_3$				2.04	
				2.13	1.97
$L_5(N_4)S$		2.02(3,4)	2.28		
		2.38	2.55		
$L_5(O_2)N_2S$		1.99			
		2.00			
			2.69		

[a] The first number in parenthesis is the mean minus the smallest value and the second is the largest value minus the mean.

Two crystallographically independent molecules differing by degree of distortion and coexisting in the same crystal have been found in several species.[510, 536, 544, 557, 559, 569, 571, 586, 588, 591, 624, 642, 647, 659, 665, 670, 721, 723, 734, 735, 743, 756, 823, 841, 855, 867, 869, 895, 915]

Two isomeric forms differing by degree of distortion are observed for [Cu(bpdz)(NCS)]NCS.[840]

In Table IIC are given six examples[943–945] where the stereochemistry about copper(II) is intermediate between square-pyramidal and trigonal bipyramidal. The donor ligands are nitrogen and oxygen and in one example also a bromide.

4 CONCLUSIONS

This review has classified over one thousand and two hundred four-and five-coordinate structures of copper(II) complexes. From two limiting configurations for each, four-coordinate species are dominated by square-planar and five-coordinate species, are dominated by square-pyramidal with various degrees of distortion. Relationship between the various structural parameters have been discussed within each section.

Three types of isomerism exist: distortion, *cis-*, *trans*-somerization and configuration isomerism, from which the distortion isomerism is most prevolent.

This review presents the first overview of structural data for four- and five-coordinate copper(II) compounds; a related review on the six- and higher coordinate, as well as oligonuclear derivatives is currently in progress. Despite the increasing avaibility of data retrieval systems, the tracing of relevant material is not always a straight forward task. Much data are only available as supplementary material and some are obscure. The systematic analysis and correlation of structural data should serve to highlight both areas of interest and those requiring more investigation.

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