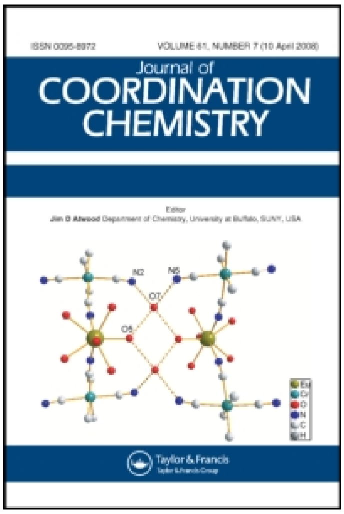

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COPPER(II) COORDINATION COMPOUNDS: CLASSIFICATION AND ANALYSIS OF CRYSTALLOGRAPHIC AND STRUCTURAL DATA II. MONONUCLEAR-, HEXA-, HEPTA-AND OCTACOORDINATE COMPOUNDS

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Review

COPPER(II) COORDINATION COMPOUNDS: CLASSIFICATION AND ANALYSIS OF CRYSTALLOGRAPHIC AND STRUCTURAL DATA II. MONONUCLEAR-, HEXA-, HEPTA- AND OCTACOORDINATE COMPOUNDS

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This review summarizes the data for over five hundred and fifty six-, seven- and eight-coordinate Cu(II) coordination compounds. The six-coordinate derivatives are mostly distorted tetragonal (elongation along a single C_4 axis). The seven-coordinate derivatives are only pentagonal-bipyramidal with different degrees of distortion and the eight-coordinate complexes are dodecahedral. The most common ligands are O- and N-donors. There is a trend for the Cu–L distance to increase with covalent radius of the coordinated atom and also increasing coordination number. In general, Cu(II) compounds "prefer" a monoclinic class and are blue or green. Several relationships were found and discussed. The data are compared and discussed with those of four- and five-coordinate Cu(II) compounds.

Keywords: Review; Cu(II); crystallography; structures

CONTENTS

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ABBREVIATIONS

aad	8-azaadenine
abpt	3,5-bis(pyridin-2-yl)-4-amino-1,2,4-triazole
abst	2-(aminobenzensulfonamide)-5-ethyl-1,3,4-tiadiazole
ac	acetate
ac-α-ala	N-acetyl-α-alaninate
acatr	3-acetylamino-1,2,4-triazole
acgl	N-acetylglycine
ac-DL-pgly	N-acetyl-DL-phenylglycinate
acsal	acetylsalicylate
act-DL	N-acetyl-DL-tryptophanate
acth	2-[(5amino4carboxamidinium)[1,2,3]triazole]
actr	5-amino-4-carboxamide[1–3]triazole
acts	5-acetamido-1,3,4-thiadiazole-2-sulfonamide
adip	adipate
aenol	2[(3-aminopropyl)amino]ethanolate
aepy	2-(2-aminoethyl)pyridine
ahb	2-amino-1-heptybenzimidazole
ahmi	2-azohexamethyleneimine
ainc	amidoisonicotinate
6-am	6-aminohexanoic acid
amb	2-amino-1-methylbenzimidazole
amcyclam	3,10-diammonio-3,10-dimethyl-1,4,8,11-tetra-azacyclotetradecane
amdza	1,3bis(2aminoethyl)5-ammonio 5-methyl 1,3-diazacyclo-hexane
ami	11-aminoundecane
amnur	6-amino-1,3-dimethyl-5-nitrosouracil
amOac	aminooxyacetate

amp	DL-α-amino-β-methylaminopropionic acid
ampr	2-amino-2-methyl-1-propanole
ampy	2-aminoethylpyridine
4-amsal	4-aminosalicylate
9-aneN_2S	1-thia-4,7-diazacyclononane
9-aneN_2Sac	dimethyl 1-thia-4,7diaza-4,7-cyclononanediacetate
10-aneN_2S_2	1,7-bis(5-methylimidazol-4-yl)-2,6-dithiaheptane
9-aneN_3	1,4,7-triazacyclononane
12-aneN_4	N,N′-dimethyl-2,11-diaza[3.3](2,6)pyridinophane
12-aneN_4ac	12-membered tetraazamacrocycle-N,N′,N″,N‴-tetra-acetic acid
12-aneO_4	1,4,7,10-tetraoxacyclododecane
14-aneS_4	1,4,8,11-tetrathiacyclotetradecane
14-aneS_2N_2	6-methyl-6-nitro-1,11-dithia-4,8-diazacyclotetradecane
15-aneN_4	1,4,8,12-tetraazacyclopentadecane
15-aneS_4	1,4,8,12-tetrathiacyclopentadecane
16-aneS_4	1,5,9,13-tetrathiacyclohexadecane
17-aneO_3N_2	pyridynyl-derivat macrocycle
17-aneO_3N_2	3,22-dioxa-11,14,28-triazatetra-cyclo[22.3.1.$0^{4,9}0^{16,21}$]octacosa-1(28),4,6,8,16,18,20,24,26 nonaene
18-aneO_4N_2	1.7.10.16 tetraoxa-4.13-diaza-cyclotetradecane
18-aneN_2S_2	3,3,7,7,11,11,15,15-octamethyl-1,9-dithia-5,13-diazacyclo-hexadecane
18-aneS_4N_2	1,4,10,13-tetrathia-7,16-diazacyclooctadecane
apy	antipyrine
asp	L-asparaginate
athal	N-(2-aminoethyl)thiophen-2-aldimine
atr	atratone
azcm	catena-μ-(4-aminoimidazole-5-carboxamidoxime)
bcmgly	N,N-bis(carboxymethyl)glycinate
bet	betaine
bheg	N,N-bis(2-hydroxyethyl)glycinate
bhdhx	1,6-bis(4(5)-imidazolyl)-2,5-dithiahexane
bim	benzimidazole
bimm	benzimidazol-2-yl-methanol
bimpa	N,N-bis(benzimidazol-2-yl-methyl)isopropylamine
bip	2,2′-bipiperidine
bipyam	2,2′-N,N′-bispyridylamine

biu	biuret
1,3-bn	1,3-diaminobutane
bpca	N-2-pyridinylcarbonyl-2-pyridinecarboximidate
bpdz	1,7-bis(2-pyridyl)-2,6-diazaheptane
bpm	2,2′-bipyrimidine
bpy	2,2′-bipyridine
bpykh	2,2′-N,N′-bipyridyl ketone hydrate
bpyO,O	2,2′-bipyridine-N,N′-dioxide
btac	(benzylthio)acetate
bz	benzoate
bzibza	N,N-bis(2-benzimidazolylmethyl)benzylamine
bzimox	1,6-bis(benzimidazol-2-yl)-2,5-dioxahexane
bzph	2-aminobenzophenone
bzpy	2-benzoylpyridine
bz-pyrpy	2,6-bis{{(2S)-2-[(benzyloxy)methyl]pyrrolidin-yl}methyl}pyridine
bzs	benzenesulphonate
c	cubic
camphs	D-camphor-10-sulphonate
cas	calix[4]arene sulphonate
cbq	1-carbamoylquanidinate
$C_5(CO_2Me)_5$	pentakis(methoxycarbonyl)cyclopentadiene
ceten	N,N′-bis(β-carbamoylethyl)trimethylenediamine
$C_2H_6O_2$	1,2-ethanediol
$C_2H_{10}N_2$	ethylenediamonium
$C_6H_5O_7$	citrate
$C_7H_{18}N_2$	N^1-isopropyl-2-methyl-1,2-propanediamine
$C_8H_8O_5$	7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylate
$C_8H_{11}NO_3$	2-methyl-oxy-4,5-di(oxymethyl)pyrioline
$C_8H_{16}N_4O_2$	N,N′-bis(β-carbamoylethyl)ethylenediamine
$C_{20}H_{28}N_4S$	quinquedentate macrocyclic ligand
$C_{22}H_{34}N_6$	3,6,12,15-tetramethyl-18{[N(2,6)-pyridino,N-1.2.1] 2-coronand-6}
Cl_2aqu	8-amino-5,7-dichloroquinoline
2-Clbquam	2-chlorobiquanide
4-Clbzs	4-chlorobenzensulphonate
2,4,6-Cl_3ph	2,4,6-trichlorophenolate
4-ClphOac	4-chlorophenoxyacetate
Clqo	4-chloro-1-benzoquinone 2-oximate
cnact	chloronitroacetamidate

1-CNgud	1-cyanoguanidine
croc	croconate
15-crown-5	macrocyclic polyethers
c-sar_2	cyclosarcosylsacorsine
cyclam	1,4,8,11-tetraazacyclotetradecane
cyclamac	1,4,8,11-tetraazacyclotetradecane-N,N′,N″,N‴-tetraacetate
cyclox	3-methyl-3-nitro-1,5,9,13-tetraazacyclohexadecane
cyt	cytosine
dacac	1,4,10,13-tetraoxa-7,16-diazacyclooctadecane-7-acetate
daco	1,5-diazacyclooctane
daes	1,7-diaza-4-thiaheptane
dafone	4,5-diazafluoren-9-one
dampr	diamine-2,3-propionique(N^2O)acid
dapsc	2,6-diacetylpyridine bis semicarbazone
dcam	dicyandiamide
debd	1,6-bis(3,5-dimethylpyrazol-1-yl)-2,5-dimethyl-2,5-diaza-hexane
degly	diethanolglycine
dempz	3,5-diethyl-4-methylpyrazole
dhmp	2,3-dihydroxy-2-methylpropanoate
dien	diethylenetriamine
dim	diimidazole
dmact	N,N-dimethyl-acetamide
dmco	2,5-dimethyloxazolidine-4-carboxylate
dmen	N,N-dimethyl-1,2-ethanediamine
dmf	dimethylformamide
dmoc	2,5-dimetyloxazolidine-4-carboxylate
dmpr	1,3-diamino-2-propanole
2,6-dnph	2,6-dinitrophenolate
dsco	3-hydroxy-1,5-dithiacyclooctane
dptp	1-(3,5-dimethyl-1-pyrazolyl)-3-thiapentane
dtpa	trihydrogen diethylenetriaminepentaacetate
dtun	1,11-diamino-3,6,9-trithiaundecane
dund	6-hydroxy-4,8-diazaundecanediamine
dzco	1,4,10,13-tetraoxa-7,16-diazacyclooctadecane-7,16-N,N′-diacetate
eac	ethylenediamine-tetraacetate
ebtb	N,N,N′,N′-tetrakis(2′-benzimidazolylmethyl)1,2-ethane diamine
ecgly	ethylenebis(N-methylcarbamylglycinate)

ecgm	N,N′-1,2-ethanediylbis[N-(carboxymethyl)glycyl-L-methionine]ethylesterate
eiphim	3,3′-ethylenedi-iminobis(o-phenyleneimino-methylidene)bis[pentane-2,dionate(2-)]
en	ethylenediamine
enphgly	ethylenebis(o-hydroxyphenyl)glycine
esbim	2-(ethylthiomethyl)benzimidazole
esop	2-(ethylthio)-4-oxopteridine
etam	ethanolamine
etapy	2-(2-diethylammonioethyl)pyridine
5,5′-Et_2barb	5,5′-diethylbarbiturate
Eten	N-ethylenediamine
EtenOH	N-(2-hydroxyethyl)ethylenediamine
Et_2en	N,N′-diethylenediamine
ethc	ethyl-1,5,9,13-tetraazabicyclo[11.2.2]hepta-decane-7-carboxylate
1-Etim	1-ethylimidazole
EtMecyclam	5,7,12,14-tetraethyl-7,14-dimethyl-1,4,8,11-tetra-azacyclotetradecane
EtOac	ethoxyacetate
Etsac	ethylthioacetate
Et_2sp	diethylthiophosphate
evda	D,L-ethylvalinate-N,N-diacetate
F_6acac	1,1,1,6,6,6-hexafluoro-2,4-pentanedionate(hexa-fluoroacetylacetonate)
fm	formiate
fmpn	4-formyl-2-methoxyphenolate
4-FphOac	4-fluorophenoxyacetate
fpsem	2-formylpyridine thiosemicarbazone
F_5Sph	pentafluorothiophenolate
ghgly	glycyl-L-histidylglycinate
ggly	glycylglycinate
gly	glycine
hbbzim	2-α-hydroxybenzylbenzimidazole
HB(3,5-Me_2pz)$_3$	hydrotris(3,5-dimethyl-1-pyrazolyl)borate
HB(pz)$_3$	hydrotris-(pyrazol-1-yl)borate
hd	3,4-hexanedione dioximate
hdmpz	1-(2-hydroxyethyl)-3,5-dimethylpyrazole
heac	dihydrogen ethylenediaminetetraacetate

hemq	9-[(2-hydroxyethoxy)methyl]quanine
himp	2-hydroxyethyliminopyruvate
hist	histidine
hmnc	N-(hydroxymethyl)nicotinamid
hpca	N-(hydroxymethyl)-3-pyridinecarboxamide
Hpth	hydrogen o-phtalate
hip	hippurate
Hpydca	hydrogen-pyridine-2,6-dicarboxylate
ibpca	N-(2-(4-imidazolyl)ethyl)-2-methyl-5-bromopyrimidine-4-carboxamide
idac	iminodiacetate
3-Ihpur	3-iodohippurate
im	imidazole
imdth	1,6-bis(5-methyl-4-imidazolyl)-2,5-dithiahexane
5′-imp	inosine-5′-monophosphate
inc	isonicotinamide
inco	isonicotinate N-oxide
ipcp	tetraisopropylmethylenediphosphonate
iprthacq	isopropylthioacetate isoquinoline
ipm-1,2-pn	N^1-isopropyl-2-methyl-1,2-propanediamine
iqu	isoquinoline
lac	lactate
lc	lignocaine
lys	L-lysin
m	monoclinic
mact	N-methylacetamide
mal	malonate
mbpy	2,6-bis(1′-methylbenzimidazol-2′-yl)pyridine
mbpym	1,3-dimethyl-2,4-dioxo-6-hydroxy-5-nitroso-1,2,3,4-tetrahydropyrimidine
mceam	β-methylmercaptoethylamine
mcgly	N,N′-methylethylene bis(N-methylcarbamylglycinate)
mdac	iminodiacetamide
9-Meade	9-methyladenine
Me_2amet	2-dimethylaminoethanole
4-Mebzcs	4-methylbenzenecyanamidosulfonate
2-Mebzim	2-methylbenzimidazole
Mecyclam	2,5,5,7,9,12,14-octamethyl-1,4,8,11-tetra-azacyclotetradecane

Me_2CO	acetone
4,4′5,5′-Me_4dim	4,4′5,5′-tetramethyldiimidazole
9-Mehpx	9-methylhypoxanthin
Meial	10-methylisoalloxazine
Meim	N-methylimidazole
Meims	bis(1-methylimidazol-2-yl)sulfide
Meimthb	4-(5-methyl-4-imidazolyl)-1-amino-3-thiabutane
Meimthp	1,3-bis(5-methyl-4-imidazolyl)-2-thiapropane
$MeNO_2$	nitromethane
mep	mepirizole
Me_2pam	3,3′-(2,2-dimethylpropylene)diiminodipropionamide
Me-picam	methyl-2-picolylamine
9-Meop	9-methyl-6-oxypurine
2Me-1,2-pn	2-methyl-1,2-propanediamine
Me_2-1,3-pn	2,2-dimethylpropane-1,3-diamine
Me_4psim	2-(2-pyridyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazolyl-1-oxy
4-MepyNO	4-methylpyridine 1-oxide
Me-pyrpy	2,6-bis{[(2S)-2-(methoxymethyl)pyrrolidin-1-yl] methyl}pyridine
4-Mepz	4-methyl-1H-pyrazole
8-Mesthp	8-methylthiotheophyllinate
9-Mequa	9-methylquanine
3,5-Me_2guapz	3,5-dimethyl-1-guanylpyrazole
5,7-Me_2tpym	5,7-dimethyl-[1,2,4]triazolo[1,5-a]pyrimidine
metri	methyltribenzo[b,f,j][1,5,9]triazacycloduodecine
mic	miconazole
mimdth	1,6-bis(5-methyl-4-imidazolyl)-2,5-dithiahexane
mmcyclam	C-meso-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetra-azacyclotradecane or C-meso-5,5,7,12,12,14hexamethyl-1,4,8,11-tetraazacyclotetradecane
mntcp	10-methyl-10-nitro-1,4,8,12-tetraazacyclopentadecane
mnim	2-methyl-5-nitroimidazole
mocpz	3,5-dimethoxycarbonylpyrazole
monp	2-methoxy-4-nitrophenolate
mor	morpholine
mpo	2-(methylaminomethyl)pyridine 1-oxide
mtpo	5-methyl[1,2,4]triazolo[1,5-a]pyrimidin-7-olate

mug	mugineic acid
nbta	1,1,1-trifluoro-4-(4′-nitrophenyl)-buta-2,4-dionate
nc	nicotinamide
ndap	N,N′-bis(2-pyridylmethylene)-1,3-diamino-2-methyl-2-nitropropane
nn	1-nitroso-2-naphtole
6-NO_2cyclam	6-(p-nitrobenzyl)-1,4,8,11-tetraazacyclo-tetradecane-1,4,8,11-tetraacetate
4-NO_2pyNO	4-nitropyridine N-oxide
npac	nitrilodi(β-propionamide)monoacetate
nphyr	1,8-naphthyridine
nphyrO	1,8-naphthyridine-N-monoxide
$N(py)_3$	2,2′,2″-tripyridylamine
odac	oxydiacetate
Opy	2,2′-(1,3,4-oxadiazole-2,5-diyl)dipyridine
OH-1,3-pn	2-hydroxy-1,3-propanediamine
2-OH-2-Mepr	2-hydroxy-2-methyl-propionate
OH-pyrpy	2,6-bis{[(2S)-2-(hydroxymethyl)pyrrolidin-1-yl]methyl}pyridine
ompa	octamethylpyrophosphoramide
opai	1-oxa-1,6,8,12,15-penta-aza-tricyclo[13,3,1.$1^{8,12}$]icosane
opca	N-oxymethylamide-pyridine-3-carbon acid (nikodine)
2-Opy	2-pyridone
or	orthorhombic
orn	σ-N-hydro-L-ornithinate
ottd	1-oxa-4,8,12-triazacyclotetradecane-4,12-diacetate
ox	oxalate
papt	1,4-di(2′-pyridyl)aminophthalazine
pbpc	1-oxo-1,2-diphenyl-3,3,5-tricarbbutoxy-1,2-2-diphosphacyclopentanone
pcam	bis(2-pyridylcarbonyl)amide
pcb	1-pyrroline-2-carboxylate (L-ornithine)
pcp	octamethylenediphosphonic diamine
pdto	1,8-diamino-3,6-dithiaoctane
peme	1,1-di(2-pyridyl)ethylmethyl ether
Ph	phenyl

phen	1,10-phenanthroline
phenO	1,10-phenanthroline-N-monoxide
phepy	2,6-bis[1-(phenylimino)ethyl]pyridine
Phnit	2-phenyl-4,4,5,5-tetramethylimidazoline-1-oxyl-3-oxide
Phimthp	1,3-bis(5-phenyl-2-imidazolyl)-2-thiopropane
phOac	phenoxyacetate
$Ph_2P(O)CH_2P(O)Ph_2$	tetraphenylmethylenediphosphonium dioxide
picl	4-amino-3,5,6-trichloropyridine-2-carboxylate
picNO	picolin-N-oxide
pipc	2-piperidinecarboxylate
2-pira	2-pyridylenaniline
pith	pyridyl, imine, thioether donor
pmca	bis(2-pyrimidylcarbonyl)aminate
pmtrz	2,4-bis(n-propylamino)-6-methoxy-1,3,5-triazine
1,2-pn	1,2-propanediamine
1,3-pn	1,3-diaminopropane
poet	bis[(diphenylphosphinyl)methyl]ethyl phosphinate
pppa	N-(2-pyridyl)-3-phenyl-2-propeneamide
pr	propionate
prcim	4-(n-propylmercaptomethyl)imidazole
prcpy	2-(n-propylmercaptomethyl)pyridine
prim	2-pyrimidinone
prol	prolinate
prometone	2,4-bis(isopropylamino)-6-methoxy-1,3,5-triazine
prtac	isopropylthioacetate
psac	phenylsulphinylacetate
psalh	N-picolinyilidene-N′-salicylhydrazine
pslh	N-picolinyilidene-N′-salicyloylhydrazinae
ptcbx	pterin-6-carboxylate
py	pyridine
pyact	pyridine-2-acetamide
pyam	pyrimidin-2-amine
pybox	pyridine-2-carboxamide
2-pyc	pyridine-2-carboxylate
pydca	pyridine-2,6-dicarboxylate
pydcaH	pyridine-2,6-dicarboxylic acid
pydoc	1,8-bis(2′-pyridyl)-3,6-diazaoctane

pym	2-pyridylmethanol
pyf	2-pyridylformamide
pyha	7-(2′-pyridyl)-3,6-diazaheptylamine
pyNO	pyridine 1-oxide
pyos	1,9-bis(2-pyridyl)-5-oxa-2,8-dithianonane
pypr	pyridinopropionate
pytrz	2,4,6-tris(2-pyridyl)-1,3,5-triazine
purp	purpurate
pz	pyrazole
pzc	pyrazinecarboxylate
pzdc	pyrazine-2,3-dicarboxamide
$(pz)_2(py)CH$	bis(pyrazol-1-yl)(pyridin-2-yl)methane
5′-qmp	guanosine 5′-monophosphate
qu	quinoline
qusp	1,5-bis(quinoline-8′-yl)-1,5-dithiapentane
rh	rhombohedral
sach	saccharin, (o-sulphobenzoimide)
sal	salicylate
salen	N-salicylidene-N′-methylenediamine
sbh	Schiff-base ligand
sbzh	thiobenzoylhydrazine
sc	semicarbazide
sim	simatone
SO_3CF_3	trifluoromethanesulphonate
suc	succinate
tach	cis,cis-1,3,5-triaminocyclohexane
taci	1,3,5-triamino-1,3,5-trideoxy-cis-inositol
tcne	O-tricyanoethyleneoate
tcnq	7,7′,8,8′-tetracyanoquinodimethane
tdac	thiodiacetate
tdc	1,2,3-triazole-4,5-dicarboxylate
tdpom	trisphenylphosphitomethane
terpy	2,2′:6′,2″-terpyridine
tfac	thenoyltrifluoroacetate
tg	tetragonal
tgly	N-tosyl-glycinate
thc	L-1,3-thiazolidine-4-carboxylate
thp	3,4,5,6-tetrahydropicolinate (L-lysine)

thr	threonine
tim	2,3,9,10-tetramethyl-1,4,8,11-tetraaza-1,3,8,10-cyclotetradecatetraene
tmic	2,2,5,5-tetramethyl-3-imidazoline-1-oxo-4-carboxylate
tmpCN	3-cyano-2,2,5,5-tetramethylpyrrolinyl-1-oxy
tmtc	tetrakis(5-methylbenzo) [b,f,j,n][1,5,9,13]tetraacyclohexadecine
tnph	2,4,6-trinitrophenolate
tocop	2,2′-(1,4,10,13-tetraoxa-7,16-diaza-7,16-cyclooctadecylene)-dipropionate
tol	toluene
tols	toluene-4-sulphonate
tpy	tetrapyridine
tr	triclinic
trg	trigonal
trien	triethylenetetramine
trioc	1,3,6,9,11,14-hexaazatricyclo[12.2.1.1^{6,9}]octadecane
trt	D-tartrate
tsval	N-tosylvalinate
ttbd	4,4,4-trifluoro-1-(2-thienyl)butanedione-1,3
ttbt	1-(2-thienyl)-4,4,4-trifluoro-1,3-butanedionate
ttcn	1,4,7-trithiacyclononane
tu	thiourea
1-vim	1-vinylimidazole

INTRODUCTION

The structural chemistry for over one thousand copper compounds has been reviewed recently.[1] Several relationships were found and discussed. The overwhelming majority of X-ray studies of transition metal compounds are of copper compounds, and of these Cu(II) is the most common. Comprehensive data on mononuclear tetra- and pentacoordinate Cu(II) compounds[2] as well as on mixed-valence Cu(I)-Cu(II) compounds[3] have also appeared.

The systems discussed in this paper are mononuclear six-, seven- and eight-coordinate Cu(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.

HEXACOORDINATE Cu(II) COMPOUNDS

Structural data for mononuclear six-coordinate Cu(II) compounds are summarized in Table I. There are five hundred and fifty examples.

Because of its electronic configuration, the Cu(II) atom is an ideal candidate for deformation studies of its coordination polyhedron. First of all, it has only one outermost electron which simplifies theoretical considerations. Secondly, if the ligand atoms around the central Cu(II) atom are identical, the coordination polyhedron is subject to the first-order Jahn–Teller effect.

There are three principal forms of distortion of the octahedron. One is tetragonal, elongation or contraction along a single C_4 axis; the resulting symmetry is only D_{4h}. Another is rhombic; changes in the lengths of two of the C_4 axes so that no two are equal; the symmetry is then only D_{2h}. The third is a trigonal distortion, elongation or contraction along one of the C_3 axes so that the symmetry is reduced to D_{3d}. All of the limiting geometries occur in the chemistry of Cu(II) with various degrees of distortion. The tetragonal distortion is most common and involves an elongation of one C_4 axis and, in the limit, two *trans* ligands are lost completely, leaving a square, four-coordinate complex.

The explanation for the axial elongation in *trans*-CuX_4Y_2 type polyhedra is still controversial. Because the highest possible site symmetry around the central Cu(II) atom would be D_{4h}, a first-order Jahn–Teller effect is ruled out. Assuming site symmetry of D_{4h}, the second-order Jahn–Teller deformation takes place only in the CuX_4 plane. On the other hand, it is well known that *d–s* mixing leads to effects of the same order of magnitude as the first-order ligand field energies. Indeed, this concept has been used to explain axial elongation in coordination polyhedra of the type CuX_4Y_2. Interestingly, *d–s* mixing predicts that the most stabilizing distortion in CuX_4Y_2 type coordination polyhedra can be produced by an asymmetric axial elongation. This means that one axial site is weakened more than its antipode. This ultimately leads to five-coordination.

There are some examples[21–25] which contain a complex cation of composition, $[Cu(pyNO)_6]^{2+}$, where six unidentate pyridine N-oxide molecules form an almost regular octahedron about the Cu(II) atoms.

Finally, there are several examples[344–358] which contain a complex cation of composition $[CuL_2X]^+$ (L = bipyridine or 1,10-phenanthroline; and X = NO_2, NO_3 or RCOO) with a fluxional CuN_4O_2 structure, which was described as a *pseudo, cis*-distorted, octahedral Cu(II) stereochemistry and consequently these structural variations can be related to the dynamic *pseudo*-Jahn–Teller effect.

TABLE I Structural data for six-coordinated Cu(II) compounds[a]

Compound	*Crystal. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	*α* [°] *β* [°] *γ* [°]	*Chromophore*	Cu-L [Å]		L-Cu-L [°]		*Ref.*
$K_2[Cu(H_2O)_6](SeO_4)_2$ (not given)	m $P2_1/a$ 2	9.165(2) 12.224(7) 6.336(2)	 103.359(8)	CuO_6	O[b]	1.936(2) × 2 2.044(2) × 2 2.297(2) × 2	O,O[b]	90.0(1, 1.9)	4
$Rb_2[Cu(H_2O)_6](SO_4)_2$ (not given) (at 293 K)	m $P2_1/a$ 2	9.26(2) 12.35(7) 6.22(5)	 105.3(1)	CuO_6	O	1.957(3) × 2 2.031(3) × 2 2.307(3) × 2	O,O	90.0(3, 0)	5
$Rb_2[Cu(H_2O)_6](SO_4)_2$ (not given) (at 77 K)	m $P2_1/a$ 2	9.28(1) 12.15(4) 6.23(1)	 105.4(1)	CuO_6	O	1.978(8) × 2 2.000(7) × 2 2.317(10) × 2	O,O	90.0(3, 2.0)	5
$Tl_2[Cu(H_2O)_6](SO_4)_2$ (not given)	m $P2_1/a$ 2	9.27(2) 12.39(7) 6.22(1)	 105.6(1)	CuO_6	O	1.957(5) × 2 2.017(4) × 2 2.317(5) × 2	O,O	90.0(2, 4)	6
$K_2[Cu(H_2O)_6](SO_4)_2$ (not given)		not given		CuO_6	O	1.943(2) × 2 2.069(2) × 2 2.278(2) × 2		not given	7
$Cs_2[Cu(H_2O)_6](SO_4)_2$ (not given)		not given		CuO_6	O	1.966(5) × 2 2.004(4) × 2 2.315(5) × 2		not given	8
$(NH_4)_2[Cu(H_2O)_6](SO_4)_2$ (not given)	m $P2_1/a$ 2	9.267(2) 12.445(15) 6.298(5)	 106.9(6)	CuO_6	O	1.969(5) × 2 2.095(5) × 2 2.219(5) × 2	O,O	90.0(1, 1.4)	9
$(NH_4)_2[Cu(H_2O)_6](SO_4)_2$ (not given)	m $P2_1/a$ 2	9.2105(14) 12.3795(17) 6.3016(13)	 106.112(18)	CuO_6	O	1.9660(11) × 2 2.0725(14) × 2 2.2300(14) × 2	O,O	90.0(1, 1.1)	10
$Sr_2[Cu(H_2O)_6]$ (blue)	m $P2_1/c$ 2	5.786(1) 6.154(1) 9.744(2)	 124.15(1)	CuO_6		not given			11
$Ba_2[Cu(H_2O)_6]$ (blue)	m $P2_1/c$ 2	6.030(2) 6.440(2) 10.115(2)	 124.03(1)	CuO_6	O_{eq} O_{ax}	1.965(4, 7) 2.805(4) × 2	O_{eq}, O_{eq} O_{eq}, O_{ax}	90.0(1, 1.1) 90.0(1, 3.1)	11

$[Cu(H_2O)_6]SiF_6$ (not given) (at 240-290 K)	rh R-3 12	18.138(2) 9.787(5)		CuO_6			not given		12
$[Cu(H_2O)_6]SiF_6$ (not given) (at 296-302 K)	rh R-3 3	9.344(2) 9.695(5)		CuO_6		not given			12
$(C_2H_{10}N_2)_3[Cu(H_2O)_6](P_4O_{12})_2\cdot 8H_2O$ (not given)	m $P2_1/n$ 2	13.162(8) 13.301(8) 12.308(8)	106.69(1)	CuO_6	O_{eq} O_{ax}	1.966(3, 19) 2.382(3) × 2	O_{eq}, O_{eq} O_{eq}, O_{ax}	90.9(1, 0) 92.1(1, 1.8)	13
$[Cu(H_2O)_6].2(PhO)_2PO_2.(gly)_2$ (not given)	tr P-1 1	17.019(6) 6.520(3) 8.107(3)	93.39(5) 89.20(5) 94.86(5)	CuO_6	O_{eq} O_{ax}	1.980(2, 7) 2.321(2) × 2	O_{eq}, O_{eq} O_{eq}, O_{ax}	90.0(1, 2) 90.0(1, 2.1)	14
$[Cu(H_2O)_6](ClO_4)_2.2(c\text{-}sar_2)$ (not given)	m $P2_1/c$ 4	13.879(7) 14.504(7) 13.083(8)	90.98(10)	CuO_6	O_{eq} O_{ax}	1.980(6, 22) 2.307(6, 18)	O_{eq}, O_{eq} O_{eq}, O_{ax} O_{ax}, O_{ax}	90.0(5, 3.5) 90.0(5, 4.5) 172.5(5)	15
$[Cu(H_2O)_6](bzs)_2$[c] (pale blue)	tr P-I 2	22.51(2) 6.26(1) 6.96(1)	92.5(2) 93.0(2) 89.5(2)	CuO_6	O_{eq} O_{ax}	1.969(3, 11) 2.259(4) × 2	O_{eq},O_{eq} O_{eq},O_{ax}	90.3(2, 0) 92.0(2, 6)	16
				CuO_6	O_{eq} O_{ax}	1.974(3, 13) 2.264(3) × 2	O_{eq},O_{eq} O_{eq},O_{ax}	90.2(2) 92.6(2, 1)	
$[Cu(H_2O)_6](tols)_2$ (not given)	m $P2_1/c$ 2	5.85(1) 25.71(2) 7.35(1)	105.4(2)	CuO_6	O_{eq} O_{ax}	1.954(2, 1) 2.423(2) × 2	O_{eq},O_{eq} O_{eq},O_{ax}	90.6(1, 0) 94.6(1, 8)	16
$[Cu(H_2O)_6](camphs)_2$ (not given)	m $P2_1$ 2	17.17(3) 7.05(2) 11.64(2)	94.1(2)	CuO_6	O_{eq} O_{ax}	2.00(3, 5) 2.20(2, 3)	O_{eq},O_{eq} O_{eq},O_{ax} O_{ax},O_{ax}	90.0(9, 1.1) 89.9(9, 6.9) 178.8(9)	16
$[Cu(H_2O)_6](4\text{-}Clbzs)_2$ (colourless)	m $P2_1/c$ 2	5.7910(5) 25.614(3) 7.3360(9)	104.350(9)	CuO_6		not given			17
$[Cu(H_2O)_6][Cu(C_8H_8O_5)_2]$[c] (pale blue)	m $P2_1/c$ 2	9.631(2) 10.725(2) 10.710(2)	103.69(1)	CuO_6	H_2O_{eq} H_2O_{ax}	1.965(2, 8) 2.321(2) × 2		not given	18
				CuO_6	O_{eq} O_{ax}	1.977(2, 18) 2.376(2) × 2		not given	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	*α* [°] *β* [°] *γ* [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
$[Cu(H_2O)_6][Cu(C_8H_8O_5)_2]^c$ (green)	tr P-1 1	6.580(1) 8.527(1) 9.859(2)	100.04(2) 101.67(2) 94.75(2)	CuO_6		not given			19
				CuO_6	O	2.20 × 6		not given	
$[Cu(2\text{-}Opy)_6](ClO_4)_2$ (not given)	m $P2_1/c$ 2	9.453(2) 10.492(3) 17.794(3)	 95.57(2)	CuO_6	O_{eq} O_{ax}	1.937(2, 15) 2.546(2) × 2	O_{eq},O_{eq} O_{eq},O_{ax}	95.9(1, 4.0) 86.81(7)	20
$[Cu(pyNO)_6](ClO_4)_2$ (not given)	rh R-3 1	9.605(1)	81.10(1)	CuO_6	O	2.076(2) × 6	O,O	90.29(7)	21
$[Cu(pyNO)_6](ClO_4)_2$ (not given)	rh R-3 1	9.620(2)	81.21(2)	CuO_6	O	2.086(2) × 6	O,O	90.0(1, 0)	22
$[Cu(pyNO)_6](BF_4)_2$ (not given)	rh R-3 1	9.621(2)	81.46(2)	CuO_6	O	2.088(1) × 6	O,O	90.0(1, 0)	22
$[Cu(pyNO)_6](ClO_4)_2\cdot 0.15dmf$ (not given) (at 20 K)	rh R-3 3	12.260(1) 18.798(2)		CuO_6	O	2.074(1) × 6	O,O	90.0(1, 0)	23
$[Cu(pyNO)_6](NO_3)_2$ (not given)	rh R-3 1	9.504(3)	83.41(5)	CuO_6	O	2.097(2) × 6	O,O	90.0(4, 5)	24
$[Cu(pyNO)_6](NO_3)_2$ (not given)	rh R-3 3	12.623(5) 18.190(6)		CuO_6	O	2.091(4) × 6	O,O	90.0(1, 3)	25
$[Cu(pyNO)_6](NO_3)_2\cdot 2H_2O$ (not given)	m $P2_1/c$ 2	9.556(2) 9.924(2) 18.658(3)	 100.43(3)	CuO_6	O_{eq} O_{ax}	1.962(2, 8) 2.478(2) × 2	O_{eq},O_{eq} O_{eq},O_{ax}	88.9(1) 88.0(1, 4.4)	26

$[Cu(4\text{-}MepyNO)_6](ClO_4)_2$	m	9.523(5)		CuO_6	O_{eq}	1.987(0, 22)	O_{eq},O_{eq}	90.3(4)	27
(not given)	$P2_1/c$	10.707(8)	92.47(6)		O_{ax}	2.385(11) × 2	O_{eq},O_{ax}	92.1(4, 7)	
	2	20.512(16)							
$Cu(dmact)_4(ClO_4)_2$	m	13.080(5)		CuO_6	O_{eq}	1.926(5, 16)	O_{eq},O_{eq}	92.3(5)	28
(not given)	$P2_1/n$	10.937(5)	109.95(4)		O_3ClO_{ax}	2.933(7) × 2	O_{eq},O_{ax}	84.8(7, 4.0)	
	2	9.605(5)							
$Cu(H_2O)_2(tsval)_2(MeOH)_2$	m	4.996(2)		CuO_6	H_2O_{eq}	1.989(3) × 2	O_{eq},O_{eq}	89.1(1)	29
(not given)	$P2_1/n$	19.304(7)	97.93(1)		$tsvalO_{eq}$	1.954(4) × 2	O_{eq},O_{ax}	92.3(1, 1.9)	
	2	17.124(6)			$MeHO_{ax}$	2.492(4) × 2			
$[Cu(ahmi)_6][Cu(ahmi)Cl_3]_2$[c]	m	10.757(2)		CuO_6	O	1.951(4) × 2	O,O	90.0(2, 3.8)	30
(not given)	$P2_1/c$	19.787(3)	101.26(1)			1.962(4) × 2			
	2	14.528(2)				2.514(4) × 2			
				$CuCl_3O$	Cl	2.239(2, 3)	Cl,Cl	99.2(1, 3)	
					O	1.954(4)		137.55(7)	
							Cl,O	95.6(1, 1.5)	
								138.3(1)	
$Cu(H_2O)_4(MeSO_3)_2$	m	9.3064(9)		CuO_6	H_2O_{eq}	1.958(2, 11)	O_{eq},O_{eq}	89.9(1, 1)	31
(not given)	$P2_1/c$	9.632(2)	122.18(1)		$MeSO_{ax}$	2.378(2) × 2	O_{eq},O_{ax}	90.1(1)	
	2	7.3076(8)							
$Cu(H_2O)_4(tols)$	m	15.789(4)		CuO_6	O_{eq}	2.020(4) × 2	O_{eq},O_{eq}	88.6(2, 1.2)	32
(light green)	$P2_1/b$	11.911(4)			H_2O_{eq}	1.973(4) × 2	O_{eq},O_{ax}	85.9(2)	
	2	5.086(4)	108.13(20)		H_2O_{ax}	2.347(4) × 2			
$[Cu(H_2O)_4(3\text{-}Ihpur)_2]\cdot H_2O$	m	45.665(5)		CuO_6	$purO_{eq}$	1.88(2) × 2		not given	33
(not given)	B2/b	8.156(5)			H_2O_{eq}	1.99(2) × 2			
	4	6.828(5)	99.6(2)		H_2O_{ax}	2.30(2) × 2			
$Cu(H_2O)_3(SO_4)(ami)$	tr	7.745(2)	80.91(3)	CuO_6	H_2O_{eq}	1.973(4, 35)	O_{eq},O_{eq}	90.4(2, 4.1)	34
(green)	P-1	9.553(4)	79.28(2)		$amiO_{eq}$	1.916(4)	O_{eq},O_{eq}	165.5(2, 8.3)	
	2	20.343(5)	87.58(3)		$amiO_{ax}$	2.785(3)	O_{eq},O_{ax}	90.1(2, 37.1)	
					O_3SO_{ax}	2.238(3)	O_{ax},O_{ax}	147.4(1)	
$Cu(MeOac)_2(H_2O)_2$	m	6.92(2)		CuO_6	O_{eq}	2.04(1, 11)		not given	35
(not given)	$P2_1/n$	7.24(2)			H_2O_{ax}	2.14(1) × 2			
	2	10.10(3)	96.7(1)						
$Cu(picNO)_2(H_2O)_2$	tr	6.634(11)	80.5(1)	CuO_6	O_{eq}	1.935(4, 13)	O,O	90.19(1)[d]	36
(not given)	P-1	7.302(14)	89.4(1)		H_2O_{ax}	2.488(5) × 2		90.0(2, 2.9)	
	1	7.968(1)	61.4(1)						

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
$Cu(4\text{-}MeOC_6H_4OCH_2CO_2)_2$ $(H_2O)_2$ (blue)	tr P-1 1	14.90(2) 6.56(1) 5.31(1)	104.4(2) 75.4(2) 94.3(2)	CuO_6	H_2O_{eq} O_{eq} O_{ax}	1.945(2) × 2 1.955(2) × 2 2.432(3) × 2	O,O	74.8(1)[e] 93.5(1, 1.5)	37
$Cu(C_6H_3O_3S)_2(H_2O)_2$ (not given)	m $P2_1/c$ 2	8.425(2) 11.532(4) 7.348(9)	 92.93(2) 	CuO_6	H_2O_{eq} O_{eq} O_{ax}	2.029(2) × 2 1.955(2) × 2 2.290(2) × 2	O,O	76.52(5)[e] 90.1(8, 8)	38
$Cu(4\text{-}ClphOac)_2(H_2O)_2$ (pale blue)	tr P-1 1	7.065(3) 13.273(11) 5.114(2)	93.72(5) 103.64(4) 81.63(5)	CuO_6	H_2O_{eq} O_{eq} O_{ax}	1.960(4) × 2 1.956(4) × 2 2.406(4) × 2	O_{eq},O_{eq} O_{eq},O_{ax}	89.0(3, 8) 74.6(3)[e]	39
$Cu(dhmp)_2(H_2O)_2$ (not given)	m C2/c 4	5.688(6) 20.79(3) 10.569(16)	 94.55(6) 	CuO_6	O_{eq} H_2O_{ax}	1.932(8, 42) 2.542(12) × 2	O_{eq},O_{eq} O_{eq},O_{ax}	83.5(3)[e] 92.0(4, 1.5)	40
$[Cu(acgly)_2(H_2O)_2]\cdot 2H_2O$ (not given)	m C2/c 4	21.13(1) 5.04(1) 17.59(1)	 124.7(1) 	CuO_6	H_2O_{eq} O_{eq} O_{ax}	1.947(3) × 2 1.955(3) × 2 2.614(3) × 2	O_{eq},O_{eq} O_{eq},O_{ax} O_{eq},O_{ax}	90.6(1) 55.5(1)[g] 88.1(1)	41
$[Cu(acgl)_2(H_2O)_2]\cdot 2H_2O$ (blue)	m Cc 4	21.145(6) 5.046(2) 18.248(5)	 127.55(4) 	CuO_6	H_2O_{eq} O_{eq} O_{ax}	1.944(2) × 2 1.952(2) × 2 2.619(2) × 2	O_{eq},O_{eq} O_{eq},O_{ax}	90.0(1, 6) 55.4(1)[f] 90.0(1, 1.6) 124.6(1)	42
$[Cu(mal)_2(H_2O)_2]\cdot 2H_2O$[c] (light blue)	tr P-1 2	7.630 10.327 5.285	103.14 96.06 108.54	CuO_6	O_{eq} H_2O_{ax}	1.97(–, 1) 2.48 × 2	O_{eq},O_{eq} O_{eq},O_{ax}	90.0(–, 1.2)[d] 90.2(–, 2.5)	43
				CuO_6	H_2O_{eq} H_2O_{ax}	1.98(–, 3) 2.47 × 2	O_{eq},O_{eq} O_{eq},O_{ax}	87.1[d] 91.5(–, 1.5)	
$Cu(mal)_2(H_2O)_2$ (not given)	m $P2_1/c$ 2	8.573(1) 7.423(1) 10.315(2)	 102.72(1) 	CuO_6	O_{eq} H_2O_{ax}	1.937(2, 25) 2.528(2) × 2	O_{eq},O_{eq}	83.17(7)[e] 96.83(7)	44

$Cu(EtOac)_2(H_2O)_2$	tr	6.60(1)	91.6(3)	CuO_6	H_2O_{eq}	1.990(7) × 2	O_{eq},O_{eq}	90.9(3)	45
(blue)	P-1	7.21(1)	91.6(3)		O_{eq}	1.970(7) × 2	O_{eq},O_{ax}	75.2(3)[e]	
	1	7.58(1)	117.3(4)		O_{ax}	2.380(7) × 2		89.8(3)	
$[Cu(4\text{-}FphOac)_2(H_2O)_2]$-	tr	14.808(2)	87.77(2)	CuO_6	H_2O_{eq}	1.940(3) × 2	O_{eq},O_{eq}	86.6(1)	46
$(4\text{-}FphOac)_2 \cdot 2H_2O$	P-1	9.832(2)	98.41(2)		O_{eq}	1.942(2) × 2	O_{eq},O_{ax}	73.0(1)[e]	
(dark green)	1	6.847(2)	112.33(2)		O_{ax}	2.471(2) × 2		89.4(1)	
$Cu(ac\text{-}\beta\text{-}ala)_2(H_2O)_2$	m	5.0135(2)		CuO_6	H_2O_{eq}	1.960(2) × 2	O_{eq},O_{eq}	89.7(1)	47a
(blue)	$P2_1/n$	8.415(1)	91.186(3)		O_{eq}	1.958(2) × 2			
	2	17.952(2)			O_{ax}	2.580(2) × 2			
$Cu(inco)_2(H_2O)_2$	m	14.136(7)		CuO_6	H_2O_{eq}	1.930(2) × 2	O_{eq},O_{eq}	90.0(1, 1.2)	47b
(royal blue)	C2/c	9.791(3)	110.91(3)		O_{eq}	1.934(4) × 2	O_{eq},O_{ax}	54.7(1)[f]	
	4	10.768(3)			O_{ax}	2.691(4) × 2		90.0(1, 2.9)	
								125.2(1)	
$Cu(Hpth)_2(H_2O)_2$	m	8.31(2)		CuO_6	H_2O_{eq}	1.930(8) × 2	O_{eq},O_{eq}	91.4(3, 0)	48
(blue)	$P2_1/c$	14.62(2)	112.2(2)		O_{eq}	1.967(8) × 2	O_{eq},O_{ax}	54.4(2)[g]	
	2	7.20(2)			O_{ax}	2.677(5) × 2		88.7(2, –)	
$trans[Cu(nbta)_2(H_2O)_2](pyNO)_2$	m	15.318(5)		CuO_6	O_{eq}	1.924(1, 1)	O_{eq},O_{eq}	92.6(0)[d]	49
(green)	$P2_1/a$	9.036(3)	114.16(1)		H_2O_{ax}	2.594(2) × 2	O_{eq},O_{ax}	93.7(1, 6)	
	2	13.253(5)							
$Cu(phOac)_2(H_2O)_2$[c]	m	16.24(4)		CuO_6	H_2O_{eq}	1.99(–, 1)	O_{eq},O_{eq}	89.3(–, 1.2)	50
(green)	$P2_1/c$	7.28(3)			O_{eq}	1.95(–, 1)	O_{eq},O_{ax}	74.7(–, 4)[e]	
	6	23.99(6)	110.4(3)		O_{ax}	2.47(–, 3)		97.0(–, 13.1)	
				CuO_6	H_2O_{eq}	1.97 × 2	O_{eq},O_{ax}	73.6[e]	
					O_{eq}	1.94 × 2		90.4(–, 1.4)	
					O_{ax}	2.50 × 2			
$Cu(MeOac)_2(H_2O)_2$	m	6.92(2)		CuO_6	O_{eq}	1.93 × 2	O,O	79.9[e]	50
(blue)	$P2_1/m$	7.26(2)				2.13 × 2		90.7	
	2	10.10(3)	96.7(3)		H_2O_{ax}	2.16 × 2		92.2	
$Cu(2\text{-}OH\text{-}2\text{-}Mepr)_2(H_2O)_2$	m	10.25(5)	105.9(5)	CuO_6	O_{eq}	1.95(–, 6)	O_{eq},O_{eq}	82.7[e]	50
(blue)	C2/m	5.80(3)			H_2O_{ax}	2.56 × 2	O_{eq},O_{ax}	90.0(–, 0)	
	2	11.24(5)							
$Cu(NO_3)_2(apy)_2$	m	13.05(2)		CuO_6	$apyO_{eq}$	1.917(16, 20)	O_{eq},O_{eq}	90.3(1.0,2.2)	51
(not given)	$P2_1/c$	17.50(3)	136.0(5)		$(NO_3)O_{eq}$	1.979(16, 3)		171.5(2.0,2.2)	
	4	15.82(3)			$(NO_3)O_{ax}$	2.481(21, 3)			

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	*α* [°] *β* [°] *γ* [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
$Cu(NO_3)_2(apy)_2$	tr	14.92(3)	117.2(5)	CuO_6	$apyO_{eq}$	1.926(12, 1)	O_{eq},O_{eq}	90.5(9, 9)	52
(not given)	P-1	10.20(2)	103.8(5)		$(NO_3)O_{eq}$	2.014(13, 44)		168.8(1.6,1.2)	
	2	9.60(2)	75.9(5)		$(NO_3)O_{ax}$	2.444(13, 15)			
$Cu(C_8H_{11}NO_3)_2(NO_3)_2$	tr	10.483(1)	73.92(2)	CuO_6	O_{eq}	1.945(3, 29)	O_{eq},O_{eq}	91.2(1)[d]	53
(light green)	P-1	6.9278(5)	67.62(2)		O_2NO_{ax}	2.443(4) × 2	O_{eq},O_{ax}	87.7(1, 5.8)	
	1	8.198(1)	97.81(2)						
$Cu(ompa)_2(ClO_4)_2$	m	10.797(1)		CuO_6	O_{eq}	1.941(2, 5)	O_{eq},O_{eq}	90.0(1, 3)[d]	54
(light blue)	$P2_1/c$	8.865(1)	109.9(1)		O_3ClO_{ax}	2.546(3) × 2	O_{eq},O_{ax}	87.4(1, 2.1)	
	2	20.047(1)							
$Cu\{C_5(CO_2Me)_5\}_2(MeOH)_2$	m	8.205(5)		CuO_6	O_{eq}	1.954(2, 8)	O,O	93.3(1, 3.4)	55
(blue green)	$P2_1/c$	20.204(9)	108.09(4)		$MeHO_{ap}$	2.314(3) × 2			
	2	11.975(5)							
$[Cu(poet)_2(EtOH)_2](ClO_4)_2$	tr	13.688(7)	110.43(4)	CuO_6	$EtHO_{eq}$	1.988(4) × 2	O,O	90.0(1)[d]	56
(pale blue)	P-1	14.424(10)	90.13(2)		O_{eq}	1.969(4) × 2		90.0(2, 3.8)	
	1	9.865(2)	115.54(4)		O_{ax}	2.312(4) × 2			
$[Cu(NO_3)_2(Ph_3PO)_2]\cdot to$	m	12.933(3)		CuO_6	$(NO_3)O_{eq}$	2.099(6) × 2	O,O	56.2(2)[f]	57
(green blue)	$P2_1/c$	15.532(3)	100.68(3)			2.331(6) × 2		87.6(2, 1.5)	
	2	10.285(3)			Ph_3PO_{ax}	1.941(4) × 2			
$[Cu(pypr)_4](ClO_4)_2$	tr	7.3760(8)	102.05(1)	CuO_6	O_{eq}	1.927(3) × 2	O_{eq},O_{eq}	93.7(1)	58
(blue)	P-1	8.558(1)	98.55(1)			1.991(4) × 2	O_{eq},O_{ax}	50.9(1)[f]	
	1	15.402(2)	99.74(1)		O_{ax}	2.834(4) × 2		90.7(1)	
$Cu(bpyO,O)(NO_3)_2(H_2O)$	m	6.635(2)		CuO_6	H_2O_{eq}	1.95	O_{eq},O_{eq}	89.8(1)[i]	59
(green)	$P2_1/c$	7.188(2)	95.54(1)		$bpyO_{eq}$	1.95 × 2		90.1(1, 3.0)	
	4	29.038(3)			$(NO_3)O_{eq}$	1.99		172.6(1, 6.1)	
					O_2NO_{eq}	2.37	O_{eq},O_{ax}	55.6(1)[f]	
					$(NO_3)O_{ax}$	2.53		94.8(1, 16.6)	
							O_{ax},O_{ax}	151.1(1)	
$[Cu(C_2H_6O_2)_3]SO_4$	m	10.166(1)		CuO_6	O_{eq}	1.966(8, 9)	O,O	81.2(3)[c]	60
(pale blue)	$P2_1/c$	9.013(1)	115.666(6)			2.027(8, 4)		93.0(4, 5.6)	
	4	15.365(1)			O_{ax}	2.328(8, 8)		171.4(3, 5.9)	

$[Cu(ompa)_3](ClO_4)_2$ (not given)	trg P-3c1 2	12.855(1) 90.5(1) 18.260(3)		CuO_6	O	2.065(2) × 6	O,O	89.5(1, 1.1)[d]	61
$[Cu(ipcp)_3](ClO_4)_2$ (not given)	m C2/c 8	29.126(6) 23.399(4) 21.696(4)	118.86	CuO_6	O	2.089(2, 22)	O,O	90.5(1.8)[d] 89.9(1, 6.1)	62
$[Cu(C_{14}H_{19}N_2)](F_6acac)_3$ (yellow green)	m $P2_1/n$ 4	12.878(7) 20.998(1) 13.620(7)	98.44(2)	CuO_6	O	2.012(9, 31) 2.179(9, 23)	O,O	87.6(4, 2.9)[d]	63
$[Cu(pcp)_3](ClO_4)_2$ (colourless)	or $Pna2_1$ 4	19.196(4) 12.131(2) 22.868(4)		CuO_6	O	2.086(3, 63)	O,O	90.0(1, 3.6)[d]	64
$[Cu\{Ph_2P(O)CH_2P(O)Ph_2\}_3]\cdot$ $[Cu_2Cl_6]\cdot Me_2CO$ (not given)	m $P2_1/c$ 4	13.144(1) 19.701(3) 30.109(4)	90.88(1)	CuO_6	O	2.022(4, 41) 2.177(4, 79)	O,O	90.7(2, 1.1)[d] 89.8(2, 4.0) 177.4(2, 1.8)	65
$Cu(F_6acac)_2(Phnit)_2$ (blue)	m $P2_1/c$ 4	12.358(6) 15.428(7) 22.61(1)	102.33(3)	CuO_6	O_{eq} $nitO_{ax}$	1.936(5, 7) 2.378(5, 16)	O_{eq},O_{eq} O_{eq},O_{ax} O_{ax},O_{ax}	92.3(1, 3)[d] 89.2(1, 2.8) 178.6(2, 8) 90.0(1, 8.3) 172.4(1)	66
$(NH_4)_4[Cu(C_6H_5O_7)_2]$ (pale blue)	m $P2_1/c$ 2	8.755(3) 13.185(4) 9.364(2)	113.73(2)	CuO_6	O	1.969(3) × 2 1.977(3) × 2 2.341(3) × 2	O,O	73.8(1)[e] 85.1(1)[d] 90.3(1)[g]	67
$[Cu(tdpom)_2](ClO_4)_2\cdot 2H_2O$ (colourless)	tr P-1 1	11.997(3) 12.264(2) 13.159(2)	90.76(1) 107.97(2) 99.03(2)	CuO_6	O	1.977(2) × 2 2.128(2) × 2 2.152(2) × 2	O,O	88.3(1, 5)[d] 90.9(1, 1.4)	68
$[Cu(im)_6](NO_3)_2$ (bright blue)	m $P2_1/c$ 2	8.65(1) 17.64(1) 8.38(1)	93.20(10)	CuN_6	N_{eq} N_{ax}	2.031(2, 19) 2.593(3) × 2	N_{eq},N_{eq} N_{eq},N_{ax}	91.7(1) 91.8(1, 4)	69
$K_2Ca[Cu(NO_2)_6]$ (greenish black)	or Fmmm 4	10.743(3) 10.325(2) 10.318(2)		CuN_6	N_{eq} N_{ax}	2.051(1, 1) 2.313(1) × 2		not given	70
$K_2Pb[Cu(NO_2)_6]$ (green black) (at 276 K)	or Fmmm 4	10.741(1) 10.734(1) 10.538(1)		CuN_6	N	2.058(9) × 2 2.153(14) × 2 2.166(13) × 2		not given	71

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
(at 193 K)				CuN_6	N	2.071(14) × 2		not given	71
						2.151(16) × 2			
						2.133(31) × 2			
$Rb_2Pb[Cu(NO_2)_6]$[c]	or	10.8296(7)		CuN_6	N	2.036(4) × 2		not given	72
(green black)	Fmmm	10.8196(7)				2.176(5) × 2			
	4	10.6113(7)				2.166(5) × 2			
				CuN_6	N	2.063(4) × 2		not given	
						2.169(5) × 2			
						2.179(5) × 2			
$Tl_2Pb[Cu(NO_2)_6]$	c	10.7344(5)		CuN_6	N	2.118(6) × 6		not given	73
(green black)	Fm3								
	4								
$K_2Ba[Cu(NO_2)_6]$	or	11.219(2)		CuN_6	N	2.038(2) × 2		not given	74
(not given)	Fmmm	10.728(2)				2.048(2) × 2			
	4	10.685(1)				2.311(2) × 2			
$K_2Sr[Cu(NO_2)_6]$	or	10.4301(7)		CuN_6	N	2.029(2) × 2		not given	75
(green)	Fmmm	10.4621(7)				2.041(2) × 2			
	4	10.9368(9)				2.310(2) × 2			
$[Cu(4\text{-}Mepy)_4(NCS)_2]\cdot$	trg	27.356(7)		CuN_6	SCN_{eq}	1.975(7) × 2	N_{eq},N_{eq}	90.0(2)	76
$0.67(4\text{-}Mepy)\cdot 0.33H_2O$	R-3				pyN_{eq}	2.060(5) × 2	N_{eq},N_{ax}	90.3(2, 2)	
(green)	9	11.303(9)			pyN_{ax}	2.503(6) × 2			
$Cu(abst)_2(NH_3)_2$	tr	8.693(7)	79.86(5)	CuN_6	H_3N_{eq}	2.019(6) × 2	N_{eq},N_{eq}	91.2(2)	77
(dark green)	P-1	9.980(14)	118.77(7)		N_{eq}	2.060(4) × 2			
	1	9.980(14)	74.34(5)		N_{ax}	2.479(6) × 2			
$Cu(phen)_2(NCS)_2$	or	13.029(21)		CuN_6	SCN_{eq}	2.013(10) × 2	N_{eq},N_{eq}	91.7(7, 1.0)	78
(green)	Pbcn	9.900(15)			N_{eq}	2.195(9) × 2		169.3(4)	
	4	17.256(23)			N_{ax}	2.125(10) × 2	N_{eq},N_{ax}	89.3(6)	
$Cu(phen)_2(NCS)_2$	or	13.250(36)		CuN_6	SCN	2.014(14) × 2	N,N	78.0(6)[e]	79
(green)	Pbcn	10.020(6)			phenN	2.150(14) × 2		92.4(6, 6.9)	
	4	17.432(10)				2.255(14) × 2		167.0(6, 2.3)	

$Cu(phen)_2(NCSe)_2$ (green)	or Pbcn 4	13.213(7) 10.077(3) 17.725		CuN_6	SeCN phenN	2.042(13) × 2 2.127(11) × 2 2.183(11) × 2	N,N	77.2(4)[e] 92.6(5, 6.6) 167.0(5, 9)	79
$Cu(aepy)_2(NCS)_2$ (blue)	m $P2_1/c$ 2	8.398(5) 14.751(10) 7.834(4)	102.35(4)	CuN_6	N_{eq} SCN_{ax}	2.042(2, 20) 2.593(3) × 2	N_{eq},N_{eq} N_{eq},N_{ax}	86.9(1)[d] 82.6(1, 8)	80
$Cu(Me_2en)_2(NCS)_2$ (not given)	m $P2_1/c$ 2	6.566(1) 14.741(3) 8.582(3)	95.09(2)	CuN_6	N_{eq} SCN_{ax}	2.063(6, 1) 2.517(7) × 2	N_{eq},N_{eq} N_{eq},N_{ax}	85.0(2)[e] 85.6(2, 1.5)	81
$Cu(1,3\text{-}pn)_2(NO_2)_2$ (violet)	m $P2_1/c$ 2	6.088(4) 16.534(7) 6.943(5)	118.20(4)	CuN_6	N_{eq} O_2N_{ax}	2.038(6, 10) 2.655(8) × 2	N_{eq},N_{eq} N_{eq},N_{ax}	86.8(2)[d] 85.8(2, 3.0)	82a
$Cu(1,3\text{-}pn)_2(acts)_2$ (not given)	m $P2_1/n$ 2	9.336(3) 10.232(1) 14.138(3)	103.80(2)	CuN_6	pnN_{eq} $actsN_{ax}$	2.046(2, 2) 2.457(2) × 2	N_{eq},N_{eq} N_{eq},N_{ax}	87.8(1, 0)[d] 90.4(1, 4)	82b
$Cu(abpt)_2(tcnq)_2$ (black)	tr P-1 1	9.194(1) 9.761(2) 12.235(2)	68.29(1) 86.72(1) 81.80(1)	CuN_6	N_{eq} $tenqN_{ax}$	2.017(5, 30) 2.442(5) × 2	N_{eq},N_{eq} N_{eq},N_{ax} N_{ax},N_{ax}	80.5(2)[c] 99.5(2) 90.0(2, 1.1) 180	83
$[Cu\{N(py)_3\}_2(MeCN)_2]\cdot$ $(SO_3CF_3)_2$ (dark green)	m $P2_1/n$ 2	11.825(2) 14.774(3) 11.516(2)	97.699(4)	CuN_6	N_{eq} $MeCN_{ax}$	2.020(4, 2) 2.526(8) × 2	N_{eq},N_{eq} N_{eq},N_{ax}	86.3(2)[e] 86.0(2, 1.0)	84
$[Cu(en)_3]SO_4$ (purple)	trg P31c 2	8.966(1) 9.597(1)		CuN_6	N	2.150(2) × 6	N,N	80.9[e] 93.5(–, 7)	85
$[Cu(en)_3]SO_4$ (blue) (at 120 K)	tr P-1 2	8.814(3) 8.896(3) 9.588(3)	90.34(4) 89.37(4) 119.80(4)	CuN_6	N_{eq}	2.055(1, 5) 2.215(1, 15)	N_{eq},N_{eq} N_{ax},N_{ax}	81.3(5, 1.5) 91.60(6, 7.0) 171.5(7, 1.7)	86
$[Cu(en)_3]Cl_2\cdot 0.75en$[g] (blue)	m C2/c 16	33.774(6) 8.756(2) 23.972(5)	99.96(4)	CuN_6	N	2.14(2, 9) 2.21(1, 3)	N,N	82.6(6)[e] 79.6(7, 2)[e] 171.06(6)	86
				CuN_6	N	2.04(3, 13) 2.41(3, 8)	N,N	76.9(11, –)[e] 91.6(9, 6.0)	
				CuN_6	N	2.10(4, 14) 2.27(4, 3)	N,N	90.0(9, 7.0) 164.5(15)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
$[Cu(1,2\text{-}pn)_3]Br_2 \cdot 2H_2O$ (not given)	m $P2_1$ 2	10.71 8.93 10.88	107.2	CuN_6	N	2.09 × 4 2.31 × 2		not given	87
$[Cu(bpy)_3](ClO_4)_2$ (dark blue)	tr P-1 2	12.673(17) 18.440(21) 7.937(7)	90.37(14) 120.56(13) 98.80(11)	CuN_6	N_{eq} N_{ax}	2.031(8, 5) 2.226(7) 2.450(7)	N_{eq},N_{eq} N_{eq},N_{ax} N_{ax},N_{ax}	80.4(3)[e] 93.3(3, 1.7) 76.1(3, 2.2)[e] 94.7(3, 11.1) 174.8(2)	88
$[Cu(phen)_3](ClO_4)_2$ (dark blue)	m C2/c 8	35.98(5) 15.97(3) 12.20(3)	101.7(3)	CuN_6	N_{eq} N_{ax}	2.037(14, 34) 2.328(11, 7)	N_{eq},N_{eq} N_{eq},N_{ax} N_{ax},N_{ax}	81.6(5)[e] 93.5(6, 2.3) 76.9(5, 3)[e] 94.3(5, 9.9) 179.2(5)	89
$[Cu(phen)_3](ClO_4)_2$ (not given)	m C2/c 8	35.98(5) 15.97(3) 12.20(3)	101.7(3)	CuN_6		not given			90
$[Cu(phen)_3](ClO_4)_2$ (not given)	m $P2_1/c$ 4	9.41(2) 30.11(6) 13.08(3)	111.7(2)	CuN_6		not given			90
$[Cu(phen)_3](tcnq)_2 \cdot 0.5MeOH$ (dark brown)	tr P-1 2	21.945(5) 11.106(3) 10.186(3)	86.50(5) 84.41(6) 83.21(4)	CuN_6	N	2.05(1, 1) 2.12(1, 1) 2.23(1, 4)	N,N	78.0(4, 2)[e] 94.5(4, 6.6) 165.7(4, 2.0)	91
$[Cu(mep)_3](PF_6)_2$ (green)	m Cc; C2/c 4	19.950(4) 20.421(5) 12.066(3)	115.90(4)	CuN_6	N_{eq} N_{ax}	2.040(9, 57) 2.432(4)	N_{eq},N_{eq} N_{eq},N_{ax}	104.5(3) 80.8(3)[e] 72.6(1)[e] 85.5(3)[e] 93.6(3)	92
$[Cu(dien)_2](NO_3)_2$ (royal blue)	or $P2_12_12_1$ 4	9.274(16) 12.192(26) 15.029(36)		CuN_6	N_{eq} N_{ax}	2.219(23, 49) 2.010(11, 8)	N_{eq},N_{eq} N_{eq},N_{ax} N_{ax},N_{ax}	91.5(5, 6.1) 81.1(5, 2.3)[e] 99.0(5, 4.7) 178.0(4)	93

$[Cu(dien)_2](NO_3)_2$ (not given)	or $P2_12_12_1$ 4	9.306(2) 12.248(3) 15.047(3)		CuN_6	N_{eq} N_{ax}	2.221(6, 66) 2.023(4, 1)		not given	94
(at 150 K)	or $P2_12_12_1$ 4	9.274(3) 12.192(15) 15.029(18)		CuN_6	N_{eq} N_{ax}	2.192(3, 52) 2.022(1, 2)		not given	94
$[Cu(dien)_2]Cl_2{\cdot}H_2O$ (not given)	m $P2_1/c$ 4	13.62(5) 8.80(5) 13.96(5)	102.7(5)	CuN_6	N_{eq} N_{ax}	2.419(7, 47) 2.065(8, 47)	N_{eq},N_{eq} N_{eq},N_{ax} N_{ax},N_{ax}	83.3(3, 2) 78.7(3, 5)[e] 156.5(3)	95
$[Cu(dien)_2]Cl(ClO_4)$ (not given)	m $P2_1/c$ 4	9.23(5) 13.92(5) 14.65(5)	116.0(5)	CuN_6	N_{eq} N_{ax}	2.451(14, 65) 2.047(13, 42)	N_{eq},N_{eq} N_{eq},N_{ax} N_{ax},N_{ax}	82.8(6, 8) 78.7(6, 9)[e] 155.3(5)	95
$[Cu(terpy)_2](NO_3)_2$ (dark green)	tg $I4_1/a$ 8	12.476(6) 36.284(13)		CuN_6	N	1.989(5, 24) 2.085(4) × 2 2.288(4) × 2	N,N	77.4(6, 1.5)[e] 92.8(6, 2.9) 154.7(6, 2.9) 180	96
$[Cu(terpy)_2]Br_2{\cdot}3H_2O$ (dark green)	tr P-1 2	19.763(4) 9.563(2) 8.537(1)	95.96(1) 93.48(1) 94.44(1)	CuN_6	N	1.970(9, 15) 2.147(9, 3) 2.203(9, 2)	N,N	78.0(9, 9)[e]	97
$[Cu(terpy)_2](PF_6)_2$ (green)	tg $P\text{-}42_1c$ 2	8.930(3) 20.623		CuN_6	N	1.977(8) × 2 2.179(7) × 4	N,N	76.9(–, 2)[e]	98
$[Cu(9\text{-}aneN_3)_2](ClO_4)_2{\cdot}2H_2O$ (blue)	m $P2_1/a$ 4	9.533(3) 16.909(8) 13.653(9)	89.22(3)	CuN_6	N	2.087(6) × 2 2.176(6) × 2 2.233(7) × 2	N,N	81.0(2, 8)[e]	99
$[Cu(taci)_2]Br_2{\cdot}4H_2O$ (not given)	or Cmcm 4	9.391(6) 11.475(7) 21.924(12)		CuN_6	N	2.086(4) × 2 2.322(6) × 2	N,N	85.7(2)[e] 91.4(2, 2.9) 180.0(1)	100
$[Cu(bpca)_2]{\cdot}H_2O$ (green)	m $P2_1/c$ 4	8.917(1) 8.932(1) 28.794(17)	95.49(2)	CuN_6	N	1.979(3, 19) 2.091(3, 7) 2.299(3, 6)	N,N	78.9(1, 2.0)[e] 95.2(1, 11.6) 163.2(1.1, 1.7)	101
$[Cu(metri)_2](BF_4)_2$ (orange)	c Pa3 4	16.621(5)		CuN_6	N	2.100(7) × 6	N,N	82.9(3)[e] 97.1(3)	102
(at 105 K)	c Pa3 4	16.445(5)		CuN_6	N	2.058(6) × 6	N,N	82.8(3)[e] 97.2(3)	102

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	*α* [°] *β* [°] *γ* [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
Cu{HB(pz)$_3$}$_2$	tr	10.309(2)	127.39(2)	CuN$_6$	N	1.998(2) × 2	N,N	81.9(1)^e	103
(not given)	P-1	13.794(3)	88.46(2)			2.082(2) × 2		87.3(1, 7)	
	2	11.677(3)	116.63(2)			2.356(4) × 2			
Cu{HB(3, 5-Me$_2$pz)$_3$}$_2$	tr	10.201(1)	83.68(1)	CuN$_6$	N	2.028(6, 15)	N,N	86.9(2, 1.7)^d	104
(blue green)	P-1	10.875(1)	101.62(1)			2.137(6, 4)			
	1	8.787(1)	117.59(1)			2.288(7, 36)			
[Cu(tach)$_2$](NO$_3$)$_2$	m	18.496(4)		CuN$_6$	N	2.169(6, 5)	N,N	87.7(1, 2.0)^d	105
(not given)	C2/m	7.289(2)	110.22(2)						
	2	7.201(2)							
[Cu(tach)$_2$](ClO$_4$)$_2$	or	9.68(1)		CuN$_6$	N	2.070(6, 9)	N,N	85.4(2, 1.4)^d	105
(not given)	Cmca	18.00(2)				2.353(7) × 2		90.3(2)	
	4	12.14(1)							
[Cu{(pz)$_2$(py)CH}$_2$](NO$_3$)$_2$	m	10.207(3)		CuN$_6$	N	1.994(3) × 2	N,N	81.8(1)	106
(blue)	P2$_1$/c	7.756(2)	113.28(3)			2.020(3) × 2		86.8(1, 1)	
	2	18.806(11)				2.385(4) × 2			
[Cu{NH(CH$_2$C$_7$H$_5$N$_2$)$_2$}$_2$](ClO$_4$)$_2$·	tr	9.576(3)	83.31(3)	CuN$_6$		not given			107
2H$_2$O·2MeOH	P-1	10.123(3)	80.93(3)						
(blue)	1	11.628(5)	87.25(2)						
[Cu(pcam)(pytrz)](CF$_3$SO$_3$)	tr	9.177(3)	102.65(2)	CuN$_6$	pcamN$_{eq}$	2.019(8, 63)	N$_{eq}$,N$_{eq}$	81.4(3, 1)^e	108
(green)	P-1	10.735(3)	106.60(2)		pytrzN$_{eq}$	2.052(7)		98.6(3, 2)	
	2	18.231(4)	93.89(3)		pytrzN$_{ax}$	2.374(10, 5)		179.6(2)	
							N$_{eq}$,N$_{ax}$	74.0(3, 4)^e	
								92.4(3, 1.8)	
								106.0(3, 2)	
							N$_{ax}$,N$_{ax}$	147.9(2)	
Cu(debd)(NCS)$_2$	tg	9.614(5)		CuN$_6$	N	2.191(4) × 2	N,N	78.7(2, 1.9)^e	109
(not given)	P4$_1$2$_1$2					2.193(4) × 2		94.2(2, 5.2)	
	4	24.854(8)			SCN	2.034(4) × 2		171.0(2, 2.9)	
(at 140 K)	tg	9.677(4)		CuN$_6$	N	2.242(4) × 2	N,N	78.5(1, 1.4)^e	
	P4$_1$2$_1$2					2.099(4) × 2		94.3(1, 5.4)	
	4	24.422(4)			SCN	2.060(4) × 2		170.5(1, 2.7)	

[Cu(edtb)]BF_4(BF_3OEt)·H_2O (blue)	m C2/c 4	14.402(2) 14.953(2) 18.846(2)	101.17(1)	CuN_6	N	1.986(7) × 2 2.039(8) × 2 2.499(8) × 2	N,N	73.8(3, 3.7)[e] 91.9(3, 1.4) 142.8(3, 2) 165.9(5)	110
[Cu($C_{22}H_{34}N_6$)][$CuCl_4$]·$2H_2O$ (green)	m $P2_1/c$ 4	15.467(4) 11.287(9) 17.459(5)	106.45(2)	CuN_6	N_{eq} N_{ax}	2.264(5, 50) 1.985(5, 2)	N,N	77.8(2, 3)[e] 155.4(2, 3) 178.2(2)	111
[Cu(ttcn)$_2$](BF_4)$_2$ (dark brown)	or Pbca 4	21.169(3) 15.193(2) 8.729(2)		CuS_6	S	2.435(3, 16)	S,S	87.8(2, 6)[e] 92.2(2, 6)	112
[Cu(ttcn)$_2$](BF_4)$_2$(MeCN)$_2$[c] (brown) (at 117 K)	m $P2_1/c$ 4	20.695(2) 14.944(1) 8.864(1)	90.797(8)	CuS_6	S	2.429(1, 30)	S,S	88.1(1, 2)[d] 91.9(1, 2) 179.9(1, 1)	113
				CuS_6	S	2.432(1, 27)	S,S	88.3(1, 4)[d] 91.7(1, 4) 179.9(1, 1)	
[Cu(ttcn)$_2$](BF_4)$_2$($MeNO_2$)$_2$ (brown)	or Pbca 4	19.746(2) 15.442(2) 9.227(1)		CuS_6	S	2.343(2) × 2 2.487(2) × 2 2.504(2) × 2	S,S	87.8(1, 8) 92.2(1, 8) 180.0	113
[Cu(H_2O)$_5$(bim)](5′-imp)·$3H_2O$ (light blue)	m $P2_1$ 2	7.013(2) 13.179(9) 14.565(9)	94.82(4)	CuO_5N	H_2O_{eq} N_{eq} H_2O_{ax}	2.017(5, 62) 1.947(5) 2.194(6) 2.732(6)	O_{eq},N_{eq} O_{eq},O_{ax} O_{ax},O_{ax}	89.8(2, 3.9) 90.0(2, 12.2) 172.6(2)	114
[Cu(9-Meade)(H_2O)$_4$(SO_4)]·H_2O (turquoise)	tr P-1 2	14.079(2) 7.150(3) 7.853(2)	100.52(2) 75.87(2) 107.98(2)	CuO_5N	H_2O_{eq} N_{eq} H_2O_{ax} O_3SO_{ax}	1.968(2, 33) 1.995(2) 2.355(2) 2.551(2)	O_{eq},O_{eq} O_{eq},N_{eq} O_{eq},O_{ax} N_{eq},O_{ax} O_{ax},O_{ax}	89.19(5, 14.5) 91.13(5, 1.05) 87.16(5, 9.53) 98.25(5, 5.40) 162.94(5)	115
Cu{Mephim(ac)$_2$}(H_2O)$_2$ (blue green)	m $P2_1/c$ 4	11.452(2) 7.595(2) 15.416(2)	101.60(1)	CuO_5N	H_2O_{eq} O_{eq} N_{eq} O_{ax} H_2O_{ax}	1.962(4) 1.935(4, 3) 2.049(5) 2.337(5) 2.424(4)	O_{eq},O_{eq} O_{eq},N_{eq} O_{eq},O_{ax} O_{ax},O_{ax}	95.9(2, 1.9) 77.5(3) 84.2(2, 8) 90.2(2, 4.3) 172.4(3)	116
Cu(F_6acac)$_2$(tmpCN)·H_2O (green yellow)	tr P-1 2	11.835(2) 11.942(2) 11.988(2)	111.21(1) 95.31(1) 118.65(1)	CuO_5N	O_{eq} CN_{ax} H_2O_{ax}	1.951(3, 6) 2.616(5) 2.255(4)	O_{eq},O_{eq}	92.57(11, 5)[d] 87.19(8, 27) 175.37(10)	117

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
							O_{eq},N_{ax}	87.32(11, 3.90)	
							N_{ax},O_{ax}	174.84(11)	
$Cu(evda)(H_2O)_2$	m	7.50(1)		CuO_5N	O_{eq}	1.95(1, 1)	O_{eq},O_{eq}	94.9(5, 4)	118
(bright blue)	$P2_1/n$	28.60(1)	91.27(1)		N_{eq}	2.04(1)	O_{eq},N_{eq}	85.3(5, 1)[e]	
	4	7.50(1)			H_2O_{eq}	1.95(1)		162.9(5)	
					O_{ax}	2.84(2)	O_{eq},O_{ax}	90.4(5, 8.7)	
					H_2O_{ax}	2.32(1)	N_{eq},O_{ax}	88.8(5, 9.3)	
							O_{ax},O_{ax}	177.5(4)	
$Cu(idac)(H_2O)_2$	or	10.56(3)		CuO_5N	H_2O_{eq}	2.00(2)		not given	119
(not given)	Pbca	13.68(3)			O_{eq}	2.00(2, 1)			
	8	10.28(3)			N_{eq}	2.07(2)			
					O_{ax}	2.50(2)			
					H_2O_{ax}	2.50(2)			
$Cu(F_6acac)_2(tmpCN)H_2O$	tr	11.835(2)	111.21(1)	CuO_5N	O_{eq}	1.951(3, 6)	O_{eq},O_{eq}	89.9(1, 32)[d]	120
(green yellow)	P-1	11.942(2)	95.31(1)		H_2O_{ax}	2.255(4)		174.6(1, 8)	
	2	11.988(2)	118.65(1)		CN_{ax}	2.616(5)	O_{eq},O_{ax}	93.1(9, 1.2)	
							O_{eq},N_{ax}	91.2(1)	
							O_{ax},O_{ax}	174.8(1)	
$[Cu(phen)_2(im)(PF_6)]\cdot PF_6$	m	16.866(5)		CuN_5F	imN_{eq}	1.982(5)	N_{eq},N_{eq}	81.9(2)[e]	121
(not given)	P2/c	14.913(3)	105.86(2)		N_{eq}	2.028(6, 15)		92.5(2, 6)	
	4	12.417(3)			N_{ax}	2.219(7)	N_{eq},N_{ax}	79.1(3)[e]	
					F_{ax}	2.782(6)		99.2(2, 8.1)	
$[Cu(mbpy)_2(ClO_4)]\cdot H_2O$	m	8.4824(22)		CuN_5O	N_{eq}	1.966(5, 8)	N_{eq},N_{eq}	100.4(8, 1.3)	122
(light green)	$P2_1/c$	29.1965(29)	95.836(17)			2.023(5, 19)	N_{eq},N_{ax}	80.0(7, 7)[e]	
	4	16.7393(24)			N_{ax}	2.510(5)	N_{eq},O_{ax}	91.5(2, 8.9)	
					O_3ClO_{ax}	2.698(7)	N_{ax},O_{ax}	165.8(2)	
$(NH_4)_2[CuF_4(H_2O)_2]$	m	10.463(3)		CuF_4O_2	F_{eq}	1.918(3, 1)	F_{eq},F_{ax}	90.99(6)	123
(blue)	C2/c	9.245(2)	108.61(2)		H_2O_{eq}	1.982(2) × 2	F_{eq},O_{eq}	88.68(8)	
	4	7.368(2)			F_{ax}	2.260(2) × 2	F_{ax},O_{eq}	88.47(9)	
							F_{ax},F_{ax}	178.0(1)	
							O_{eq},O_{eq}	177.4(2)	

$Cu(H_2O)_4SiF_6$	m	5.346(2)		CuO_4F_2	H_2O_{eq}	1.957(2, 3)	O_{eq},O_{eq}	88.79(6)	124
(dark blue)	$P2_1/b$	7.221(2)			F_{ax}	2.333(1) × 2	O_{eq},F_{ax}	88.26(5, 82)	
	2	9.618(3)	105.21(1)						
$[Cu(H_2O)_4(9\text{-Meade})_2]Cl_2\cdot 2H_2O$	m	15.482(7)		CuO_4N_2	H_2O_{eq}	2.162(2) × 4	O_{eq},O_{eq}	90.6(2, 0)	125
(green)	C2/m; C2	6.894(10)	114.42(3)		N_{ax}	2.008(2) × 2	O_{eq},N_{eq}	90.7(2, 0)	
	2	11.269(5)							
$[Cu(H_2O)_4(opca)_2](NO_3)_2$	tr	8.197(6)	116.90(5)	CuO_4N_2	H_2O_{eq}	2.131(10, 81)	O_{eq},O_{eq}	159.9(4)	126
(not given)	P-1	10.107(5)	87.56(4)		N_{eq}	1.923(6)	N_{eq},O_{eq}	89.6(4, 9.2)	
	2	15.534(4)	101.30(6)		H_2O_{ax}	2.403(11)	N_{eq},N_{eq}	172.0(3)	
					N_{ax}	2.243(6)	O_{eq},O_{ax}	89.7(4, 13.0)	
							N_{eq},O_{ax}	89.8(5, 9.0)	
							O_{ax},O_{ax}	170.5(3)	
$[Cu(H_2O)_4(hmnc)_2](NO_3)_2$	tr	8.154(1)	101.31(1)	CuO_4N_2	N_{eq}	2.031(7) × 2	N_{eq},O_{eq}	90.6(3)	127
(light blue)	P-1	8.575(1)	104.67(1)		H_2O_{eq}	2.120(7) × 2	N_{eq},O_{ax}	90.9(3)	
	1	8.761(1)	115.53(1)		H_2O_{ax}	2.193(7) × 2	O_{eq},O_{ax}	91.5(3)	
$[Cu(H_2O)_4(sach)_2]\cdot 2H_2O$	m	8.384(2)		CuO_4N_2	N_{eq}	2.061(2) × 2	O_{eq},N_{eq}	90.2(1)	128
(not given)	$P2_1/c$	16.327(2)	101.08(2)		H_2O_{eq}	1.956(2) × 2	O_{eq},O_{ax}	94.0(1)	
	2	7.327(2)			H_2O_{ax}	2.489(2) × 2	N_{eq},O_{ax}	90.3(1)	
$Cu(H_2O)_4(mtpo)_2$	m	9.497(3)		CuO_4N_2	H_2O_{eq}	2.066(2) × 2	O_{eq},N_{eq}	90.5(7, 1.3)	129
(light green)	$P2_1/c$	13.748(2)	110.34(2)		N_{eq}	1.962(2) × 2	O_{eq},N_{ax}	90.0(8, 5.3)	
	2	6.850(4)			H_2O_{ax}	2.391(2) × 2	N_{eq},O_{ax}	90.0(7, 1.6)	
$Ca[Cu(H_2O)_4(5'\text{-imp})_2]\cdot 6.7H_2O$	or	not given		CuO_4N_2	N_{eq}	2.04(1) × 2	N_{eq},N_{eq}	88.1(6)	130
(not given)	$C222_1$				H_2O_{eq}	1.97(1) × 2	N_{eq},O_{eq}	89.6(6)	
	4				H_2O_{ax}	2.52(1) × 2		177.3(6)	
							O_{eq},O_{eq}	88.8(7, 4.0)	
							N_{eq},O_{ax}	95.1(6, 1.0)	
							O_{eq},O_{ax}	85.4(7)	
							O_{ax},O_{ax}	165.7(7)	
$[Cu(H_2O)_4(9\text{-Mehpx})_2]SO_4$	m	8.709(3)		CuO_4N_2	N_{eq}	2.026(2, 4)		not given	131
(not given)	$P2_1/c$	13.348(3)	105.44(2)		H_2O_{eq}	1.953(2, 6)			
	4	16.778(1)			H_2O_{ax}	2.409(2, 4)			
$[Cu(H_2O)_4(8\text{-aad})_2](NO_3)_2$	m	7.582(2)		CuO_4N_2	H_2O_{eq}	1.961(2) × 2	O_{eq},N_{eq}	88.8(1)	132
(not given)	$P2_1/n$	11.538(2)	95.02(2)		N_{eq}	1.961(2) × 2	O_{eq},O_{ax}	89.9(1)	
	2	10.773(1)			H_2O_{ax}	2.624(2) × 2	N_{eq},O_{ax}	89.0(1)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
$[Cu(H_2O)_4(1\text{-}CNgud)_2](NO_3)_2$	tr	3.508(2)	102.45(3)	CuO_4N_2	H_2O_{eq}	1.96 × 2		not given	133
(not given)	P-1	10.201(3)	101.58(3)		N_{eq}	1.92 × 2			
	1	11.927(3)	101.60(3)						
$[Cu(H_2O)_4(hpca)_2](NO_3)_2$	tr	8.197(6)	116.90(5)	CuO_4N_2	H_2O_{eq}	2.246(11, 15)		not given	134
(not given)	P-1	10.107(5)	87.56(4)			2.060(8)			
	2	15.534(4)	101.30(6)		N_{ax}	1.923(6)			
						2.243(6)			
$[Cu(H_2O)_4(py)_2](cas)\cdot 10H_2O$	tr	15.438(4)	112.74(4)	CuO_4N_2	H_2O_{eq}	2.11(2, 1)		not given	135
(blue green)	P-1	15.727(6)	102.02(4)		N_{eq}	2.00(1, 1)			
	2	12.121(9)	85.35(4)		H_2O_{ax}	2.35(2, 1)			
$Cu(py)_4(bzs)_2$	m	15.180(6)		CuO_4N_2	pyN_{eq}	2.013(9, 7)	N_{eq},N_{eq}	90.0(2, 2)	136
(not given)	C2/c	14.431(5)	96.38(4)		O_{ax}	2.471(8) × 2	O_{ax},N_{eq}	90.3(3, 2.6)	
	4	15.269(6)							
$[Cu(py)_4(F_3ac)_2]\cdot[Cu(py)_2(F_3ac)_2]^c$	m	10.451(5)		CuO_4N_2	O_{eq}	2.067(5)	O_{eq},O_{ax}	87.8(2)	137
(not given)	P2/c	14.596(6)	98.81(13)		pyN_{eq}	2.075(10, 23)			
	4	17.881(4)			O_{ax}	2.143(6)			
				CuN_4O_2	pyN_{eq}	2.049(11, 7)		not given	
					O_{ax}	2.343(6) × 2			
$Cu(H_2O)_2(py)_2(act\text{-}DL)_2$	m	9.377(6)		CuO_4N_2	O_{eq}	2.02(1) × 2	O_{eq},N_{eq}	87.9(6)	138
(blue)	$P2_1/c$	19.341(14)	123.2(2)		pyN_{eq}	1.95(1) × 2			
	2	11.615(7)			H_2O_{ax}	2.61(1) × 2			
$Cu(H_2O)_2(py)_2(fm)_2$	m	16.493(1)		CuO_4N_2	O_{eq}	1.977 × 2		not given	139
(blue)	C2/c; Cc	6.320(2)	113.11(1)		N_{eq}	2.017 × 2			
	4	15.184(1)			H_2O_{ax}	2.455 × 2			
$Cu(H_2O)_2(py)_2(inco)_2$	tr	7.036(5)	110.05(3)	CuO_4N_2	O_{eq}	1.973(1) × 2	O_{eq},N_{eq}	90.00(3, 1.4)	140
(blue)	P-1	9.640(3)	70.95(3)		N_{eq}	2.006(1) × 2	N_{eq},O_{ax}	90.00(2, 2.4)	
	1	9.752(4)	104.28(5)		N_{ax}	2.509(1) × 2	O_{eq},O_{ax}	90.00(3, 1.3)	
$Cu(H_2O)_2(py)_2(psac)_2$	m	23.58(1)		CuO_4N_2	O_{eq}	1.99(2, 2)	O_{eq},O_{eq}	179.2(7)	189
(blue)	C2	7.747(3)	107.05(3)		pyN_{eq}	2.02(2, 3)	N_{eq},N_{eq}	90.0(7, 1.9)	
	4	16.082(8)			H_2O_{ax}	2.55(2, 4)	O_{eq},O_{ax}	90.0(7, 3.6)	

							O_{ax},O_{ax}	177.8(6)	
							N_{eq},O_{ax}	90.0(7, 5.2)	
							N_{eq},N_{eq}	178.9(8)	
$Cu(H_2O)_2(ac)_2(ainc)_2$	m	7.782(4)		CuO_4N_2	O_{eq}	1.944(5) × 2	N_{eq},O_{eq}	88.4(2)	141
(not given)	$P2_1/n$	11.137(9)	97.67(4)		N_{eq}	2.046(5) × 2	O_{eq},O_{ax}	95.3(2)	
	2	11.324(4)			H_2O_{ax}	2.594(5) × 2	N_{eq},O_{ax}	91.5(2)	
$Cu(H_2O)_2(iqu)_2(ClO_4)_2$	tr	7.487(2)	100.82(2)	CuO_4N_2	N_{eq}	1.999(2) × 2	N_{eq},O_{eq}	89.8(1)	142
(bright green)	P-1	7.621(2)	108.33(3)		H_2O_{eq}	1.999(1) × 2	O_{eq},O_{ax}	84.0(1)	
	1	10.271(4)	99.03(2)		O_3ClO_{ax}	2.461(2) × 2	N_{eq},O_{ax}	87.5(1)	
$Cu(H_2O)_2(inc)_2(fm)_2$	m	7.349(4)		CuO_4N_2	N_{eq}	2.035(7) × 2	O_{eq},N_{eq}	87.8(3)	143
(dark blue)	$P2_1/a$	14.40(1)	104.62(5)		O_{eq}	1.978(6) × 2	O_{eq},O_{ax}	88.4(3)	
	2	8.738(5)			H_2O_{ax}	2.458(6) × 2	N_{eq},O_{ax}	93.5(3)	
$[Cu(H_2O)_2(fm)_2(nc)_2]\cdot 2H_2O$	m	14.417(8)		CuO_4N_2	O_{eq}	1.981(2) × 2	O_{eq},N_{eq}	90.1(3)	144
(dark blue)	C2/c	9.856(6)	109.25(5)		N_{eq}	2.019(3) × 2	O_{eq},O_{ax}	98.11(1)	
	4	15.089(9)			H_2O_{ax}	2.626(5) × 2	N_{eq},O_{ax}	86.4(1)	
$Cu(H_2O)_2(NO_3)_2(xan)_2$	tr	7.111(2)	108.63(1)	CuO_4N_2	H_2O_{eq}	1.938(1) × 2	O,O	90.0(1, 7)	145
(green)	P-1	7.528(1)	98.29(2)		N_{eq}	2.050(1) × 2	N,N	180	
	1	8.888(1)	102.39(2)		O_2NO_{ax}	2.540(1) × 2	O,N	90.0(1, 3.6)	
$[Cu(H_2O)_2(im)_2(ac\text{-DL-pgly})_2]$	tr	10.156(7)	84.45(3)	CuO_4N_2	imN_{eq}	1.989(3) × 2	O_{eq},N_{eq}	88.4(2)	146
(deep blue)	P-1	9.488(6)	93.39(3)		O_{eq}	1.956(3) × 2			
	1	8.452(3)	63.55(3)		H_2O_{ax}	2.912(5) × 2			
$Cu(9\text{-Mequa})_2\ (NO_3)_2(H_2O)_2$	m	5.4087(8)		CuO_4N_2	H_2O_{eq}	1.960(3) × 2	N_{eq},O_{eq}	87.57(2)	147
(not given)	$P2_1/c$	16.696(15)	109.874(15)		N_{eq}	2.004(3) × 2	N_{eq},O_{ax}	85.92(2)	
	2	11.8414(7)			O_2NO_{ax}	2.484(3) × 2	O_{eq},O_{ax}	89.97(2)	
$Cu(im)_2(mact)_2(ClO_4)_2$	m	7.720(2)		CuO_4N_2	imN_{eq}	1.97(6) × 2	N_{eq},O_{eq}	90.0(2, 1)	148
(blue)	$P2_1/c$	16.169(3)	96.08(1)		O_{eq}	1.982(5) × 2	N_{eq},N_{eq}	180.0(1)	
	2	8.742(2)			O_3ClO_{ax}	2.760(10) × 2	N_{eq},O_{ax}	89.2(4, 4.2)	
							O_{eq},O_{ax}	90.0(4, 9.0)	
$[Cu(H_2O)_3(bpy)(NO_3)]\cdot NO_3$	tr	9.52(1)	110.4(2)	CuO_4N_2	H_2O_{eq}	2.01(1) × 2	N_{eq},O_{ax}	91.0(4, 6.1)	149
(not given)	P-1	7.80(1)	124.3(2)		N_{eq}	2.01(1, 2)			
	2	13.62(2)	77.3(1)		H_2O_{ax}	2.36(1)			
					O_2NO_{ax}	2.70(1)			
$[Cu(F_3ac)_2(py)_2]\cdot[Cu(F_3ac)_2(py)_4]$[c]	m	10.451(5)		CuO_4N_2	acO_{eq}	2.067(5) × 2	O_{eq},N_{eq}	89.6(2, 5)	150
(not given)	P2/c	14.596(6)	98.81(13)		N_{eq}	2.075(10, 2.2)	O_{eq},O_{ax}	87.8(2)[d]	
	4	17.881(4)			acO_{ax}	2.143(6) × 2			

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
				CuN_4O_2	N_{eq}	2.049(11, 7)	N_{eq},N_{eq}	90.0(2, 6)	
					acO_{ax}	2.343(6) × 2	N_{eq},O_{ax}	90.5(3, 1.5)	
$Cu(bz)_2(4\text{-}Mepy)_2(H_2O)$	m	12.404(1)		CuO_4N_2	N_{eq}	2.039(–, 5)	O_{eq},O_{ax}	98.4(1, 1.3)	151
(not given)	$P2_1/c$	15.369(3)	108.88(1)		bzO_{eq}	1.960(–, 10)	O_{eq},N_{eq}	89.8(1, 1.8)	
	4	13.264(3)			H_2O_{ax}	2.291	N_{eq},O_{ax}	91.7(1, 3.0)	
					bzO_{ax}	2.780	O_{eq},O_{eq}	163.1(1)	
							N_{eq},N_{eq}	176.2(1)	
$Cu(pc)_2(H_2O)_2$	tr	7.64(1)	95.5(3)	CuO_4N_2	O_{eq}	1.935(9)	O_{eq},N_{eq}	83.5(3)[e]	152
(not given)	P-1	9.23(2)	108.7(3)		N_{eq}	1.974(12)	N_{eq},O_{ax}	88.8(3)	
	1	5.13(1)	74.9(3)		H_2O_{ax}	2.754(11)	O_{eq},O_{ax}	85.4(3)	
$Cu(ac)_2(3\text{-}Mepy)(H_2O)$	or	8.892(6)		CuO_4N_2	acO_{eq}	1.94(1) × 2	N_{eq},N_{eq}	175.3(6)	196
(not given)	$P2_12_12_1$	9.151(6)			pyN_{eq}	2.05(1)	N_{eq},O_{ax}	90.6(5, 2.7)	
	4	21.845(9)			H_2O_{ax}	2.34(1)	O_{eq},N_{eq}	89.8(5, 2.6)	
					acO_{ax}	2.64(1)	O_{eq},O_{ax}	54.0(4)[f]	
								90.0(5, 36.0)	
							O_{eq},O_{eq}	163.7(5)	
							O_{ax},O_{ax}	151.6(4)	
$[Cu(etam)_2(OH)_2]\cdot 2H_2O$	m	8.90(4)		CuO_4N_2	O_{eq}	1.91(50) × 2	O_{eq},N_{eq}	90.0(2.5,7)	153
(blue)	$P2_1/c$	12.33(5)	100.0(5)		N_{eq}	2.06(50) × 2	O_{eq},O_{ax}	90.2(2.5,1)	
	2	7.15(3)			HO_{ax}	2.37(50) × 2	N_{eq},O_{ax}	90.0(2.5,6.8)[e]	
$Cu(dmco)_2(H_2O)_2$	m	11.32(2)		CuO_4N_2	O_{eq}	1.962(15) × 2	N_{eq},O_{eq}	83.86(72)[e]	154
(not given)	$P2_1/c$	7.17(2)	100(1)		N_{eq}	2.013(14) × 2	O_{eq},O_{ax}	95.46(59)	
	2	10.62(2)			H_2O_{ax}	2.542(20) × 2	N_{eq},O_{ax}	98.75(69)	
$Cu(2\text{-}pyc)_2(H_2O)_2$	tr	5.122	101.07	CuO_4N_2	O_{eq}	1.940(2) × 2	N_{eq},O_{eq}	83.6(1)[e]	155
(not given)	P-1	7.717	95.60		N_{eq}	1.963(2) × 2	O_{eq},O_{ax}	85.1(1)	
	1	9.216	110.45		H_2O_{ax}	2.752(2) × 2	N_{eq},O_{ax}	89.5(1)	
$\alpha\text{-}Cu(pipc)_2(H_2O)_2$	m	11.723(4)		CuO_4N_2	O_{eq}	1.989(2) × 2	O_{eq},N_{eq}	83.1(1)[e]	156
(light blue)	$P2_1/c$	5.749(3)	104.11(3)		N_{eq}	2.022(3) × 2	O_{eq},O_{ax}	90.4(1)	
	2	11.174(3)			H_2O_{ax}	2.401(3) × 2	N_{eq},O_{ax}	90.6(1)	

β-$Cu(pipc)_2(H_2O)_2$	m	5.875(2)		CuO_4N_2	O_{eq}	1.966(2) × 2	N_{eq},O_{eq}	84.1(1)[e]	156
(dark blue)	$P2_1/n$	18.618(5)	106.40(3)		N_{eq}	2.002(2) × 2	O_{eq},O_{ax}	93.0(1)	
	2	7.014(2)			H_2O_{ax}	2.611(4) × 2	N_{eq},O_{ax}	90.5(1)	
$Cu(pzc)_2(H_2O)_2$	m	5.438(1)		CuO_4N_2	O_{eq}	1.98(1) × 2	O_{eq},N_{eq}	82.9(2)[e]	157
(blue)	$P2_1/c$	10.880(2)	98.24(1)		N_{eq}	2.00(1) × 2	N_{eq},O_{ax}	94.0(2)	
	2	10.385(2)			H_2O_{ax}	2.39(1) × 2	O_{eq},O_{ax}	86.9(2)	
$Cu(prol)_2(H_2O)_2$	m	5.62		CuO_4N_2	O_{eq}	2.03 × 2	N_{eq},O_{eq}	82[e]	158
(blue)	$P2_1/n$	17.85	108(−)		N_{eq}	1.99 × 2	O_{eq},O_{ax}	72	
	2	7.13			H_2O_{ax}	2.52 × 2	N_{eq},O_{ax}	93	
$Cu(mbpym)_2(H_2O)_2$	m	13.181(1)		CuO_4N_2	O_{eq}	2.045(3) × 2	N_{eq},O_{eq}	81.39(4)[e]	159
(dark green)	$P2_1/c$	8.973(1)	103.7(1)		N_{eq}	1.977(2) × 2	N_{eq},O_{ax}	91.07(16)	
	2	7.637(1)			H_2O_{ax}	2.285(3) × 2	O_{eq},O_{ax}	90.54(2)	
$Cu(bz\text{-}L\text{-}val)_2(H_2O)_2$	tr	9.827(5)	102.80(5)	CuO_4N_2	O_{eq}	1.94(1) × 2	O,N	85.2(7)[e]	160
(blue)	P-1	11.435(5)	93.15(5)		N_{eq}	2.03(2) × 2		94.8(7)	
	1	5.975(3)	95.20(5)		H_2O_{ax}	2.82(1) × 2	O,O	180.0(7)	
$Cu(thc)_2(H_2O)_2$	tr	6.670(1)	95.83(1)	CuO_4N_2	O_{eq}	1.970(12, 9)	O_{eq},N_{eq}	85.2(5, 2)[e]	161
(not given)	P-1	9.404(1)	106.12(1)		N_{eq}	2.008(13, 8)		90.3(5, 5.6)	
	1	5.608(1)	97.15(1)		H_2O_{ax}	2.639(13)	O_{ax},N_{eq}	90.0(5, 6.0)	
						2.408(11)	O_{ax},O_{eq}	90.0(5, 8.6)	
							N_{eq},N_{eq}	170.2(6)	
							O_{eq},O_{eq}	169.4(4)	
							O_{ax},O_{ax}	178.4(5)	
$[Cu(tmic)_2(H_2O)_2]\cdot 2H_2O$	m	9.973(2)		CuO_4N_2	O_{eq}	2.02(1, 8)	O_{eq},N_{eq}	82.0(−, 4.1)[e]	162
(green)	$P2_1$	8.947(2)	111.10(2)		N_{eq}	2.05(1, 5)	O_{eq},O_{ax}	86.8(−, 3)	
	2	13.400(3)			H_2O_{ax}	2.31(1, 14)			
$[Cu(tdc)_2(H_2O)_2]\cdot 2H_2O$	tr	5.203(1)	77.99(2)	CuO_4N_2	O_{eq}	1.952(2) × 2	O_{eq},N_{eq}	89.3(1)[e]	163
(blue)	P-1	6.583(2)	98.92(2)		N_{eq}	1.994(1) × 2	O_{eq},O_{ax}	89.9(1)	
	1	11.835(2)	105.87(2)		H_2O_{ax}	2.490(2) × 2	N_{eq},O_{ax}	74.6(1)	
$[Cu(himp)_2(H_2O)_2]\cdot 2H_2O$	m	6.50(1)		CuO_4N_2	O_{eq}	1.92 × 2	N_{eq},O_{eq}	84.6[e]	164
(pale blue)	$P2_1/n$	1.975(2)	113.0(2)		N_{eq}	2.00 × 2	O_{eq},O_{ax}	92.0	
	2	7.26(1)			H_2O_{ax}	2.57 × 2	N_{eq},O_{ax}	86.0	
$[Cu(aoac)_2(H_2O)_2]\cdot 2H_2O$	or	5.2092(3)		CuO_4N_2	O_{eq}	1.967 × 2	N_{eq},O_{eq}	94.28[d]	165
(blue)	Pbca	18.8395(9)			N_{eq}	1.978 × 2	O_{eq},O_{ax}	95.35	
	4	11.1252(6)			H_2O_{ax}	2.545(1) × 2	N_{eq},O_{ax}	89.12	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
$[Cu(pcb)_2(H_2O)_2]\cdot 6H_2O$ (blue)	m $P2_1/n$ 2	6.849(4) 20.552(4) 7.291(4)	 108.79(5)	CuO_4N_2	O_{eq} N_{eq} H_2O_{ax}	1.974(3) × 2 1.980(4) × 2 2.580 × 2	O_{eq},N_{eq}	82.4(1)[e]	166
$[Cu(thp)_2(H_2O)_2]\cdot 6H_2O$ (dark green)	tr P-1 1	10.713(5) 7.321(4) 6.904(4)	107.66(5) 90.55(5) 95.85(5)	CuO_4N_2	O_{eq} N_{eq} H_2O_{ax}	1.959(1) × 2 1.965(1) × 2 2.630 × 2	N_{eq},O_{eq}	82.53(8)[e]	167
$[Cu(pybox)_2(H_2O)_2]Cl_2$ (blue)	m $P2_1/c$ 2	6.32(2) 10.34(1) 14.69(1)	 114.9(2)	CuO_4N_2	O_{eq} N_{eq} H_2O_{ax}	1.99(1) × 2 1.97(1) × 2 2.54(1) × 2	O_{eq},N_{eq} O_{eq},O_{ax} N_{eq},O_{ax}	79.5(3)[e] 89.2(3) 84.4(3)	168
$[Cu(hist)_2(H_2O)_2](NO_3)_2$ (blue violet)	tr P-1 1	5.4582(10) 7.1533(13) 13.8444(11)	98.617(16) 87.070(25) 109.830(6)	CuO_4N_2	O_{eq} N_{eq} H_2O_{ax}	1.958(7, 28) 1.987(7, 9) 2.461(7) 2.778(7)	N_{eq},O_{eq} O_{eq},O_{ax} N_{eq},O_{ax}	84.0(3)[e] 92.1(3, 1) 83.5(3, 3.5)	169
$[Cu(phenO)_2(H_2O)_2](NO_3)_2$ (not given)	m C2/c 4	15.724(2) 8.995(2) 18.432(3)	 112.06(2)	CuO_4N_2	O_{eq} N_{eq} H_2O_{ax}	1.935(3) × 2 2.016(3) × 2 2.462(3) × 2	N_{eq},O_{eq} N_{eq},O_{ax} O_{eq},O_{ax}	86.0(2)[d] 91.6(3) 89.4(3)	170
$[Cu(bzpy)_2(H_2O)_2](NO_3)_2$ (green)	m $P2_1/c$ 2	7.872(1) 14.573(3) 11.132(1)	 102.79(1)	CuO_4N_2	O_{eq} N_{eq} H_2O_{ax}	2.068(2) × 2 1.965(2) × 2 2.256(3) × 2	O_{eq},O_{ax} O_{eq},N_{eq} N_{eq},O_{ax}	90.0(1, 3.2) 90.0(1, 9.7)[e] 90.0(1, 9)	171
$[Cu(acatr)_2(H_2O)_2](SO_4)\cdot 5H_2O$ (blue)	m $P2_1/a$ 4	24.834(6) 8.796(4) 9.751(4)	 92.21(2)	CuO_4N_2	O_{eq} N_{eq} H_2O_{ax}	1.978(3, 10) 1.939(3, 6) 2.467(3, 67)	N_{eq},O_{eq} O_{eq},O_{eq} N_{eq},N_{eq} O_{eq},O_{ax} N_{eq},O_{ax} O_{ax},O_{ax}	88.8(1)[d] 89.8(1, 3.7) 175.0(1) 177.0(1) 90.1(1, 4.2) 90.0(1, 2.6) 175.3(1)	172
$[Cu(Meial)_2(H_2O)_2](ClO_4)_2\cdot 2H_2O$ (brown orange)	m $P2_1/c$ 4	8.439(8) 12.208(12) 15.37(2)	 111.08(5)	CuO_4N_2	H_2O_{eq} O_{eq} N_{ax}	1.926(2) × 2 2.040(2) × 2 2.414(2) × 2	O_{eq},O_{eq} O_{eq},N_{eq}	88.03(8) 80.63(8, 4.77)[e]	173

$[Cu(bpm)(ox)(H_2O)_2]\cdot 5H_2O$	or	6.554(2)		CuO_4N_2	bpmN_{eq}	2.189(6, 13)	O_{eq},O_{eq}	85.5(1)[e]	174
(blue)	$P2_12_12_1$	13.838(4)			oxO_{eq}	1.935(6, 1)	N_{eq},N_{eq}	81.5(3)[e]	
	4	19.319(7)			H_2O_{ax}	2.529(7, 26)	O_{eq},N_{eq}	96.5(3, 1.4)	
							O_{eq},O_{ax}	93.1(3, 4.7)	
							N_{eq},O_{ax}	87.1(3, 3.9)	
$Cu(Me_4en)(NO_2)_2$	m	7.570(2)		CuO_4N_2	N_{eq}	2.03(1, 1)	O_{eq},O_{eq}	89.0(6)	175
(green)	$P2_1/n$	12.506(2)	102.08		O_{eq}	2.02(1, 2)	O_{eq},O_{ax}	55.2(5, 1.0)[f]	
	4	12.500(4)			O_{ax}	2.44(1, 3)		86.4(5, 2)	
							O_{ax},O_{ax}	127.1(6)	
							N_{eq},O_{ax}	108.9(6, 4.5)	
							N_{eq},O_{eq}	93.4(6, 1.1)	
								167.2(5, 7)	
							N_{eq},N_{eq}	87.0(6)[e]	
$Cu(dmpz)_2(NO_3)_2$	tr	8.708(3)	88.02(3)	CuO_4N_2	N_{eq}	1.955(−, 5)	O_{eq},O_{ax}	55.6(4, 7)[f]	176
(not given)	P-1	13.481(4)	88.50(3)		O_{eq}	2.005(−, 5)		84.6(4, 2.0)	
	2	9.717(3)	100.39(3)		O_{ax}	2.46(−, 1)	O_{ax},O_{ax}	126.4(4)	
							O_{eq},O_{eq}	85.5(4)	
							N_{eq},O_{ax}	96.3(4)	
								118.6(4, 1.2)	
							N_{eq},O_{eq}	92.3(4, 5.7)	
								172.5(4, 1.3)	
							N_{eq},N_{eq}	95.9(4)	
$Cu(hdmpz)_2(NO_3)_2$	m	7.8176(8)		CuO_4N_2	O_{eq}	1.991(2) × 2	O_{eq},N_{eq}	88.91(7)[d]	177
(blue)	$P2_1/c$	14.93(2)	92.62(2)		N_{eq}	1.974(2) × 2		90.0(7, 1.09)	
	2	8.4076(8)			O_{ax}	2.561(2) × 2	O_{eq},O_{ax}	90.0(1, 7.04)	
							N_{eq},O_{ax}	90.0(6, 1.81)	
$Cu(nphyrO)_2(NO_3)_2$	m	7.768(2)		CuO_4N_2	O_{eq}	1.951(3) × 2	O_{eq},N_{eq}	90.00(1, 6.8)[e]	178
(dark blue)	$P2_1/n$	13.976(2)	113.12(3)		N_{eq}	1.963(3) × 2	O_{eq},O_{ax}	90.00(1, 5)	
	2	9.045(3)			O_2NO_{ax}	2.410(3) × 2	N_{eq},O_{ax}	90.00(1, 3.0)	
$[Cu(etapy)_2(NO_3)_2](NO_3)_2$	tr	8.320(6)	102.38(5)	CuO_4N_2	N_{eq}	1.984(2) × 2	N_{eq},O_{eq}	88.95(9)	179
(purple)	P-1	8.639(7)	99.95(7)		O_2NO_{eq}	1.992(2) × 2	N_{eq},O_{ax}	92.29(9)	
	1	11.096(11)	89.85(7)		O_2NO_{ax}	2.562(3) × 2	O_{eq},O_{ax}	54.85(8)[f]	
$Cu(amp)_2(ClO_4)_2$	m	9.893(1)		CuO_4N_2	O_{eq}	1.942(1) × 2	O_{eq},N_{eq}	84.8(2)[e]	180
(not given)	$P2_1/a$	11.192(5)	101.62(1)		N_{eq}	1.976(5) × 2	N_{eq},O_{ax}	84.0(2)	
	2	8.367(1)			O_3ClO_{ax}	2.457(6) × 2	O_{eq},O_{ax}	86.2(2)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*	Cu-L [Å]		L-Cu-L [°]		*Ref.*
$Cu(pyact)_2(ClO_4)_2$	m	10.957(3)		CuO_4N_2	O_{eq}	1.98(1) × 2	N_{eq},O_{eq}	89.9(3)[d]	181
(blue)	C2/c	12.178(6)	108.74(2)		N_{eq}	2.01(1) × 2	N_{eq},O_{ax}	89.1(5)	
	4	15.566(4)			O_3ClO_{ax}	2.52(2) × 2	O_{eq},O_{ax}	89.1(5)	
$Cu(pzdc)_2(ClO_4)_2$	tr	10.959(4)	116.63(3)	CuO_4N_2	O_{eq}	1.899(5) × 2	N_{eq},O_{eq}	81.9(2)[e]	182
(yellowish green)	P-1	6.970(3)	78.14(5)		N_{eq}	1.972(5) × 2	N_{eq},O_{ax}	87.5(2)	
	1	7.666(3)	97.27(5)		O_3ClO_{ax}	2.495(5) × 2	O_{eq},O_{ax}	90.6(3)	
$Cu(mpo)_2(ClO_4)_2$	or	13.0888(5)		CuO_4N_2	O_{eq}	1.953(4) × 2	O_{eq},N_{eq}	91.8(7)[d]	183
(purple)	Pbca	14.7638(6)			N_{eq}	1.999(4) × 2	N_{eq},O_{ax}	91.2(7)	
	4	10.3534(4)			O_3ClO_{ax}	2.747(4) × 2	O_{eq},O_{ax}	86.6(7)	
$[Cu(dampr)_2(ClO_4)_2]\cdot 2H_2O$	m	7.913(5)		CuO_4N_2	O_{eq}	1.949(3) × 2	O_{eq},N_{eq}	85.0(2)[e]	184
(blue)	$P2_1/c$	11.214(5)	94.86(2)		N_{eq}	1.980(4) × 2	O_{eq},O_{ax}	84.2(2)	
	2	9.756(6)			O_3ClO_{ax}	2.506(4) × 2	N_{eq},O_{ax}	94.0(2)	
$Cu(2\text{-}NO_2bz)_2(py)_2$	tr	8.380(8)	103.98(6)	CuO_4N_2	O_{eq}	1.94(1) × 2	O_{eq},N_{eq}	90.5(5, 2)	185
(not given)	P-1	5.773(5)	91.06(7)		N_{eq}	2.06(1) × 2	O_{eq},O_{ax}	53.7(5)[f]	
	1	13.095(8)	103.99(7)		O_{ax}	2.76(1) × 2		126.3(5)	
							O_{ax},N_{eq}	90.0(5, 2)	
							O_{eq},O_{eq}	180.0(5, 1)	
							O_{ax},O_{ax}	180.0(4)	
$Cu(tnph)_2(py)_2$	or	9.476(4)		CuO_4N_2	O_{eq}	1.957(4) × 2	O_{eq},N_{eq}	87.1(2)	186
(green)	Pccn	12.455(5)			pyN_{eq}	1.992(7) × 2	O_{eq},O_{eq}	90.2(2)[d]	
	4	22.401(9)			O_{ax}	2.438(6) × 2	N_{eq},N_{eq}	96.5(4)	
$Cu(monp)_2(4\text{-}Mepy)_2$[c]	tr	10.537(1)	121.031(5)	CuO_4N_2	pyN_{eq}	2.040(6) × 2	O_{eq},N_{eq}	90.6(2)	187
(not given)	P-1	10.521(1)	110.958(5)		O_{eq}	1.927(5) × 2	O_{eq},O_{ax}	88.7(2)	
	2	15.377(2)	86.105(3)		O_{ax}	2.458(3) × 2	O_{ax},O_{eq}	74.6(2)[e]	
				CuO_4N_2	pyN_{eq}	2.038(6) × 2	O_{eq},N_{eq}	90.2(2)	
					O_{eq}	1.933(4) × 2	O_{ax},N_{eq}	89.5(2)	
					O_{ax}	2.042(3) × 2	O_{ax},O_{eq}	75.1(2)[e]	
$Cu(acsal)_2(py)_2$	m	17.823(5)		CuO_4N_2	O_{eq}	1.949(3) × 2	O_{eq},N_{eq}	89.6(1)	188
(purple)	$P2_1/n$	10.903(4)	95.74(2)		pyN_{eq}	2.003(4) × 2	O_{eq},O_{ax}	55.2(1)[f]	
	2	6.598(2)			O_{ax}	2.623(3) × 2	N_{eq},O_{ax}	89.0(1)	

$Cu(btac)_2(py)_2$ (purple)	tr P-1 1	8.413(2) 8.370(3) 10.988(3)	98.14(3) 84.43(2) 119.62(2)	CuO_4N_2	O_{eq} pyN_{eq} O_{ax}	2.012(3) × 2 1.993(3) × 2 2.510(5) × 2	O_{eq},N_{eq} O_{eq},O_{ax} N_{eq},O_{ax}	91.4(1) 57.5(1)[f] 89.7(2)	189
$Cu(Ph_3ac)_2(py)_2$ (blue green)	m $P2_1/c$ 2	8.931(1) 12.602(1) 19.578(1)	118.17(40)	CuO_4N_2	pyN_{eq} O_{eq} O_{ax}	2.015(2) × 2 1.964(1) × 2 2.673(2) × 2	N_{eq},O_{eq} N_{eq},O_{ax} O_{eq},O_{ax}	91.51(6) 80.99(6) 54.15(6)[f]	190
$Cu(monp)_2(py)_2$ (dark green)	or Pbca 8	37.54(2) 16.76(1) 7.947(5)		CuO_4N_2	O_{eq} pyN_{eq} O_{ax}	1.94(2, 1) 2.07(2, 2) 2.52(2, 6)	N_{eq},N_{eq} O_{eq},O_{eq} O_{ax},O_{ax} N_{eq},O_{eq} N_{eq},O_{ax} O_{eq},O_{ax}	178.6(2) 177.5(2) 178.1(2) 90.0(2, 1.9) 90.0(2, 2.3) 71.6(2, 1.1)[e]	191
$Cu(F_6acac)_2(py)_2$ (green)	m $P2_1/c$ 4	15.7643(4) 10.3651(3) 16.8517(6)	99.37(1)	CuO_4N_2	pyN_{eq} O_{eq} O_{ax}	2.012(7, 1) 1.998(6, 1) 2.263(6, 37)	O_{eq},O_{ax} O_{ax},O_{ax} N_{eq},N_{eq} N_{eq},O_{ax} N_{eq},O_{eq}	87.5(3, 2.0)[d] 167.4(3) 93.0(3) 94.7(3, 1.6) 90.6(3, 1.7) 176.8(3, 4)	192
$[Cu(MeOac)_2(py)_2]\cdot 4H_2O$ (blue)	tr P-1 1	8.55(2) 9.25(2) 7.50(2)	97.5(4) 70.1(4) 86.4(4)	CuO_4N_2	O_{eq} pyN_{eq} O_{ax}	1.94(1) × 2 2.01(1) × 2 2.36(1) × 2	N_{eq},O_{eq} O_{eq},O_{ax} N_{eq},O_{ax}	80.1(3) 75.5(3)[e] 91.2(3)	193
$Cu(Cl_2ac)_2(2\text{-}Mepy)_2$ (blue)	m $P2_1/n$ 4	10.511(15) 16.091(23) 12.275(17)	93°24′(6′)	CuO_4N_2	pyN_{eq} O_{eq} O_{ax}	2.011(2, 21) 2.007(7, 8) 2.493(9) 2.711(10)	O_{eq},O_{eq} N_{eq},N_{eq} O_{eq},O_{ax} O_{eq},N_{eq} O_{ax},N_{eq}	158.3(4) 169.8(5) 55.3(3, 2.6)[f] 91.0(4, 2.5) 90.7(4, 6.5)	194
$Cu(Clac)_2(2\text{-}Mepy)_2$ (purple)	tr P1 1	8.166(10) 9.231(12) 7.818(9)	118°25′(5′) 107°40′(5′) 100°26′(5′)	CuO_4N_2	pyN_{eq} O_{eq} O_{ax}	1.989(6) × 2 1.975(6) × 2 2.707(7) × 2	N_{eq},N_{eq} N_{eq},O_{ax} O_{eq},O_{ax}	90.5(2) 91.4(2) 53.9(2)[f]	195
$Cu(ttbt)_2(4\text{-}Mepy)_2$ (not given)	m C2/c 4	9.357(3) 17.784(5) 18.138(5)	95.4(4)	CuO_4N_2	O_{eq} pyN_{eq} O_{ax}	2.066(6) × 2 2.174(5) × 2 2.125(5) × 2	O_{eq},O_{ax} O_{eq},N_{eq} N_{eq},N_{eq} N_{eq},O_{ax}	90.3(−, 1.5)[d] 91.4(−, 2.1) 94.9 90.8	197
$Cu(ac)_2(2,6\text{-}Me_2py)_2$ (not given)	tr P-1	8.424(3) 8.456(2)	60.01(2) 64.41(2)	CuO_4N_2	O_{eq} pyN_{eq}	1.997(4) × 2 2.046(3) × 2	N_{eq},O_{eq} N_{eq},O_{ax}	90.9(1) 91.3(1)	198

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
	1	8.736(2)	62.34(2)		O_{ax}	2.711(9) × 2	O_{ax},O_{eq}	127.0(2)	
[$Cu(ac)_2(3,4\text{-}Me_2py)_2]\cdot H_2O$	m	14.442(12)		CuO_4N_2	O_{eq}	1.953(3) × 2	O_{eq},O_{ax}	84.60(8)	199
(not given)	C2/c	12.578(11)	93.49(6)		pyN_{eq}	1.998(3) × 2	N_{eq},O_{eq}	90.00(1, 1.30)	
	4	10.817(5)			O_{ax}	2.810(2) × 2	N_{eq},O_{ax}	89.55(8, 0)	
[$Cu(pr)_2(3,4\text{-}Me_2py)_2]\cdot H_2O$	m	15.024(1)		CuO_4N_2	O_{eq}	1.952(5) × 2	O_{eq},N_{eq}	89.95(20, 7.5)	199
(not given)	C2/c	13.498(1)	97.433(9)		pyN_{eq}	2.003(5) × 2	N_{eq},O_{ax}	92.7(2)	
	4	11.086(1)			O_{ax}	2.960(3) × 2	O_{ax},O_{eq}	83.2(2)	
$Cu(ac)_2(2,4,6\text{-}Me_3py)_2$	m	7.842(1)		CuO_4N_2	O_{eq}	1.963(2) × 2	O_{eq},N_{eq}	90.00(8, 33)	200
(violet)	$P2_1/c$	16.384(2)	101.91(1)		pyN_{eq}	2.042(2) × 2	O_{eq},O_{ax}	52.02(9)[f]	
	2	8.320(2)			O_{ax}	2.788(3) × 2			
$Cu(ac)_2(amb)_2$[c]	m	15.302(8)		CuO_4N_2	O_{eq}	1.99(2, 1)	O_{eq},N_{eq}	154.2(–, 1.7)	201
(not given)	$P2_1/n$	17.373(6)	103.06(4)		N_{eq}	2.01(2, 2)	O_{ax},O_{ax}	142.2	
	4	18.449(10)			O_{ax}	2.66(2, 75)			
				CuO_4N_2	O_{eq}	2.00(2) × 2	O_{eq},N_{eq}	153.2(–, 1.8)	
					N_{eq}	2.03(2, 3)	O_{ax},O_{ax}	137.6	
					O_{ax}	2.61(2, 4)			
$Cu(ac)_2(ahb)_2$	tr	9.782(5)	100.70(4)	CuO_4N_2	O_{eq}	2.07(1, 1)	O_{eq},N_{eq}	158.2(–, 1)	201
(not given)	P-1	13.557(7)	89.90(4)		N_{eq}	1.95(1, 3)	O_{ax},O_{ax}	136.6	
	2	14.188(6)	110.56(5)		O_{ax}	2.57(1, 8)			
$Cu(fm)_2(2\text{-}Mebzim)_2$	m	6.3306(5)		CuO_4N_2	fmO_{eq}	1.985(1) × 2	O_{eq},O_{ax}	54.2(1)[f]	202
(purple)	$P2_1/n$	13.4855(11)	105.471(5)		fmN_{eq}	1.971(1) × 2	O_{eq},N_{eq}	90.0(1)	
	2	11.1863(5)			$bzimO_{ax}$	2.668(1) × 2			
$Cu(ac)_2(im)_2$	or	11.660(3)		CuO_4N_2	imN_{eq}	2.004(8) × 2	O_{eq},N_{eq}	89.97(35)	203
(violet)	Pccn	12.284(4)			O_{eq}	1.921(9) × 2	O_{eq},O_{ax}	52.21(28)[f]	
	4	9.375(3)			O_{ax}	2.799(8) × 2	N_{eq},O_{ax}	85.94(32)	
$Cu(tgly)_2(Meim)_2$	m	13.733(3)		CuO_4N_2	imN_{eq}	1.970(4) × 2	N_{eq},O_{eq}	90.4(2)	204
(blue violet)	$P2_1/n$	8.766(2)	105.97(5)		O_{eq}	1.967(3) × 2			
	2	13.641(3)			O_{ax}	2.758(4) × 2			

$[Cu(ac)_2(mor)_2]\cdot 2H_2O$	m	9.60(1)	113.9(1)	CuO_4N_2	$morN_{eq}$	2.035(4) × 2	O_{ax},O_{eq}	52.7(1)[f]	205
(not given)	$P2_1/c$	15.93(1)			acO_{eq}	1.958(4) × 2	N_{eq},O_{ax}	89.6(3)	
	2	6.28(1)			acO_{ax}	2.738(4) × 2	N_{eq},O_{eq}	100.6(3)	
$Cu(sal)_2(pym)_2$	m	15.786(1)		CuO_4N_2	$salO_{eq}$	1.981(2) × 2	N_{eq},O_{ax}	77.62(7)[e]	206
(blue)	C2/c	13.299(2)	97.22(1)		$pymN_{eq}$	1.981(1) × 2	N_{eq},O_{eq}	90.06(6)	
	4	12.083(1)			$pymO_{ax}$	2.331(1) × 2	O_{eq},O_{ax}	95.13(5)	
$Cu(sal)_2(nc)_2$	or	14.625(7)		CuO_4N_2	ncN_{eq}	1.944(7) × 2	O_{eq},N_{eq}	89.4(2)	207
(violet)	Pbca	9.572(5)			$salO_{eq}$	1.935(6) × 2	O_{eq},O_{ax}	55.2(2)[f]	
	4	18.671(9)			$salO_{ax}$	2.609(6) × 2	N_{eq},O_{ax}	88.2(2)	
$Cu(pppa)_2(CF_3SO_3)_2$[c]	tr	10.648(9)	81.86(4)	CuO_4N_2	O_{eq}	1.926(4) × 2	O_{eq},O_{ax}	90.3(2, 4.7)	208
(green)	P1	14.080(7)	77.06(6)		N_{eq}	2.069(6) × 2	O_{eq},N_{eq}	88.2(2, 1.0)[d]	
	3	18.294(10)	71.21(5)		O_2SO_{ax}	2.356(5) × 2	O_{ax},O_{ax}	180	
							O_{ax},N_{eq}	92.8(2)	
							O_{eq},O_{eq}	180	
							N_{eq},N_{eq}	180	
				CuO_4N_2	O_{eq}	1.917(4, 2)	O_{ax},O_{ax}	174.4(2)	
					N_{eq}	2.017(4, 2)	O_{ax},O_{eq}	90.0(2, 10.9)	
					O_2SO_{ax}	2.633(5, 167)	O_{ax},N_{eq}	90.0(2, 4.2)	
							O_{eq},O_{eq}	174.2(2)	
							N_{eq},O_{eq}	90.3(2, 1)[d]	
								90.1(2, 2)	
							N_{eq},N_{eq}	173.6(2)	
$Cu(2\text{-}Mepy)_2(NO_3)_2$	m	8.31(3)		CuO_4N_2	pyN_{eq}	1.985(14, 15)	O_{eq},O_{ax}	53.9(5, 2.2)[f]	209
(not given)	$P2_1/c$	14.81(3)	123.9(2)		O_{eq}	1.999(16, 28)		142.9(5, 2.3)	
	4	14.14(3)			O_{ax}	2.398(14, 91)	O_{ax},O_{ax}	89.1(5)	
							O_{ax},N_{eq}	91.1(5, 3.0)	
							O_{eq},O_{eq}	163.2(5)	
							O_{eq},N_{eq}	89.8(6, 8)	
							N_{eq},N_{eq}	176.9(5)	
$Cu(2\text{-}Mepy)_2(NO_3)_2$	m	8.57(3)		CuO_4N_2	pyN_{eq}	2.000(10, 1)	O_{eq},O_{ax}	55.1(4, 2)[f]	209
(not given)	$P2_1/c$	14.39(3)	119.5(2)		O_{eq}	1.994(10, 11)		129.8(4, 3)	
	4	14.20(3)			O_{ax}	2.534(8, 17)	O_{ax},O_{ax}	74.8(4)	
							O_{ax},N_{eq}	93.4(4, 1.9)	
							O_{eq},O_{eq}	175.1(1)	
							O_{eq},N_{eq}	89.8(5, 1.4)	
							N_{eq},N_{eq}	171.5(4)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
$Cu(F_6acac)_2(4\text{-}Mepz)_2$	tr	9.301(3)	104.71(2)	CuO_4N_2	pzN_{eq}	1.988(3) × 2	O_{ax},O_{eq}	86.1(1)[d]	210
(light green)	P-1	10.815(2)	101.38(2)		O_{eq}	1.975(3) × 2	N_{eq},O_{ax}	90.5(1)	
	1	6.457(1)	75.41(2)		O_{ax}	2.346(3) × 2	O_{eq},N_{eq}	88.3(1)	
$Cu(hip)_2(im)_2$	m	10.4863(4)		CuO_4N_2	imN_{eq}	1.964(3) × 2	O_{eq},N_{eq}	89.6(2)	211
(violet)	$P2_1/c$	11.4758(3)	102.234(1)		$hipO_{eq}$	1.976(3) × 2			
	2	10.3410(4)			$hipO_{ax}$	2.736(4) × 2			
$[Cu(phen)(NO_3)(H_2O)_2]\cdot NO_3$	m	7.03(1)		CuO_4N_2	N_{eq}	2.007(6, 2)	N_{eq},N_{eq}	83.1(2)[e]	212
(pale blue)	$P2_1/c$	20.20(1)	109.9(1)		H_2O_{eq}	2.005(6)	N_{eq},O_{eq}	92.2(2, 9)	
	4	11.49(1)			O_2NO_{eq}	1.983(5)		171.9(2, 1.1)	
					H_2O_{ax}	2.261(6)	N_{eq},O_{ax}	102.8(2, 17.5)	
					O_2NO_{ax}	2.594(6)	O_{eq},O_{ax}	54.0(2)[f]	
								86.6(2, 6.0)	
							O_{eq},O_{eq}	91.8(2)	
							O_{ax},O_{ax}	142.9(2)	
$Cu(nn)_2(Me_2CO)_2$	m	8.001(5)		CuO_4N_2	nnN_{eq}	1.988(5) × 2	N_{eq},O_{eq}	82.4(2)[e]	213
(dark brown)	$P2_1/c$	13.806(11)	98.0(1)		nnO_{eq}	1.951(4) × 2	N_{eq},O_{ax}	89.8(2)	
	2	11.012(18)			Me_2CO_{ax}	2.651(6) × 2	O_{eq},O_{ax}	91.2(2)	
$Cu(NO_2bz)_2(ampr)_2$	or	10.933(3)		CuO_4N_2	N_{eq}	2.000(4, 10)	N_{eq},O_{eq}	78.0(1, 1)[e]	214
(green)	$Pna2_1$	23.188(9)			O_{eq}	2.018(3) × 2		89.8(1, 14.2)	
	4	9.921(2)			bzO_{ax}	2.457(4, 28)	N_{eq},N_{eq}	176.5(1)	
							O_{eq},O_{eq}	177.0(1)	
							N_{eq},O_{ax}	89.9(2, 3.3)	
							O_{eq},O_{ax}	90.0(1, 10.8)	
							O_{ax},O_{ax}	173.2(1)	
$Cu(ttbd)_2(qu)_2$	tr	9.782(2)	91.62(2)	CuO_4N_2	O_{eq}	1.924(1) × 4	O_{eq},O_{eq}	92.0(1)	215
(not given)	P-1	9.978(2)	111.09(1)		quN_{ax}	2.545(3) × 2	O_{eq},N_{ax}	92.2(1)	
	1	9.562(2)	104.75(2)						
$Cu(Clac)_2(Me_4en)$[c]	or	13.013(3)		CuO_4N_2	N_{eq}	2.059(6) × 2	N_{eq},N_{eq}	88.5(2)[e]	216
(dark blue)	Pccn	19.182(12)			O_{eq}	1.970(6) × 2	O_{eq},O_{eq}	90.6(2, 1)	
	8	15.372(5)			O_{ax}	2.645(5) × 2	O_{eq},N_{eq}	156.2(3)	

							O_{eq},N_{eq}	95.3(2, 1)[f]	
							O_{ax},O_{ax}	152.4(2)	
							O_{ax},O_{eq}	55.2(2)[f]	
								103.7(2)	
							O_{ax},N_{eq}	99.9(3, 1.3)	
				CuO_4N_2	N_{eq}	2.071(6) × 2	N_{eq},N_{eq}	84.7(2)[e]	
					O_{eq}	1.973(6) × 2	O_{eq},N_{eq}	94.6(2)	
					O_{ax}	2.676(6) × 2	O_{eq},O_{eq}	89.8(2)	
							O_{eq},N_{eq}	160.8(2)	
							O_{ax},O_{ax}	150.1(2)	
							O_{ax},O_{eq}	54.0(2)[f]	
								102.9(2)	
							O_{ax},N_{eq}	100.8(3, 6.0)	
$Cu(Clac)_2(Me_4en)$	m	7.266(3)		CuO_4N_2	O_{eq}	1.976(3, 1)	N_{eq},N_{eq}	86.9(1)[e]	217
(not given)	$P2_1$	14.846(7)	103.41(3)		N_{eq}	2.038(3, 1)	O_{eq},O_{ax}	55.7(1, 1)[f]	
	2	7.260(2)			O_{ax}	2.626(3, 2)	O_{eq},O_{eq}	93.7(3, 2)	
$Cu(lac)_2(Me_4en)$	or	10.019(2)		CuO_4N_2	O_{eq}	1.982(7) × 2	N_{eq},N_{eq}	85.3(3)[e]	217
(not given)	$P4_12_12_1$	10.019(2)			N_{eq}	2.099(7) × 2	O_{eq},O_{eq}	94.4(3)	
	4	16.123(6)			O_{ax}	2.310(7) × 2	O_{eq},O_{ax}	55.7(3)[f]	
								83.8(3, 8.1)	
							N_{eq},O_{ax}	96.7(2, 3.1)	
							O_{ax},O_{ax}	161.9(2)	
$Cu(sal)_2(Me_4en)$	m	7.389(4)		CuO_4N_2	O_{eq}	1.988(8, 13)	O_{eq},O_{ax}	56.2(3, 9)[f]	218
(blue)	$P2_1/n$	13.807(6)	90.50(5)		N_{eq}	2.030(10, 10)		89.5(3, 2.7)	
	4	21.188(11)			O_{ax}	2.558(9, 38)	O_{eq},O_{eq}	91.3(3)	
							O_{eq},N_{eq}	93.0(4, 8)	
								164.4(4, 7)	
							O_{ax},O_{ax}	132.2(3)	
							O_{ax},N_{eq}	107.08(3, 3.5)	
							N_{eq},N_{eq}	86.9(4)[e]	
$Cu(fmpn)_2(Me_4en)$	tg	13.8046(3)		CuO_4N_2	enN_{eq}	2.240(8) × 2	O_{eq},O_{ax}	77.1(1)[e]	219
(red)	$P4_12_12$				O_{eq}	2.317(4) × 2	N_{eq},N_{eq}	83.2(1)[e]	
	4	12.1131(3)			O_{ax}	1.901(3) × 2	O_{ax},N_{eq}	94.7(1, 4.0)	
							O_{eq},O_{eq}	94.4(1, 6)	
							O_{eq},N_{eq}	93.4(1, 6)	
								166.5(1)	
							O_{ax},O_{ax}	167.7(1)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	a [Å] b [Å] c [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
$[Cu(monp)_2(Me_4en)]\cdot 2H_2O$	or	16.160(3)		CuO_4N_2	O_{eq}	1.932(3) × 2	O_{eq},O_{ax}	79.14(12, 7.69)[e]	220a
(dark brown)	Pbcn	18.538(3)			N_{eq}	2.049(4) × 2	O_{eq},N_{eq}	91.84(14)	
	4	8.263(1)			O_{ax}	2.565(3) × 2		175.01(14)	
							N_{eq},O_{ax}	101.22(13, 3.17)	
							O_{eq},O_{eq}	90.69(4)	
							O_{ax},O_{ax}	149.19(13)	
							N_{eq},N_{eq}	85.98(15)[e]	
$Cu(2,6\text{-}dnph)_2(Me_4en)$[c]	m	14.780(3)		CuO_4N_2	enN_{eq}	2.038(2) × 2	O_{eq},O_{ax}	76.0(1)[e]	220b
(green)	$P2_1/n$	10.984(2)	116.63(3)		phO_{eq}	1.946(1) × 2		85.3(1)	
	4	15.490(3)			phO_{ax}	2.432(2) × 2	N_{eq},O_{ax}	100.2(1, 6)	
							N_{eq},O_{eq}	172.5(1)	
								88.8(1)	
							N_{eq},N_{eq}	86.0(1)[e]	
							O_{eq},O_{eq}	96.9(1)	
							O_{ax},O_{ax}	151.9(1)	
				CuO_4N_2	enN_{eq}	2.024(2) × 2	O_{eq},O_{ax}	75.2(1)[e]	
					phO_{eq}	1.938(2) × 2		86.9(1)	
					phO_{ax}	2.436(2) × 2	N_{eq},O_{ax}	99.8(1, 2.7)	
							N_{eq},O_{eq}	89.1(1)	
								174.0(1)	
							N_{eq},N_{eq}	85.7(1)[e]	
							O_{eq},O_{eq}	96.2(1)	
							O_{ax},O_{ax}	153.2(1)	
$[Cu(fmpn)_2(Me_4en)]\cdot 4H_2O$	m	8.3080(3)		CuO_4N_2	enN_{eq}	2.059(2, 16)	O_{eq},O_{ax}	71.77(6, 71)[e]	221
(not given)	$P2_1/c$	15.0715(6)	97.158(3)		O_{eq}	1.955(2, 3)		86.09(8, 1.59)	
	4	21.5856(9)			O_{ax}	2.530(4, 38)	O_{ax},N_{eq}	101.54(8, 2.37)	
							O_{eq},N_{eq}	98.21(8, 4.58)	
								175.10(8, 30)	
							O_{ax},O_{ax}	148.70(7)	
							O_{eq},O_{eq}	90.02(7)	

$Cu(F_6acac)_2(Me_4pim)$	tr	9.317(4)	95.24(1)	CuO_4N_2	N_{eq}	2.012(4, 9)	O_{ax},N_{eq}	94.8(2, 2.7)	222
(orange)	P-1	12.922(5)	109.71(1)		acO_{eq}	1.962(4, 6)	N_{eq},O_{eq}	90.9(2)	
	2	13.525(6)	110.92(1)		acO_{ax}	2.288(4, 5)		174.2(2, 2.8)	
							N_{eq},N_{eq}	80.5(2)	
							O_{ax},O_{ax}	167.4(2)	
							O_{eq},O_{eq}	90.6(2)[d]	
$[Cu(Me_2amet)_2(bz)]\cdot bz$	or	9.166(3)		CuO_4N_2	N_{eq}	2.059(6, 1)	O_{ax},O_{eq}	57.1(2)[f]	223
(blue)	$P2_12_12_1$	13.293(7)			O_{eq}	2.168(6)		101.5(2, 8.7)	
	4	19.274(7)			bzO_{eq}	2.126(6)	O_{ax},N_{eq}	81.3(2)[e]	
					O_{ax}	2.179(6)		93.4(2, 5.8)	
					bzO_{ax}	2.376(6)	O_{ax},O_{ax}	158.8(2)	
							O_{eq},N_{eq}	90.3(2, 7.8)	
							O_{eq},O_{eq}	159.5(2)	
							N_{eq},N_{eq}	174.0(2)	
$Cu(NO_2)_2(Et_2en)$	m	11.939(12)		CuO_4N_2	N_{eq}	2.026(9, 29)	O_{eq},O_{eq}	87.8(3)	224
(not given)	$P2_1/c$	7.699(4)	99.75(9)		O_{eq}	2.007(8, 6)	N_{eq},O_{ax}	115.8(4, 2)	
	4	12.561(10)			O_{ax}	2.452(11, 28)	O_{eq},O_{ax}	54.8(3, 3)[f]	
							O_{eq},N_{eq}	90.6(3, 3)	
								170.5(4, 7)	
							N_{eq},N_{eq}	86.3(3)[e]	
							O_{ax},O_{ax}	176.1(3)	
$Cu(NO_2)_2(Et_2en)$	or	17.722(8)		CuO_4N_2	N_{eq}	1.994(7) × 2	N_{eq},N_{eq}	88.5(3)[e]	225
(not given)	Pbcn	8.126(2)			O_{eq}	2.235(10) × 2	O_{eq},O_{ax}	47.4(3)[f]	
	4	8.104(2)			O_{ax}	2.509(12) × 2	N_{eq},O_{eq}	86.6(3)	
							N_{eq},O_{ax}	100.7(3)	
$Cu(NO_2)_2(Me_4en)$	m	7.570(2)		CuO_4N_2	O_{eq}	2.01(1, 2)	N_{eq},N_{eq}	87.0(6)[e]	226
(dark green)	$P2_1/n$	12.506(2)	102.08(2)		N_{eq}	2.03(2, 1)	N_{eq},O_{ax}	108.9(6, 4.5)	
	4	12.500(4)			O_{ax}	2.43(1, 4)	N_{eq},O_{eq}	93.4(6, 1.1)	
								167.2(5, 7)	
							O_{eq},O_{ax}	55.2(5, 1.0)[f]	
								86.4(6, 3)	
								127.1(6)	
							O_{eq},O_{eq}	89.0(6)	
$Cu(NO_3)_2(Me_4en)$	m	13.8971		CuO_4N_2	N_{eq}	2.003(2) × 2	N_{eq},N_{eq}	88.0(1)[e]	227
(blue)	$C2/c$	7.4956	103.62(1)		$(NO_3)O_{eq}$	2.007(2) × 2	O_{eq},O_{ax}	56.9(1)[f]	
	4	12.2960			$(NO_3)O_{ax}$	2.440(2) × 2	O_{eq},N_{eq}	99.8(1, 6.3)	

TABLE I (*Continued*)

Compound	Cryst. Cl. Space G. Z	a [Å] b [Å] c [Å]	α [°] β [°] γ [°]	Chromophore		Cu-L [Å]		L-Cu-L [°]	Ref.
								164.3(1)	
							O_{eq},O_{eq}	89.3(1)	
$Cu(NO_3)_2(Me_4en)$	or	11.724(4)		CuO_4N_2	N_{eq}	2.022(5) × 2	N_{eq},O_{ax}	113.1(2, 12.0)	228
(not given)	Pnma	15.725(6)			$(NO_3)O_{eq}$	1.989(5) × 2	O_{eq},O_{ax}	53.9(2, 0)[f]	
	4	8.815(2)			$(NO_3)O_{ax}$	2.612(6) × 2		80.5(2, 0)	
							O_{ax},O_{ax}	115.7(2)	
							O_{eq},N_{eq}	178.3(2)	
								91.1(2, 0)	
							N_{eq},N_{eq}	87.9(2)[e]	
							O_{eq},O_{eq}	89.8(2)	
$Cu(NO_3)_2(daco)$	m	8.56(2)		CuO_4N_2	N_{eq}	1.977(5, 2)	N_{eq},N_{eq}	86.9(2)[d]	229
(not given)	$P2_1/c$	10.39(5)	78.52(3)		$(NO_3)O_{eq}$	1.995(4, 8)	O_{eq},N_{eq}	92.6(2, 3)	
	4	13.38(5)			$(NO_3)O_{ax}$	2.556(4, 24)		168.9(2, 1.5)	
							O_{ax},N_{eq}	111.5(2, 5.7)	
							O_{eq},O_{ax}	54.5(2, 6)[f]	
								82.5(2, 1.2)	
							O_{eq},O_{eq}	90.1(2)	
							O_{ax},O_{ax}	119.4(2)	
$Cu(NO_3)_2(Cl_2aqu)$	m	20.901(5)		CuO_4N_2	N_{eq}	1.983(4, 20)	N_{eq},N_{eq}	83.5(1)[e]	230
(not given)	C2/c	7.439(2)	114.59(3)		O_{eq}	2.015(3, 25)	O_{eq},N_{eq}	94.1(1, 4)	
	8	18.708(4)			O_{ax}	2.481(3, 8)		172.3(1, 2.9)	
							O_{ax},N_{eq}	91.6(1, 3.7)	
								131.5(1, 3.5)	
							O_{ax},O_{eq}	55.7(1, 8)[f]	
							O_{eq},O_{eq}	89.2(1)	
							O_{ax},O_{ax}	123.8(1)	
$[Cu(bimm)_2(NO_3)]NO_3 \cdot H_2O$	tr	8.562(4)	90.16(2)	CuO_4N_2	O_{eq}	2.045(1)	O_{eq},O_{ax}	55.3(2)[f]	231
(green)	P-1	9.990(4)	100.86(2)		N_{eq}	1.948(1, 8)		101.6(3, 10.2)	
	2	13.546(1)	118.29(4)		$(NO_3)O_{eq}$	2.055(1)	O_{eq},O_{eq}	157.6(3)	
					O_{ax}	2.285(1)	O_{eq},N_{eq}	80.7(2)[e]	
					$(NO_3)O_{ax}$	2.501(1)		90.7(3, 10.0)	

							O_{ax},O_{ax}	146.4(2)	
							O_{ax},N_{eq}	77.2(2)[e]	
								91.6(3, 14.4)	
							N_{eq},N_{eq}	166.0(3)	
$Cu(C_{10}H_{10}NO_4)_2$	m	9.141(2)		CuO_4N_2	O_{eq}	1.949(2) × 2	O,O	93.4(1)	232
(deep blue)	$P2_1/n$	7.335(3)	103.87(2)		N_{eq}	1.991(3) × 2	O,N	85.5(1, 8)[e]	
	2	11.112(3)			O_{ax}	2.582(3) × 2			
$Cu(degly)_2$	m	9.73(2)		CuO_4N_2	N_{eq}	2.14		not given	233
(blue)	$P2_1/b$	7.07(2)			O_{eq}	1.90			
	2	12.22(3)	111		O_{ax}	2.41			
$[Cu(bcmgly)_2]\cdot 2H_2O$	m	6.845(1)		CuO_4N_2	O_{eq}	1.954(2) × 2	O_{eq},O_{eq}	180	234
(pale blue)	$P2_1/c$	14.095(4)	91.95(2)		N_{eq}	2.062(2) × 2	O_{eq},N_{eq}	86.11(9)[e]	
	2	9.427(3)			O_{ax}	2.321(2) × 2	O_{eq},O_{ax}	86.8(1)	
							N_{eq},O_{ax}	77.97(9)[e]	
$[Cu(npac)_2]\cdot 2H_2O$	m	8.636(2)		CuO_4N_2	N_{eq}	2.071(2) × 2	O_{eq},N_{eq}	85.3(1)[e]	235
(not given)	$P2_1/c$	14.361(4)	94.78(2)		O_{eq}	1.939(2) × 2	N_{eq},O_{ax}	90.9(1)[d]	
	2	9.247(2)			O_{ax}	2.416(2) × 2	O_{eq},O_{ax}	88.5(1)	
$[Cu(Hpydca)_2]\cdot 3H_2O$[c]	m	14.74(1)		CuO_4N_2	N_{eq}	1.947(11, 48)	O_{eq},N_{eq}	100.5(3, 6)	236
(blue)	Pc	10.30(1)	123.9(1)		O_{eq}	2.051(8, 7)		79.6(4, 3)[e]	
	4	13.77(1)			O_{ax}	2.349(9, 27)	O_{ax},N_{eq}	103.8(4, 1.2)	
								77.1(4)[e]	
							O_{eq},O_{ax}	92.5(3, 3.0)	
								75.4(3)[e]	
							O_{ax},O_{ax}	152.4(3)	
							N_{eq},N_{eq}	179.1(4)	
							O_{eq},O_{eq}	159.1(3)	
				CuO_4N_2	N_{eq}	1.952(12, 50)	O_{eq},N_{eq}	80.0(4, 6)[e]	
					O_{eq}	2.026(10, 7)		108.0(4, 2)	
					O_{ax}	2.389(11, 63)	O_{ax},N_{eq}	107.1(4)	
								75.0(4, 1.0)[e]	
							O_{ax},O_{eq}	92.6(4, 8)	
							O_{ax},O_{ax}	150.0(4)	
							N_{eq},N_{eq}	176.9(4)	
							O_{eq},O_{eq}	160.0(4)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
$[Cu(purp)_2]\cdot 7.6H_2O$	tr	12.187(4)	73.57(3)	CuO_4N_2	N_{eq}	1.997(6, 24)	N_{eq},O_{eq}	81.9(2)[e]	237
(not given)	P-1	11.889(5)	83.72(3)		O_{eq}	2.026(7, 3)		90.0(3, 8.1)	
	2	10.447(3)	75.09(2)		O_{ax}	2.296(5, 7)	N_{eq},N_{eq}	179.0(7)	
							N_{eq},O_{ax}	76.8(2, 2)[e]	
								103.3(2, 1.2)	
							O_{eq},O_{eq}	164.2(2)	
							O_{eq},O_{ax}	91.8(2, 1.3)	
							O_{ax},O_{ax}	153.5(2)	
$K_2[Cu(idac)_2]\cdot H_2O$	m	15.53(3)		CuO_4N_2	N_{eq}	1.97(2) × 2		not given	238
(not given)	B2/b	13.17(3)			O_{eq}	1.95(2) × 2			
	4	6.28(3)	95.5(5)		O_{ax}	2.43(2) × 2			
$K_2[Cu(pydcaH)_2]\cdot 7H_2O$	or	20.823(5)		CuO_4N_2	O_{eq}	2.189(5, 29)	O_{eq},O_{eq}	87.9(3, 2.5)	239
(not given)	Pnna	13.398(5)			N_{ax}	1.936(5)		154.7(3)	
	4	8.183(3)					O_{eq},N_{ax}	77.6(2, 3)[e]	
							N_{ax},N_{ax}	173.7(3)	
$[Cu(pydca)(pydcaH)]\cdot H_2O$[c]	m	14.76(9)		CuO_4N_2	O_{eq}	2.06(1, 1)	N_{ax},O_{eq}	78.2(4, 2.7)[e]	240
(not given)	Pc	10.27(3)	124.0(1)			2.315(1, 50)	N_{ax},N_{ax}	179.5(7)	
	4	13.76(8)			N_{ax}	1.93(1, 5)	O_{eq},O_{eq}	92.3(4, 2.3)	
								156.5(4, 3.7)	
				CuO_4N_2	O_{eq}	2.02(1, 1)	N_{ax},O_{eq}	77.5(5, 4.3)[e]	
						2.375(2, 75)	N_{ax},N_{ax}	177.1(5)	
					N_{ax}	1.97(1, 5)	O_{eq},O_{eq}	92.5(9, 3.0)	
								155.0(5, 5.5)	
$[Cu(mdac)_2]\cdot ClO_4)_2$	m	6.183(2)		CuO_4N_2	O_{eq}	1.952(2) × 2	O_{eq},N_{eq}	85.5(1)[e]	241
(not given)	$P2_1/c$	17.617(4)	110.2(1)		N_{eq}	2.021(2) × 2	O_{eq},O_{ax}	91.1(1)	
	2	8.900(2)			O_{ax}	2.471(3) × 2	N_{eq},O_{ax}	71.7(1)[e]	
$[Ba(idac)_2(H_2O)_{10}][Cu(idac)_2]$	tr	9.050(4)	108.05(3)	CuO_4N_2	N_{eq}	2.005(5)	N_{eq},O_{eq}	85.8(2)[e]	242
(blue)	P-1	9.437(5)	93.68(4)		O_{eq}	1.948(5)	N_{eq},O_{ax}	70.6(1)[e]	
	1	11.468(5)	112.55(4)		O_{ax}	2.578(4)			
$[Cu(odac)(bpy)(H_2O)]\cdot 4H_2O$	tr	14.069(9)	114.1(1)	CuO_4N_2	bpyN_{eq}	2.018(4, 6)	O_{eq},N_{eq}	93.2(7, 1.0)	243
(light blue)	P1	8.898(5)	52.0(2)		O_{eq}	1.963(3, 9)		172.7(1, 2.1)	
	2	11.078(7)	118.6(1)		O_{ax}	2.458(4)	N_{eq},O_{ax}	97.8(1, 7.5)	

					H_2O_{ax}	2.307(3)	N_{eq},N_{eq}	80.7(1)[e]	
							O_{eq},O_{ax}	76.0(1, 2)[e]	
								90.2(1, 3.7)	
							O_{eq},O_{eq}	93.0(1)	
							O_{ax},O_{ax}	159.1(1)	
$Cu(dund)(ClO_4)_2$	m	13.997(7)	not given	CuO_4N_2	O_{eq}	1.968(7, 2)	O_{eq},N_{eq}	93.3(3, 2)[d]	244
(deep blue)	$P2_1/c$	10.656(9)			N_{eq}	2.003(10, 5)	N_{eq},N_{eq}	93.1(2)[d]	
	4	14.254(12)			O_3ClO_{ax}	2.545(21, 97)	O_{ax},O_{ax}	81.2(3)	
$[Cu(Me_2pam)(ClO_4)_2]\cdot H_2O$	m	16.757(4)		CuO_4N_2	O_{eq}	1.9735(2, 5)	O_{eq},O_{eq}	81.0(1)	245
(blue)	$P2_1/c$	11.290(3)	108.28(2)		N_{eq}	2.025(3, 4)	O_{eq},N_{eq}	94.5(1, 7)[d]	
	4	11.531(3)			O_3ClO_{ax}	2.464(3)		172.3((1, 2.9)	
						2.744(3)	N_{eq},N_{eq}	90.4(1)[d]	
$[Cu(ceten)(H_2O)(ClO_4)]\cdot ClO_4\cdot H_2O$	tr	8.103(2)	110.93(2)	CuO_4N_2	O_{eq}	1.980(4, 8)	O_{eq},N_{eq}	93.5(2, 2)[d]	246
(blue)	P-1	10.853(2)	100.74(2)		N_{eq}	2.008(5, 2)		170.1(2, 2.2)	
	2	12.198(2)	94.88(2)		O_3ClO_{ax}	2.500(4)	N_{eq},N_{eq}	94.1(2)[d]	
					H_2O_{ax}	2.702(5)	O_{eq},O_{eq}	79.5(2)	
							O_{ax},O_{ax}	169.1(2)	
$[Cu(C_8H_{16}N_4O_2)(NO_3)(H_2O)]\cdot$	tr	7.663(3)	91.82(4)	CuO_4N_2	O_{eq}	1.966(6, 11)	O_{eq},O_{eq}	86.0(2)	247
$NO_3\cdot H_2O$	P-1	10.725(6)	108.18(3)		N_{eq}	1.933(7, 10)	O_{eq},N_{eq}	95.2(2, 2)[d]	
(blue)	2	10.767(5)	90.14(4)		O_2NO_{ax}	2.548(9)	N_{eq},N_{eq}	85.6(3)[e]	
					H_2O_{ax}	2.399(9)			
$Cu(heac)(H_2O)$	m	11.641(28)		CuO_4N_2	H_2O_{eq}	1.978(3)	O_{eq},O_{ax}	99.0(1)	248
(blue)	$P2_1/c$	7.005(15)	91.50(10)		N_{eq}	2.066(2)	O_{eq},N_{ax}	102.2(1)	
	4	16.576(46)			O_{eq}	1.950(2, 21)	N_{eq},O_{ax}	75.0(1)[e]	
					N_{ax}	2.291(2)	N_{eq},N_{ax}	84.6(1)[e]	
					O_{ax}	2.467(2)	N_{eq},O_{eq}	172.9(1)	
							N_{ax},O_{eq}	80.1(1)[e]	
								102.1(1)	
							O_{ax},O_{eq}	88.8(1, 2.7)	
							N_{ax},O_{ax}	154.6(1)	
Cu(dzco)	tr	7.010(1)	81.33(1)	CuO_4N_2	O_{eq}	1.943(3) × 2	O_{eq},N_{eq}	84.2(2)[e]	249
(not given)	P-1	7.621(1)	70.54(1)		N_{eq}	2.055(4) × 2	N_{eq},O_{ax}	101.8(1)[h]	
	1	9.074(1)	86.35(1)		O_{ax}	2.645(4) × 2	O_{eq},O_{ax}	86.9(1)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	*α* [°] *β* [°] *γ* [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
Cu(tocop)	m	7.032(5)		CuO_4N_2	N_{eq}	2.050(3) × 2	N_{eq},O_{ax}	100.9(1)	250
(black)	$P2_1/c$	15.533(2)	113.46(4)		O_{eq}	1.924(3) × 2	N_{eq},N_{eq}	83.9(1)	
	2	9.836(2)			O_{ax}	2.615(3) × 2	O_{ax},O_{eq}	87.3(1)	
Cu(mug)	m	6.069(1)		CuO_4N_2	O_{eq}	1.955(4, 10)	O_{eq},O_{ax}	81.1(1, 7.8)[e]	251
(blue)	$P2_1$	13.617(1)	106.4(1)		N_{eq}	2.021(4, 3)		103.6(1, 9.0)	
	2	9.005(1)			O_{ax}	2.517(4, 40)	O_{eq},O_{eq}	86.2(2)	
							O_{eq},N_{eq}	84.8(2)[e]	
								99.6(2)[i]	
								168.7(2, 1)	
							O_{ax},O_{ax}	144.3(1)	
							N_{eq},O_{ax}	76.4(2, 2.2)[e]	
								99.0(2)[e]	
								103.8(2)	
							N_{eq},N_{eq}	90.5(2)	
Cu(dzco)	tr	7.608(3)	109.51(3)	CuO_4N_2	N_{eq}	2.045(1) × 2	N_{eq},O_{eq}	84.37(6)[e]	252
(not given)	P-1	9.064(2)	93.97(3)		O_{eq}	1.935(1) × 2	N_{eq},O_{ax}	101.60(4)	
	1	7.000(2)	81.32(3)		O_{ax}	2.636(2) × 2	O_{eq},O_{ax}	86.92(5)	
[Cu(ecgm)]·3/2H_2O	or	8.962(2)		CuO_4N_2	O_{eq}	1.954(3, 8)	O_{eq},O_{ax}	96.8(1, 8.3)	253
(blue)	$P2_12_12_1$	11.595(2)			N_{eq}	2.034(3, 3)	O_{eq},O_{eq}	106.3(1)	
	4	31.491(2)			O_{ax}	2.393(3, 25)	O_{ax},N_{eq}	78.1(1)[e]	
								85.2(1, 7.1)	
							O_{eq},N_{eq}	83.8(1)[e]	
								166.9(1)	
							N_{eq},N_{eq}	88.5(1)[e]	
[Cu(mcgly)]·2H_2O	or	13.451(2)		CuO_4N_2	O_{eq}	1.963(6, 9)	O_{eq},O_{eq}	108.0(3)	254
(not given)	$Pca2_1$	9.166(1)			N_{eq}	2.021(6, 16)	O_{eq},O_{ax}	89.7(3, 11.3)	
	4	13.138(2)			O_{ax}	2.343(6, 45)	O_{eq},N_{eq}	84.6(3, 1.8)[e]	
								161.4(3, 3.5)	
							O_{ax},O_{ax}	171.1(2)	
							O_{ax},N_{eq}	79.5(2, 6)[e]	
								101.6(3, 5.4)	
							N_{eq},N_{eq}	86.8(3)[e]	

[Cu(ecgly)]·$2H_2O$	or	13.745(1)		CuO_4N_2	O_{eq}	1.954(9, 23)	O_{eq},O_{eq}	106.7(4)	254
(not given)	$Pca2_1$	9.301(2)			N_{eq}	2.032(12, 15)	O_{eq},O_{ax}	90.3(4, 10.4)	
	4	13.275(4)			O_{ax}	2.368(10, 40)	O_{eq},N_{eq}	84.8(4, 1.9)[e]	
								162.7(5, 3.3)	
							O_{ax},O_{ax}	171.1(2)	
							O_{ax},N_{eq}	79.5(2, 6)[e]	
								101.6(3, 5.4)	
							N_{eq},N_{eq}	87.0(4)[e]	
Na_2[Cu(enphgly)]·$5.5H_2O$	or	14.195(1)		CuO_4N_2	O_{eq}	1.941(3, 4)		not given	255
(dark blue)	Pbcn	22.607(3)			N_{eq}	2.005(3, 6)			
	8	14.242(1)			O_{ax}	2.433(3, 29)			
K_2[Cu(eac)]·$3H_2O$	or	12.93(2)		CuO_4N_2	O_{eq}	1.978(16, 45)	O_{eq},N_{eq}	86.0(–, 1.1)[e]	256
(not given)	Pbca	22.90(3)			N_{eq}	2.095(17, 1)	N_{eq},O_{ax}	79.7(–, 2.0)[e]	
	8	11.45(2)			O_{ax}	2.302(16, 78)		100.0(–, 2.2)	
							N_{eq},N_{eq}	89.0[e]	
							O_{eq},O_{eq}	103.3	
							O_{eq},O_{ax}	90.2(– 10.2)	
Cu(4-NO_2pyNO)$_2$(H_2O)$_2Cl_2$	m	13.540(6)		CuO_4Cl_2	H_2O_{eq}	1.950(3) × 2	Cl_{eq},O_{eq}	91.0(1)	257
(golden brown)	$P2_1/c$	5.487(2)	93°37′(2′)		Cl_{eq}	2.266(1) × 2	Cl_{eq},O_{ax}	88.8(1)	
	2	11.153(5)			O_{ax}	2.635(2) × 2	O_{eq},O_{ax}	94.9(1)	
Cu(biu)$_2Cl_2$	or	6.776(6)		CuO_4Cl_2	O_{eq}	1.935(3) × 2	O_{eq},O_{eq}	90.6[d]	258
(blue green)	Pnnm Pnn2	8.025(12)			Cl_{ax}	2.960(1) × 2	O_{eq},Cl_{ax}	94.8	
	2	10.734(12)							
Cu(12-aneO_4)$_2Cl_2$	or	7.062(3)		CuO_4Cl_2	O_{eq}	2.121(3, 8)	Cl_{eq},Cl_{eq}	95.85(7)	259
(deep green)	$P2_12_12_1$	13.661(8)			Cl_{eq}	2.221(2, 7)	Cl_{eq},O_{ax}	104.72(9, 5.08)	
	4	12.337(7)			O_{ax}	2.373(4, 30)	Cl_{eq},O_{eq}	90.05(1, 1.05)	
								173.65(1, 1.15)	
							O_{eq},O_{ax}	73.7(2, 3.0)[e]	
							O_{ax},O_{ax}	135.2(1)	
							O_{eq},O_{eq}	84.2(1)	
Cu(Etsac)$_2$(H_2O)$_2$	tr	7.554(1)	104.83(1)	CuO_4S_2	O_{eq}	1.916(2) × 2	S_{eq},O_{eq}	86.49(1)[e]	260
(deep green)	P-1	9.001(1)	99.20(1)		S_{eq}	2.381(1) × 2	S_{eq},O_{ax}	96.29(1)	
	1	5.345(1)	71.02(1)		H_2O_{ax}	2.457(1) × 2	O_{eq},O_{ax}	88.97(5)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
$Cu(NO_3)_2(dptp)_2$	or	11.55(1)		CuO_4NS	N_{eq}	1.943(4)	S_{eq},N_{eq}	93.3(1)[d]	261
(red)	$Pca2_1$	7.877(2)			$(NO_3)O_{eq}$	2.000(4, 21)	S_{eq},O_{eq}	94.0(1, 5.4)	
	4	16.866(5)			S_{eq}	2.332(1)		164.7(1)	
					$(NO_3)O_{ax}$	2.445(4, 34)	N_{eq},O_{eq}	91.8(2)	
								169.1(1)	
							O_{eq},O_{eq}	89.0(2)	
							N_{eq},O_{ax}	103.0(1, 9.3)	
							O_{eq},O_{ax}	56.5(2, 3)[f]	
								93.8(2, 1.9)	
							O_{ax},O_{ax}	140.1(1)	
							S_{eq},O_{ax}	109.0(1)	
$Cu(bheg)(Br)(H_2O)$	or	8.7672(9)		CuO_4NBr	O_{eq}	1.95(1)	Br_{eq},O_{ax}	103.8(3, 3.2)	262
(blue)	$P2_12_12_1$	15.594(3)			H_2O_{eq}	1.96(1)	Br_{eq},O_{eq}	91.1(4, 1)	
	4	7.4996(5)			N_{eq}	2.07(1)	Br_{eq},N_{eq}	174.8(4)	
					Br_{eq}	2.41(1)	O_{ax},O_{ax}	151.0(4)	
					O_{ax}	2.48(1, 19)	O_{eq},O_{ax}	93.1(5, 3.3)	
								79.8(5)	
							O_{eq},O_{eq}	172.0(5)	
							O_{ax},N_{eq}	76.8(4, 2.5)[e]	
							O_{eq},N_{eq}	83.9(6)[e]	
								93.9(6)	
$Cu(cyclam)(BH_4)_2$	m	7.374(1)		CuN_4H_2	N_{eq}	2.021(4, 3)	N_{eq},N_{eq}	85.4(2)[e]	263
(not given)	$P2_1/c$	12.660(2)	111.09(1)		H_3BH_{ax}	2.28(1)		94.6(2)[d]	
	2	8.858(1)							
$Cu(Me_4cyclam)(BH_4)_2$	m	12.254(2)		CuN_4H_2	N_{eq}	2.024(5, 10)	N_{eq},N_{eq}	86.6(3)[e]	263
(not given)	C2/c	11.719(2)	107.83(2)		H_3BH_{ax}	2.25(1)		93.4(3)[d]	
	4	14.826(2)							
$Cu(en)_2(BF_4)_2$	tr	7.42(2)	100°54′	CuN_4F_2	N_{eq}	2.03(1, 1)	N_{eq},N_{eq}	86.4(5)[e]	264
(violet)	P-1	8.22(2)	105°12′		F_{ax}	2.56(1) × 2	N_{eq},F_{ax}	93.9(5, 8)	
	1	5.92(2)	160°0′						

$Cu(trien)(PF_6)_2$ (dark blue)	or B2mb 4	7.362(1) 14.708(5) 15.551(6)		CuN_4F_2	N_{eq} F_{ax}	1.982 2.596(–, 6)		not given	265
$Cu(Bu_2cyclam)(PF_6)$ (pink)	tr P-1 1	9.357(2) 9.297(2) 8.552(2)	112.60(2) 103.63(2) 77.31(1)	CuN_4F_2	N_{eq} F_{ax}	2.034(2, 29) 2.840(2) × 2	N_{eq},N_{eq}	86.8(8)[e]	266
$[Cu(en)_2(PF_6)(H_2O)]PF_6$ (dark blue)	or B2mb 4	8.66036(1) 14.51489(5) 13.25635(6)		CuN_4FO	N_{eq} F_{ax} H_2O_{ax}	2.003(–, 28) 2.7371 2.3968	N_{eq},N_{eq}	84.35[e]	267
$Cu(NH_3)_4(cnact)_2$ (blue violet)	tr P-1 1	6.827(1) 7.842(1) 8.018(1)	112.80(1) 103.40(1) 100.98(1)	CuN_4O_2	N_{eq} O_{ax}	2.008(1) × 4 2.577(1) × 2	N_{eq},N_{eq} N_{eq},O_{ax} O_{ax},O_{ax}	90.0(5, 2) 90.0(5, 7.9) 180	268
$Cu(py)_4(F_3ac)_2$ (not given)	tr P-1 2	9.156(3) 9.505(4) 17.160(6)	98.04(14) 89.91(13) 118.44(15)	CuN_4O_2	pyN_{eq} acO_{ax}	2.044(4, 8) 2.355(4, 5)	N_{eq},N_{eq} N_{eq},O_{eq}	90.5(1, 3) 178.5(2, 3) 90.0(1, 3.5)	137 150
$Cu(py)_4(F_3ac)_2$ (green)	tr P-1 2	9.528(6) 9.218(5) 18.471(10)	104.57(5) 98.50(6) 118.65(4)	CuN_4O_2	pyN_{eq} acO_{ax}	2.046(7, 4) 2.367(7, 2)	N_{eq},N_{eq} N_{eq},O_{ax} O_{ax},O_{ax}	90.0(3, 1.1) 178.5(3) 90.0(3, 3.3) 172.9(3)	269
$Cu(py)_4(CF_3SO_3)_2$ (blue)	or Pbcn 4	10.5618(7) 16.287(1) 16.830(2)		CuN_4O_2	N_{eq} O_{ax}	2.039(6, 19) 2.425(4) × 2	N_{eq},N_{eq} N_{eq},O_{ax} N_{eq},N_{eq} O_{ax},O_{ax}	90.00(15, 1.59) 90.00(11, 1.90) 178.4(3, 1.6) 179.8(2)	270
$Cu(py)_4(PhPO_3H)_2$ (blue)	m $P2_1$ 2	9.821(1) 17.776(1) 10.688(1)	117.269(6)	CuN_4O_2	N_{eq} O_{ax}	2.071 2.320(7, 22)	N_{eq},N_{eq} N_{eq},O_{ax} O_{ax},O_{ax}	90.0 90.0 176.9(3)	271
$[Cu(py)_4(PhPO_3H)_2]\cdot 2MeOH$ (blue)	tr P-1 2	9.148(3) 11.366(4) 17.466(5)	84.43(8) 86.89(8) 84.62(8)	CuN_4O_2	N_{eq} O_{ax}	2.049 2.490(4, 11)	N_{eq},N_{eq} N_{eq},O_{ax} O_{ax},O_{ax}	90.0 90.0 177.7(1)	271
$Cu(3\text{-}Mepy)_2(5,5'\text{-}Et_2barb)_2(H_2O)_2$ (light purple)	m $P2_1/c$ 2	11.196(5) 15.124(5) 9.449(5)	102.0(2)	CuN_4O_2	pyN_{eq} N_{eq} H_2O_{ax}	2.18(3) × 2 1.980(5) × 2 2.857(4) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	90.0(1, 3) 90.0(5, 38.7)	272
$[Cu(3\text{-}Mepy)_4(H_2O)_2](ClO_4)_2$ (blue)	m C2/c 4	15.292(4) 9.672(2) 20.579(5)	94.73(2)	CuN_4O_2	N_{eq} H_2O_{ax}	2.028(5, 13) 2.493(12, 23)	N_{eq},N_{eq} N_{eq},O_{ax} O_{ax},O_{ax}	90.3(2) 90.9(2, 1.7) 180	273

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
$Cu(iqu)_4(CF_3SO_3)_2$[c] (blue)	tr P-1 4	10.882(3) 18.219(8) 22.384(3)	67.49(2) 88.64(2) 83.34(2)	CuN_4O_2	N_{eq} O_{ax}	2.02(9, 1) 2.45(9, 2)	N_{eq},N_{eq} N_{eq},O_{ax}	90.0(5, 1.1) 90.0(4, 1.6)	141
				CuN_4O_2	N_{eq} O_{ax}	2.03(1, 1) 2.45(1, 4)	N_{eq},N_{eq} N_{eq},O_{ax}	90.0(5, 9) 90.0(4, 3.8)	
$[Cu(im)_4(H_2O)_2]F_2$ (dark blue)	m C2/c 4	12.708(3) 10.299(2) 13.915(3)	 106.63(2) 	CuN_4O_2	N_{eq} H_2O_{ax}	2.009(2, 25) 2.638(2) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	88.84(6) 88.38(7, 1.99)	274
$Cu(im)_4(NO_3)_2$ (purple)	or $Pna2_1$ 4	13.85(1) 9.83(1) 13.39(1)		CuN_4O_2	N_{eq} O_2NO_{ax}	2.011(7, 7) 2.566(6, 40)	N_{eq},N_{eq} N_{eq},O_{ax} O_{ax},O_{ax}	90.0(2, 8) 179.0(2, 5) 90.0(2, 3.4) 178.5(2)	275
$Cu(im)_4(MeOac)_2$ (not given)	m $P2_1/a$ 2	8.35(3) 9.85(3) 14.77(4)	94.8	CuN_4O_2	N_{eq} O_{ax}	1.979(7, 66) 2.825(7) × 2	N_{eq},N_{eq}	92.3(3, 1.1)	276
$Cu(im)_4(tsval)_2$ (pink red)	m C2/c 4	18.252(5) 12.372(2) 17.534(3)	 93.77(2) 	CuN_4O_2	N_{eq} O_{ax}	1.985(3, 5) 2.947(2) × 2	N_{eq},N_{eq} N_{eq},O_{ax} O_{ax},O_{ax}	90.1(2, 7) 176.2(1) 90.0(1, 7.1) 167.8(1)	277
$Cu(im)_4(ac)_2$ (blue violet)	m C2/c 4	13.187(2) 8.591(1) 17.644(2)	 104.13(1) 	CuN_4O_2	imN_{eq} acO_{ax}	2.047(2) × 2 1.977(1) × 2 2.649 × 2	N_{eq},N_{eq}	89.1(3)	278
$Cu(im)_4\{P(PhO)_2O_2\}_2$ (violet blue)	m $P2_1/c$ 2	8.264(3) 25.339(8) 10.216(3)	 114.82(4) 	CuN_4O_2	N_{eq} O_{ax}	2.019(3, 1) 2.556(2) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	90.0(1, 1.6) 87.6(1)	279
$[Cu(Meim)_4(H_2O)_2]Cl_2 \cdot H_2O$[c] (dark green)	tr P-1 2	9.198(1) 9.338(1) 15.520(2)	99.41(1) 105.59(1) 103.36(1)	CuN_4O_2	N_{eq} H_2O_{ax}	2.018(3, 16) 2.518(3) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	90.1(1) 89.3(1, 2.1)	280
				CuN_4O_2	N_{eq} H_2O_{ax}	2.018(3, 10) 2.511(3) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	90.8(1) 89.8(1, 4)	

$Cu(4\text{-}Meim)_4(ClO_4)_2$ (purple)	m C2/c 4	15.742(5) 10.052(3) 16.654(5)	111.81(2)	CuN_4O_2	N_{eq} O_3ClO_{ax}	2.000(5, 7) 2.659(4) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	90.0(2, 1.2) 180.0(1) 91.2(2, 1)	281
$Cu(1,2\text{-}Me_2im)_4(ClO_4)_2$ (blue purple)	m $P2_1/n$ 4	15.9011(7) 16.730(3) 10.919(1)	98.413(7)	CuN_4O_2	N_{eq} O_3ClO_{ax}	1.999(10, 12) 2.752(20, 32)	N_{eq},N_{eq} N_{eq},O_{ax} O_{ax},O_{ax}	90.0(2, 13) 178.1(2, 4) 90.0(4, 60) 174.1(3)	282
$Cu(pz)_4(F_3ac)_2$ (violet)	tr P-1 1	9.600(2) 10.666(3) 8.703(2)	115.52(2) 113.58(2) 59.71(1)	CuN_4O_2	N_{eq} acO_{ax}	2.013(3, 1) 2.452(3) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	90.5(1) 88.8(1, 3.4)	283
$[Cu(5,7\text{-}Me_2tpym)_4(H_2O)_2](PF_6)_2$ (blue)	m $P2_1/c$ 2	11.826(2) 9.463(2) 17.673(3)	97.50(1)	CuN_4O_2	N_{eq} H_2O_{ax}	2.035(3, 16) 2.456(3) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	90.1(1) 93.5(1, 1.3)	284
$Cu(H_2O)_2(NH_3)_2(mtpo)_2$ (purple)	m $P2_1/c$ 2	8.917(2) 13.998(2) 7.234(5)	106.77(3)	CuN_4O_2	N_{eq} H_3N_{eq} H_2O_{ax}	2.016(3) × 2 1.997(3) × 2 2.554(3) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	90.0(2, 8) 90.0(2, 4)	128
$Ca[Cu(en)(5'\text{-}qmp)_2(H_2O)_2]\cdot 8H_2O$ (blue)	m $P2_1$ 2	10.997(2) 21.693(4) 8.872(2)	94.69(1)	CuN_4O_2	N_{eq} N_{eq} H_2O_{ax}	2.02(2, 4) 2.04(2, 2) 2.76(2, 2.6)	N_{eq},N_{eq} N_{eq},O_{ax} O_{ax},O_{ax}	84.9(7)[d] 90.1(8, 5.1) 175.0(10, 4.4) 89.9(8, 11.8) 161.6(9)	129
$[Cu(en)_2(H_2O)_2]F_2\cdot 4H_2O$ (mauve)	m C2/m 2	8.179(2) 15.854(2) 7.123(3)	101.98(3)	CuN_4O_2	N_{eq} H_2O_{ax}	2.021(5, 2) 2.571(6) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	84.6(2)[e] 90.0(2, 2.3)	285
$[Cu(en)_2(H_2O)_2](Ph_4B)_2\cdot 2Me_2SO$ (not given)	tr P-1 1	9.871(2) 10.077(3) 14.612(3)	95.75(2) 91.59(2) 111.13(2)	CuN_4O_2	N_{eq} H_2O_{ax}	2.038(10, 17) 2.693(9) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	84.9(4)[e] 86.5(5, 7.1)	286
$[Cu(en)_2(H_2O)_2](4\text{-}amsal)$ (not given)	or Pbca 4	29.196(6) 10.788(2) 7.318(1)		CuN_4O_2	N_{eq} H_2O_{ax}	2.004(4, 1) 2.659(3) × 2		not given	287
$[Cu(en)_2(H_2O)_2](pbpc)\cdot 2MeOH$ (lilac)	tr P-1 1	9.943(1) 13.740(1) 15.968(1)	69.26(1) 83.27(1) 68.98(1)	CuN_4O_2		not given		not given	288
$Cu(en)_2(acts)_2$ (not given)	tr P-1 1	8.196(7) 9.094(4) 9.352(3)	84.51(3) 74.83(6) 63.57(5)	CuN_4O_2	enN_{eq} O_{ax}	2.005(3, 4) 2.652(1) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	84.77(6)[e] 97.43(5, 2)	82b

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
$[Cu(Meen)_2(H_2O)_2](ox)$ (not given)	m $P2_1/n$ 2	7.198(3) 12.674(4) 7.693(2)	97.32(3)	CuN_4O_2	N_{eq} H_2O_{ax}	2.032(5, 24) 2.503(5) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	85.9(2)[e] 90.9(18, 3.6)	289
$[Cu(Meen)_2(H_2O)_2](mal)$ (not given)	or Pbcn 8	23.861(16) 10.312(6) 12.663(10)		CuN_4O_2	N_{eq} H_2O_{ax}	2.033(7, 32) 2.513(7) 2.681(6)	N_{eq},N_{eq} O_{ax},N_{eq} O_{ax},O_{ax}	85.4(5)[e] 90.1(5, 8.1) 174.4(4)	290a
$Cu(Meen)_2(ClO_4)_2$ (not given)	m $P2_1/c$ 2	8.351(7) 11.850(3) 8.439(6)	113.93(5)	CuN_4O_2	N_{eq} O_{ax}	2.035(5, 31) 2.575(6) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	84.6(2)[e] 87.45(20, 2.75)	290b
$[Cu(Meen)_2(H_2O)_2](adip)$ (not given)	tr P-1 1	7.241(2) 8.271(3) 8.304(3)	89.92(3) 114.87(2) 90.45(2)	CuN_4O_2	N_{eq} H_2O_{ax}	2.028(2, 20) 2.561(2) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	85.4(1)[e] 91.5(1, 2.6)	291a
$Cu(Meen)_2(NO_3)_2$ (not given)	m $P2_1/c$ 2	8.143(7) 11.939(4) 7.509(4)	111.18(3)	CuN_4O_2	N_{eq} O_{ax}	2.03(1, 2) 2.54(1) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	86.2(4)[e] 93.9(4, 6)	291b
$[Cu(Et_2en)_2(H_2O)_2](NO_3)_2$ (not given)	m $P2_1/c$ 2	7.123(3) 15.264(6) 10.011(3)	92.21(3)	CuN_4O_2	N_{eq} H_2O_{ax}	2.068(4, 13) 2.498(4) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	85.1(2)[e] 92.2(2, 2.3)	292
$[Cu(1,3\text{-}pn)_2(H_2O)_2]F_2$ (mauve)	or Pccn 4	16.350(2) 11.383(4) 6.983(4)		CuN_4O_2	N_{eq} H_2O_{ax}	2.025(6, 5) 2.637(6) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	90.0(2, 8)[d] 87.8(2, 6)	293
$[Cu(bip)_2(H_2O)_2]Br_2$ (dark blue)	m C2/c 4	9.865(2) 12.790(2) 20.878(2)	101.98(1)	CuN_4O_2		not given		not given	294
$[Cu(Meims)_2(H_2O)_2](ClO_4)_2 \cdot 2H_2O$ (blue)	m $P2_1/n$ 2	7.696(2) 13.875(3) 13.186(2)	95.98(2)	CuN_4O_2	N_{eq} H_2O_{ax}	1.997(3, 7) 2.501(4) × 2	N_{eq},N_{eq}	88.7(1)[d]	295
$[Cu(dim)_2(H_2O)_2](ClO_4)_2 \cdot 2H_2O$ (not given)	m C2/m	11.520(2) 19.517(3)	105.24(2)	CuN_4O_2	N_{eq} H_2O_{ax}	1.996(4) × 4 2.624(3) × 2	N_{eq},N_{eq}	90.0(2, 6)[i] 180	296

	2	7.131(1)							
$Cu(amnur)_2(H_2O)_2$	m	13.190(2)		CuN_4O_2	N_{eq}	2.006(3, 15)	N_{eq},N_{eq}	81.1(1)[e]	297
(deep green)	$P2_1/c$	8.934(2)	103.81(2)		H_2O_{ax}	2.325(3) × 2	N_{eq},O_{ax}	91.2(1, 4)	
	2	7.649(1)							
$[Cu(odpy)_2(H_2O)_2](ClO_4)_2$	m	13.579(2)		CuN_4O_2	N_{eq}	2.005(6, 39)	N_{eq},N_{eq}	82.8(5)[e]	298
(green)	$P2_1/n$	10.904(3)	103.5		H_2O_{ax}	2.365(6) × 2	N_{eq},O_{ax}	90.7(5, 1.9)	
	2	10.329(2)							
$[Cu(Meims)_2(H_2O)_2]\cdot 2MeSO_4$	m	8.460(3)		CuN_4O_2	N_{eq}	2.005(6, 4)	N_{eq},N_{eq}	88.7(2)[d]	299
(blue)	$P2_1/n$	8.503(3)	98.41(3)		H_2O_{ax}	2.46(1) × 2		90.0(3, 1.3)	
	2	20.341(8)							
$[Cu(papt)_2(H_2O)_2](BF_4)_4$	tr	9.856(1)	101.69(8)	CuN_4O_2	N_{eq}	1.988(10, 8)	N_{eq},N_{eq}	86.5(4)[d]	300
(brown)	P-1	12.724(1)	96.717(9)		H_2O_{ax}	2.497(9) × 2		93.5(5)	
	1	9.401(1)	70.145(8)					180	
							N_{eq},O_{ax}	90.0(4, 4.7)	
							O_{ax},O_{ax}	180	
$[Cu(papt)_2(H_2O)_2](BF_4)_4$	m	12.663(4)		CuN_4O_2	N_{eq}	2.016(11, 19)	N_{eq},N_{eq}	85.5(4)[d]	300
(green)	$P2_1/n$	9.573(3)	107.16(2)		H_2O_{ax}	2.426(9) × 2		94.5(4)	
	2	18.813(4)						180	
							O_{ax},O_{ax}	180	
							O_{ax},N_{eq}	90.0(4, 2.3)	
$K_2[Cu(ggly)_2(H_2O)_2]\cdot 4H_2O$	m	13.730(14)		CuN_4O_2	N_{eq}	2.005(60, 35)	N_{eq},N_{eq}	83.0(2, 1)[e]	301
(red purple)	$P2_1/a$	6.240(14)	102°33′(13′)		H_2O_{ax}	2.770(70) × 2	N_{eq},O_{ax}	84.0(2)	
	2	11.670(10)							
$[Cu(hist)_2(H_2O)_2]\cdot 4H_2O$	tr	6.894(1)	98.61(1)	CuN_4O_2	N_{eq}	2.015(5, 19)	N_{eq},N_{eq}	90.6(2)[d]	302
(dark blue)	P-1	8.478(1)	116.13(1)		H_2O_{ax}	2.570(5) × 2	N_{eq},O_{ax}	92.4(2, 1.8)	
	1	9.553(1)	35.88(1)						
$Cu((bzpy)_2(N_3)_2)$	tr	7.598(4)	96.24(3)	CuN_4O_2	N_3N_{eq}	1.989(4) × 2	N_{eq},N_{eq}	90.0(1, 2.2)	303
(dark green)	P-1	7.655(3)	110.10(3)		N_{eq}	2.005(3) × 2	N_{eq},O_{ax}	74.1(1)[e]	
	1	10.796(5)	90.24(3)		O_{ax}	2.467(3) × 2		95.0(1, 10.9)	
$Cu(acatr)_2(NCS)_2$	or	9.669(6)		CuN_4O_2	N_{eq}	1.943(2) × 2	N_{eq},O_{eq}	89.06(8)[d]	304
(grass green)	Pbca	12.192(3)			O_{eq}	1.984(2) × 2	O_{eq},N_{ax}	91.78(7)	
	4	14.266(3)			SCN_{ax}	2.521(3) × 2	N_{eq},N_{ax}	92.20(8)	
$[Cu(hb\text{-}bzim)_2(NCS)_2]\cdot 2Me_2CO$	m	8.696(9)		CuN_4O_2	SCN_{eq}	1.956(5) × 2	N_{eq},N_{eq}	88.1(2)	305
(green)	$P2_1/n$	11.052(4)	85.24(5)		N_{eq}	1.995(5) × 2	N_{eq},O_{ax}	70.9(2)[e]	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
	2	19.105(7)			O_{ax}	2.575(6) × 2		93.3(2)	
$Cu(dmen)_2(NO_3)_2$ (blue violet)	m $P2_1/c$ 2	7.425(2) 8.533(2) 13.072(3)	 105.56(3)	CuN_4O_2	N_{eq} O_2NO_{ax}	2.017(7, 17) 2.57(4) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	84.8(3)[e] 89.9(3, 4.4)	306
$Cu(1,2\text{-}pn)_2(NO_3)_2$ (not given)	m $P2_1/c$ 2	8.793(10) 10.193(4) 7.960(6)	 105.02(7)	CuN_4O_2	N_{eq} O_2NO_{ax}	2.06(4, 1) 2.57(4) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	87(1)[e] 91(1, 2)	307
$Cu(2Me\text{-}1,2\text{-}pn)_2(NO_3)_2$ (not given)	m $P2_1/c$ 4	9.263(2) 18.441(6) 9.296(3)	 92.55(2)	CuN_4O_2		not given		not given	308
$Cu(1,3\text{-}pn)_2(NO_3)_2$ (not given)	or Pbca 4	8.180(5) 16.335(16) 10.240(4)		CuN_4O_2	N_{eq} O_2NO_{ax}	2.065(10, 25) 2.55(1) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	94.9(5)[d] 94.6(5, 2.3)	309
$Cu(Me_2\text{-}1,3\text{-}pn)_2(NO_3)_2$ (blue violet)	m $P2_1/n$ 2	5.951(1) 19.333(3) 7.457(2)	 91.00(1)	CuN_4O_2	N_{eq} O_2NO_{ax}	2.025(4, 4) 2.566(3) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	92.56(2)[d] 90.28(2, 7.35)	310
$Cu(Mepicam)_2(NO_3)_2$ (blue)	m $P2_1/c$ 2	7.04(2) 14.60(4) 10.08(3)	 123.4(1)	CuN_4O_2	N_{eq} O_2NO_{ax}	2.027(9, 5) 2.507(9) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	81.9(4)[e] 91.8(3, 3.1)	311
$Cu(3,5Me_2guapz)_2(NO_3)_2$ (blue)	tr P-1 1	9.708(3) 5.464(2) 9.367(3)	92.99(3) 101.24(3) 108.54(3)	CuN_4O_2	N_{eq} O_2NO_{ax}	1.989(4, 39) 2.597(5) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	101.0(2) 92.6(2, 6)	312
$Cu(Meen)_2(ClO_4)_2$ (not given)	m $P2_1/c$ 2	8.351(7) 11.850(3) 8.439(6)	 113.93(5)	CuN_4O_2	N_{eq} O_3ClO_{ax}	2.035(3, 51) 2.575(6) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	84.6(2)[e] 87.5(2, 2.8)	313a
$Cu(Eten)_2(ClO_4)_2$ (violet)	tr P-1 1	8.131(8) 8.762(13) 9.786(12)	65.33(16) 65.98(11) 63.34(8)	CuN_4O_2	N_{eq} O_3ClO_{ax}	2.022(3, 9) 2.594(3) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	85.0(1)[e] 85.9(1, 4.3)	313b
$Cu(ampy)_2(ClO_4)_2$	tr	7.630(2)	106.67(3)	CuN_4O_2	N_{eq}	2.005(8, 30)	O_{ax},O_{ax}	177.0(4)	314

(blue)	P1 1	7.980(1) 7.972(5)	108.75(3) 95.90(2)		O_3ClO_{ax}	2.598(9, 34)	O_{ax},N_{eq} N_{eq},N_{eq}	90.0(3, 12.3) 81.3(3, 3)[e] 98.6(3, 1.2) 176.6(5, 7)	
$Cu(aepy)_2(ClO_4)_2$ (not given)	tr P-1 1	8.275(3) 9.772(4) 7.894(4)	126.88(2) 82.20(3) 111.22(3)	CuN_4O_2	N_{eq} O_3ClO_{ax}	2.015(2, 10) 2.883(2) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	86.54(7)[d] 93.46(7) 90.00(7, 10.98)	315
$Cu(1,2\text{-pn})_2(ClO_4)_2$ (not given)	tr P1,P-1 1	5.82(1) 7.66(1) 9.42(2)	102.0(1) 102.8(1) 77.6(1)	CuN_4O_2	N_{eq} O_3ClO_{ax}	2.03(3, 1) 2.61(2) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	86(1)[d] 93(1, 4)	316
$Cu(1,3\text{-bn})_2(ClO_4)_2$ (red violet)	m $P2_1/c$ 2	6.807(3) 15.952(7) 8.524(3)	 105.92(2)	CuN_4O_2	N_{eq} O_3ClO_{ax}	2.028(7, 2) 2.676(10) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	88.9(3)[d] 89.2(3, 2.9)	317
$Cu(1,3\text{-bn})_2(ClO_4)_2$ (blue violet)	m $P2_1/c$ 2	9.626(9) 11.545(4) 7.856(4)	 102.46(2)	CuN_4O_2	N_{eq} O_3ClO_{ax}	2.027(6, 10) 2.579(6) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	83.3(2)[d] 90.0(2, 2.1)	317
$Cu(Me_2\text{-}1,3\text{-pn})(ClO_4)_2$ (light blue)	m $P2_1/c$ 2	9.724(2) 6.287(1) 16.191(3)	 97.66(1)	CuN_4O_2	N_{eq} O_3ClO_{ax}	2.025(3, 4) 2.602(3) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	88.1(1)[d] 90.0(1, 1.9) 88.9(1, 3.0)	318
$Cu(athal)_2(ClO_4)_2$ (purple)	m $P2_1/c$ 2	11.562(3) 9.282(2) 10.028(3)	 94.20(1)	CuN_4O_2	N_{eq} O_3ClO_{ax}	2.008(8, 11) 2.571(8) × 2	N_{eq},N_{eq}	82.9(3)[e]	319
$Cu\{N(py)_3\}_2(ClO_4)_2$ (yellowish brown)	m $P2_1/n$ 2	18.638(2) 8.552(3) 9.822(1)	 91.44(1)	CuN_4O_2	N_{eq} O_3ClO_{ax}	1.999(3, 7) 2.593(8) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	84.5(1)[d] 92.7(2, 3.6)	320
$Cu(Me_2en)_2(F_6acac)_2$ (purple)	tr P-1 1	8.174 8.495 11.910	120.32 109.02 94.65	CuN_4O_2	N_{eq} O_{ax}	2.06(2, 5) 2.76(1) × 2		not given	321
$[Cu(1,3\text{-pn})_2(3\text{-Ibz})(H_2O)]\cdot(3\text{-Ibz})$ (dark blue)	or $P2_12_12$ 4	34.987(2) 11.839(2) 6.362(2)		CuN_4O_2	N_{eq} bzO_{ax} H_2O_{ax}	2.04(8, 4) 2.67(3) 2.51(5)	N_{eq},N_{eq} N_{eq},O_{ax}	92(2, 3)[d] 90(2, 5) 91(8, 5)	322
$[Cu(Meen)_2(trt)(H_2O)]\cdot H_2O$ (violet)	or $P2_12_12_1$ 4	9.561(7) 9.578(8) 18.037(9)		CuN_4O_2	N_{eq} O_{ax} H_2O_{ax}	2.032(8, 22) 2.630(7) 2.439(8)	N_{eq},N_{eq} N_{eq},O_{ax} O_{ax},O_{ax}	84.6(3, 1)[e] 90.0(3, 5.8) 173.0(3)	323

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
$Cu(1,3\text{-}pn)_2(bz)_2$ (blue)	m $P2_1/c$ 2	11.498(2) 8.295(2) 11.383(2)	 91.84(1)	CuN_4O_2	N_{eq} bzO_{ax}	2.035(3, 8) 2.468(3) × 2	N_{eq},N_{eq}	94.4(5)[d]	324
$Cu(imp\text{-}1,2\text{-}pn)_2(sal)_2$ (not given)	m $P2_1/c$ 2	8.774(6) 19.885(12) 8.771(6)	 97.15(7)	CuN_4O_2	N_{eq} $salO_{ax}$	2.019(4, 30) 2.606(4) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	83.3(3)[c] 93.8(1, 4.3)	325
$Cu(1,3\text{-}pn)_2(2\text{-}Mebz)_2$ (blue)	or Pbca 4	10.188(3) 21.821(12) 10.567(4)		CuN_4O_2	N_{eq} O_{ax}	2.037(5, 8) 2.501(4) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	87.2(2)[d] 87.6(2, 2)	326
$Cu(1,3\text{-}pn)_2(3\text{-}NO_2bz)_2$ (blue green)	tr P-1 1	8.337(2) 11.281(3) 6.737(2)	98.72(2) 90.43(2) 111.63(2)	CuN_4O_2	N_{eq} O_{ax}	2.031(2, 2) 2.665(2) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	89.3(1)[d] 93.1(1, 2)	327
$Cu(1,3\text{-}pn)_2(3\text{-}Mebz)_2$ (not given)	m $P2_1/c$ 2	12.571(4) 8.243(2) 11.480(4)	 102.39(2)	CuN_4O_2	N_{eq} O_{ax}	2.042(10, 15) 2.486(6) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	87.4(3)[d] 87.0(3, 7)	328
$Cu(1,3\text{-}pn)_2(4\text{-}Mebz)_2$ (not given)	m $P2_1/c$ 2	12.408(5) 8.466(2) 11.199(3)	 90.049(49)	CuN_4O_2	N_{eq} O_{ax}	2.034(7, 4) 2.546(5) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	87.9(3)[d] 86.1(2, 2.3)	329
$Cu(1,3\text{-}pn)_2(4\text{-}NO_2bz)_2$ (not given)	m $P2_1/c$ 2	12.473(1) 8.174(1) 11.586(1)	 92.20(1)	CuN_4O_2	N_{eq} O_{ax}	2.044(7, 4) 2.528(8) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	87.3(3)[d] 86.7(3, 3.1)	330
$Cu(1,3\text{-}pn)_2(3\text{-}Clbz)_2$ (blue)	m $P2_1/c$ 2	12.514(6) 8.198(4) 11.449(5)	 103.10(4)	CuN_4O_2	N_{eq} O_{ax}	2.04(1) × 4 2.48(1) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	87.6(3)[d] 94.0(3)	331
$Cu(1,3\text{-}pn)_2(4\text{-}Clbz)_2$ (blue)	m $P2_1/c$ 2	12.458(3) 8.989(3) 10.605(3)	 91.72(2)	CuN_4O_2	N_{eq} O_{ax}	2.04(1, 1) 2.53(1) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	87.8(5)[d] 95.5(5)	331
$Cu(1,3\text{-}pn)_2(3\text{-}Brbz)_2$ (bluish green)	m $P2_1/c$	12.72(1) 8.24(1)	 104.02(8)	CuN_4O_2	N_{eq} O_{ax}	2.051(9, 1) 2.481(8) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	89.2(4)[d] 93.3(3, 1.6)	332

	2	11.50(1)							
Cu(1, 3-pn)$_2$(4-Brbz)$_2$ (not given)	m P2$_1$/c 2	14.503(5) 11.093(4) 7.636(3)	102.54(3)	CuN$_4$O$_2$	N_{eq} O_{ax}	2.036(10, 3) 2.496(11) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	88.9(4)[d] 92.9(4, 6)	333
Cu(1, 3-pn)$_2$(3-Ibz)$_2$ (blue)	m P2$_1$/a 2	11.717(2) 8.283(2) 13.000(1)	107.79(1)	CuN$_4$O$_2$	N_{eq} bzO_{ax}	2.035(3, 6) 2.500(3) × 2	N_{eq},N_{eq} N_{eq},O_{ax} O_{ax},O_{ax}	87.9(1)[d] 90.0(1, 2.1) 86.7(1, 9) 180	334
Cu(1, 3-pn)$_2$(4-Fbz)$_2$ (dark blue)	m P2$_1$/c 2	11.808(7) 8.632(4) 10.979(4)	90.29(6)	CuN$_4$O$_2$	N_{eq} O_{ax}	2.035(6, 1) 2.503(5) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	87.2(2)[d] 93.2(2, 3.0)	335
Cu(1, 3-pn)$_2$(4-Ibz)$_2$ (not given)	m P2$_1$/c 2	14.80(1) 11.15(1) 7.74(1)	105.38(8)	CuN$_4$O$_2$	N_{eq} O_{ax}	2.014(21, 9) 2.548(18) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	89.1(8)[d] 92.15(80, 1.55)	336
Cu(8-Mesthp)$_2$(py)$_2$ (red violet)	m P2$_1$/c 2	7.502(2) 20.352(4) 9.757(2)	98.67(3)	CuN$_4$O$_2$	pyN_{eq} N_{eq} O_{ax}	2.032(2) × 2 1.999(2) × 2 2.825(2) × 2	N_{eq},N_{eq} N_{eq},O_{ax} O_{ax},O_{ax}	90.0(1, 8) 74.5(1)[e] 90.0(1, 15.5) 180.0(1)	337
Cu(4-Mebzcs)$_2$(py)$_2$ (blue)	tr P-1 1	7.150(4) 9.314(5) 10.523(7)	93.55(5) 97.15(5) 109.06(4)	CuN$_4$O$_2$	pyN_{eq} N_{eq} O_{ax}	2.010(2) × 2 1.936(2) × 2 2.616(4) × 2	N_{eq},N_{eq}	90.2(2)	338
Cu(mocpz)$_2$(py)$_2$ (violet)	m P2$_1$ 2	11.441(2) 9.339(3) 12.493(3)	99.95(1)	CuN$_4$O$_2$	pyN_{eq} N_{eq} O_{ax}	2.057(2) × 2 1.950(2) × 2 2.680(2) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	89.28(2) 72.21(8)[e] 83.07(8)	339
Cu(5, 5′-Et$_2$barb)$_2$(py)$_2$ (not given)	m P2$_1$/c 2	11.235(5) 9.958(4) 12.624(5)	102.6(2)	CuN$_4$O$_2$	pyN_{eq} N_{eq} O_{ax}	2.032(5) × 2 1.983(5) × 2 2.723(5) × 2	N_{eq},N_{eq}	90.0(2, 5)	340
Cu(picl)$_2$(pyam)$_2$ (dark green)	m P2$_1$/c 4	12.311(5) 15.435(5) 15.320(6)	115.95(3)	CuN$_4$O$_2$	pyamN_{eq} piclO_{eq} piclN_{ax}	2.051(6, 3) 1.951(7, 10) 2.599(7, 13)	O_{eq},N_{ax} N_{ax},N_{ax} N_{eq},N_{eq} N_{eq},N_{ax} O_{eq},N_{eq} O_{eq},O_{eq}	73.8(5, 3)[e] 106.2(5, 2.5) 176.9(4) 178.8(4) 86.1(5) 90.3(5, 1.8) 177.1(4)	341

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* Z	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
Cu(bipyam)$_2$(tcne)$_2$	tr	10.075(2)	107.98(2)	CuN_4O_2	bipyamN_{eq}	2.003(6, 14)	N_{eq},N_{eq}	86.28(23)[e]	342
(golden brown)	P-1	10.911(2)	104.78(2)		tcneO_{ax}	2.250(4) × 2		89.78(17, 48)	
	1	7.841(2)	108.40(2)						
[Cu(prim)$_4$](ClO$_4$)$_2$·EtOH	or	20.022(2)		CuN_4O_2	N_{eq}	1.998(6, 6)	N_{eq},N_{eq}	90.1(3, 3)	343
(purple)	Aba2;Acam	12.263(1)			O_{ax}	2.839(6, 63)		176.9(3)	
	4	11.073(1)					N_{eq},O_{ax}	52.1(2, 1.5)[f]	
[Cu(bpy)$_2$(NO$_2$)$_2$]BF$_4$	m	10.839(3)		CuN_4O_2	(NO_3)O_{eq}	2.117(6)	N_{eq},N_{ax}	80.1(2, 7)[e]	344
(not given)	P2$_1$/n	12.367(3)	105.25(5)			2.463(6)		99.4(2, 1.6)	
	4	16.219(3)			bpyN_{eq}	2.097(5, 44)	N_{ax},N_{ax}	178.6(1)	
					bpyN_{ax}	1.998(5, 8)	N_{eq},N_{eq}	98.5(2)	
							O_{eq},N_{ax}	90.4(2, 3.2)	
							O_{eq},N_{eq}	164.1(1)	
								149.2(1)	
								111.9(2)	
								97.3(2)	
							O_{eq},O_{eq}	52.7(2)[f]	
[Cu(2-pira)$_2$(NO$_3$)]NO$_3$	m	14.817(4)		CuN_4O_2	(NO_3)O_{eq}	2.317(9, 75)	O_{eq},O_{eq}	54.3(4)[f]	345
(not given)	P2$_1$/n	14.872(3)	94.28(2)		N_{eq}	2.085(9, 16)	O_{eq},N_{eq}	145.8(4, 2.6)	
	4	11.595(2)			N_{ax}	1.974(9, 5)	O_{eq},N_{ax}	95.2(4, 14.8)	
							N_{eq},N_{ax}	87.0(4, 11.3)[e]	
							N_{ax},N_{ax}	179.4(4)	
[Cu(bpy)$_2$(NO$_2$)]NO$_3$	m	11.101(18)		CuN_4O_2	(NO_3)O_{eq}	2.283(10, 45)	N_{eq},N_{eq}	103.0(4)	346
(not given)	P2$_1$/n	12.058(23)	99.10(10)		bpyN_{eq}	2.083(10, 18)	N_{eq},N_{ax}	80.7(4, 4)[e]	
	4	15.385(30)			bpyN_{ax}	1.993(10, 15)		99.0(4, 4)	
							O_{eq},O_{eq}	52.5(4)[f]	
							N_{eq},O_{eq}	102.4(4, 3.2)	
								154.6(4, 3.5)	
							O_{eq},N_{ax}	90.2(4, 3.4)	
							N_{ax},N_{ax}	179.6(4)	
[Cu(bpy)$_2$(NO$_2$)]NO$_3$	m	11.225(2)		CuN_4O_2	bpyN_{eq}	2.083(10, 18)	N_{eq},N_{ax}	80.7(4, 4)[e]	347
(not given)	P2$_1$/n	12.035(5)	99.55(2)		(NO_3)O_{eq}	2.284(10, 46)		89.9(4, 9.6)	348

	4	15.109(5)			bpyN_{ax}	1.993(11, 13)	O_{eq},N_{ax}	90.5(4, 3.7)	
							O_{eq},O_{eq}	52.5(4)[f]	
							O_{eq},N_{eq}	98.0(4, 8.9)	
								154.5(4, 3.4)	
							N_{eq},N_{eq}	103.0(4)	
							N_{ax},N_{ax}	179.6(4)	
$[Cu(bpy)_2(NO_2)]NO_3$	m	11.217(2)		CuN_4O_2	bpyN_{eq}	2.085(2, 14)	N_{eq},N_{ax}	80.24(9, 27)[e]	347
(not given)	$P2_1/n$	11.936(5)	99.14(2)		$(NO_3)O_{eq}$	2.278(3, 74)		99.79(9, 26)	348
(at 165 K)	4	14.969(3)			bpyN_{ax}	2.987(2, 3)	N_{eq},N_{eq}	102.85(9)	
							N_{eq},O_{eq}	102.02(9, 3.01)	
								154.84(9, 3.18)	
							N_{ax},N_{ax}	179.96(9)	
							N_{ax},O_{eq}	89.98(9, 3.45)	
							O_{eq},O_{eq}	53.5(9)[f]	
$[Cu(bpy)_2(NO_2)]NO_3$	m	11.168(4)		CuN_4O_2	bpyN_{eq}	2.085(2, 25)	N_{eq},N_{ax}	80.37(8, 3.4)[e]	347
(not given)	$P2_1/n$	11.945(5)	99.32(3)		$(NO_3)O_{eq}$	2.155(2)		99.69(8, 62)	
(at 100 K)	4	14.909(6)				2.414(2)	N_{eq},N_{eq}	102.08(8)	
					bpyN_{ax}	1.989(2, 3)	N_{eq},O_{eq}	102.36(8, 3.45)	
								155.22(7, 3.69)	
							N_{ax},N_{ax}	179.63(8)	
							N_{ax},O_{eq}	89.97(8, 3.51)	
							O_{eq},O_{eq}	53.62(7)[f]	
$[Cu(bpy)_2(NO_2)]NO_3$	m	11.067(2)		CuN_4O_2	bpyN_{eq}	2.085(2, 57)	N_{eq},N_{ax}	80.39(7, 84)[e]	347
(not given)	$P2_1/n$	12.014(3)	100.01(3)		$(NO_3)O_{eq}$	2.051(2)		99.87(7, 1.62)	
(at 20 K)	4	14.855(7)				2.536(2)	N_{eq},N_{eq}	100.68(7)	
					bpyN_{ax}	1.990(2, 8)	N_{eq},O_{eq}	103.02(6, 4.55)	
								155.82(7, 4.91)	
							N_{ax},N_{ax}	178.91(7)	
							N_{ax},O_{eq}	89.86(8, 2.89)	
							O_{eq},O_{eq}	53.83(4)[f]	
$[Cu(4,4',5,5'-Me_4dim)_2(NO_3)]NO_3$	tr	7.854(1)	78.46(2)	CuN_4O_2	N_{eq}	2.119(6, 91)	N_{eq},N_{ax}	84.2(2, 4.0)[e]	349
(red purple)	P-1	14.303(2)	94.96(2)		$(NO_3)O_{eq}$	2.180(7)		99.4(2, 1)	
	2	11.852(2)	91.92(1)			2.569(8)	O_{eq},N_{ax}	89.3(3, 6.1)	
					N_{ax}	2.000(5, 12)	O_{eq},O_{eq}	53.1(2)[f]	
							O_{eq},N_{eq}	91.4(2)	
								114.3(2)	

TABLE 1 (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	*α* [°] *β* [°] *γ* [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
								140.4(2)	
								163.8(2)	
							N_{eq},N_{eq}	104.8(2)	
							N_{ax},N_{ax}	178.3(4)	
$[Cu(bpy)_2(NO_3)]NO_3 \cdot H_2O$	tr	7.488(2)	106.183(4)	CuN_4O_2	$bpyN_{eq}$	2.037(5, 14)	N_{eq},N_{ax}	$81.3(2, 3)^e$	350
(not given)	P-1	10.017(2)	91.335(3)		$(NO_3)O_{eq}$	2.301(5)		101.9(2, 1.9)	
	2	15.061(2)	89.662(3)			2.832(5)	N_{ax},N_{ax}	170.7(1)	
					$bpyN_{ax}$	1.980(5, 7)	N_{eq},N_{eq}	140.7(1)	
							O_{eq},N_{ax}	87.9(2, 3.9)	
								127.5(2)	
$[Cu(bpy)_2(NO_3)]NO_3 \cdot H_2O$	tr	7.464(3)	111.50(5)	CuN_4O_2	$bpyN_{eq}$	2.034(5, 12)	N_{eq},N_{eq}	140.2(3)	351
(not given)	P-1	10.002(3)	91.43(5)		$(NO_3)O_{eq}$	2.299(7)	O_{eq},O_{eq}	$47.7(3)^f$	
	2	15.503(6)	90.47(4)			2.818(7)	N_{eq},O_{eq}	86.2(3, 5.9)	
					$bpyN_{ax}$	1.983(3, 1)		133.7(3, 6.4)	
							O_{eq},N_{ax}	85.9(3, 4.1)	
							N_{eq},N_{ax}	$81.5(3, 4)^e$	
								101.8(3, 1.8)	
							N_{ax},N_{ax}	170.9(3)	
$[Cu(bpy)_2(fm)]BF_4 \cdot 0.5H_2O$	tr	7.570(2)	100.376(4)	CuN_4O_2	$bpyN_{eq}$	2.110(5, 49)	N_{eq},N_{eq}	113.2(2)	352
(blue)	P-1	9.742(2)	96.806(3)		fmO_{eq}	2.024(5)	N_{eq},N_{ax}	$79.6(2, 7)^e$	
	2	14.994(2)	86.107(3)			2.869(12)		98.3(2, 8)	
					$bpyN_{ax}$	1.990(5, 12)	N_{ax},N_{ax}	175.8(1)	
							O_{eq},N_{ax}	91.4(2, 1.5)	
							O_{eq},N_{eq}	100.5(2)	
								146.1(1)	
$[Cu(phen)_2(fm)]ClO_4$	m	16.772(6)		CuN_4O_2	N_{eq}	2.111(3) × 2	N_{eq},N_{ax}	$81.3(1)^e$	353
(turquoise)	C2/c	11.5806(3)	111.370(2)		fmO_{eq}	2.353(6) × 2		99.0(1)	
	4	12.5735(3)			N_{ax}	1.985(3) × 2	O_{eq},N_{ax}	89.8(2, 5)	
							N_{ax},N_{ax}	179.4(2)	
$[Cu(bpy)_2(ac)]BF_4$	m	7.333(2)		CuN_4O_2	N_{eq}	2.121(6, 88)	N_{eq},N_{ax}	$79.5(2, 1.2)^e$	354
(purple blue)	$P2_1/c$	28.078(4)	111.42(5)		O_{eq}	1.980(4)		99.8(2, 2.0)	

	4	11.601(3)				2.785(5)	N_{ax},N_{ax}	178.3(1)	
					N_{ax}	2.006(6, 11)	N_{eq},N_{eq}	111.0(2)	
							O_{eq},N_{ax}	90.8(2, 8)	
							O_{eq},N_{eq}	92.3(2)	
								156.5(1)	
[Cy(bpy)$_2$(ac)]$ClO_4 \cdot H_2O$	tr	8.338(2)	100.35(5)	CuN_4O_2	N_{eq}	2.112(5, 56)	N_{eq},N_{ax}	79.6(2, 8)[e]	354
(turquoise green)	P-1	9.660(2)	95.99(5)		O_{eq}	2.031(5)		97.6(2, 1.2)	
	2	14.912(3)	84.90(5)			2.648(5)	N_{ax},N_{ax}	174.5(1)	
					N_{ax}	1.983(5, 12)	N_{eq},N_{eq}	111.6(2)	
							O_{eq},N_{ax}	91.8(2, 1.3)	
							O_{eq},N_{eq}	100.7(1)	
								147.6(1)	
[Cu(phen)$_2$(ac)]ClO_4	m	8.258(3)		CuN_4O_2	N_{eq}	2.114(4, 16)	N_{eq},N_{eq}	114.1(2)	355
(not given)	$P2_1/c$	19.070(9)	111.19(3)		O_{eq}	2.220(4)	N_{eq},O_{eq}	154.7(2)	
	4	16.755(3)			N_{ax}	2.421(5)		97.2(2, 6.1)	
						2.000(4, 6)	O_{eq},O_{eq}	52.1(1)[f]	
							O_{eq},N_{ax}	90.2(2, 3.7)	
							N_{eq},N_{ax}	80.6(2)[e]	
								103.6(2, 10.5)	
							N_{ax},N_{ax}	177.9(2)	
[Cu(phen)$_2$(ac)]ClO_4	m	8.246(9)		CuN_4O_2	N_{eq}	2.119(3, 22)	O_{eq},O_{eq}	52.3(1)[f]	355
(not given)	$P2_1/c$	19.009(4)	111.61(1)		O_{eq}	2.155(4)	O_{eq},N_{eq}	97.5(1, 6.2)	
(at 173 K)	4	16.717(3)				2.421(5)		148.5(1, 6.5)	
					N_{ax}	2.007(3, 5)	N_{eq},N_{eq}	113.6(1)	
							O_{eq},N_{ax}	89.8(1, 3.3)	
							N_{eq},N_{ax}	80.7(1, 2.1)[e]	
								103.4(1, 10.1)	
							N_{ax},N_{ax}	178.1(1)	
[Cu(phen)$_2$(ac)]BF_4	tr	15.087(3)	106.43(2)	CuN_4O_2	N_{eq}	2.140(2, 78)	N_{eq},N_{eq}	103.5(1)	356
(turquoise green)	P-1	10.615(2)	76.64(2)		O_{eq}	1.996(2)	N_{eq},N_{ax}	80.2(1, 1.1)[e]	
	2	8.443(2)	109.40(2)			2.670(3)		96.4(1, 1.3)	
					N_{ax}	2.018(2, 8)	O_{eq},N_{ax}	92.3(1, 1)	
							O_{eq},O_{eq}	53.9(2)[f]	
							N_{ax},N_{ax}	174.6(1)	
							O_{eq},N_{eq}	160.5(1)	
								95.7(1)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	*α* [°] *β* [°] *γ* [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
[Cu(phen)$_2$(ac)]BF$_4$·2H$_2$O	m	9.639(2)		CuN$_4$O$_2$	N$_{eq}$	2.123(4) × 2	N$_{eq}$,N$_{eq}$	114.7(2)	357
(not given)	P2/c	8.237(2)	108.66(2)		O$_{eq}$	2.261(5) × 2	O$_{eq}$,N$_{ax}$	92.0(2, 5)	
	2	17.575(4)			N$_{ax}$	2.000(4) × 2	N$_{eq}$,N$_{ax}$	80.2(2)[e]	
								97.5(2)	
							O$_{eq}$,O$_{eq}$	55.4(1)[f]	
							O$_{eq}$,N$_{eq}$	95.4(2)	
								149.5(2)	
							N$_{ax}$,N$_{ax}$	175.7(2)	
[Cu(phen)$_2$(NO$_2$)]BF$_4$	tr	10.442(4)	93.12(2)	CuN$_4$O$_2$	N$_{eq}$	2.167(3) × 2	N$_{eq}$,N$_{ax}$	80.8(1, 9)[e]	357
(not given)	P-1	16.022(3)	101.86(2)		O$_{eq}$	2.072(4)		98.4(1)	
	2	7.408(2)	110.13(2)			2.597(4)	N$_{eq}$,N$_{eq}$	112.1(1)	
					N$_{ax}$	2.022(4, 27)	N$_{eq}$,O$_{eq}$	93.2(1)	
								105.3(1)	
								141.3(1)	
								154.5(1)	
							O$_{eq}$,N$_{ax}$	90.6(1, 5.8)	
							N$_{ax}$,N$_{ax}$	178.2(1)	
							O$_{eq}$,O$_{eq}$	50.7(1)[f]	
[Cu(phen)$_2$(ac)]ClO$_4$·2H$_2$O	m	9.671(3)		CuN$_4$O$_2$	N$_{eq}$	2.124(4) × 2	N$_{eq}$,N$_{eq}$	113.4(2)	358
(blue)	P2/c	8.282(3)	109.63(2)		O$_{eq}$	2.257(5) × 2	N$_{eq}$,O$_{eq}$	150.2(2)	
	2	17.595(4)			N$_{ax}$	1.994(5) × 2		95.9(2)	
[Cu(phen)$_2$(ac)]NO$_3$·2H$_2$O	tr	14.728(2)	104.19(5)	CuN$_4$O$_2$	N$_{eq}$	2.127(3, 44)	N$_{eq}$,N$_{eq}$	104.3(1)	358
(not given)	P-1	10.499(2)	83.97(5)		O$_{eq}$	2.123(5)	N$_{eq}$,O$_{eq}$	157.7(2)	
	2	8.603(2)	96.81(5)			2.448(5)		97.6(1)	
					N$_{ax}$	2.010(3, 10)			
Cu(Clqo)$_2$(bpy)[c]	tr	15.499(14)	71.26(8)	CuN$_4$O$_2$	N$_{eq}$	2.010(6, 11)	N$_{eq}$,N$_{eq}$	91.5(3, 2.2)	359
(dark red)	P-1	14.260(13)	75.25(4)		O$_{eq}$	2.028(4)		177.0(3)	
	4	11.097(15)	81.07(5)		bpyN$_{eq}$	2.055(6)	N$_{eq}$,N$_{ax}$	76.0(3)[e]	
					bpyN$_{ax}$	2.181(5)		100.2(3, 3.8)	
					O$_{ax}$	2.320(4)	N$_{eq}$,O$_{ax}$	76.0(3)[e]	
								95.0(3, 8)	

							N_{eq},O_{eq}	162.5(3)	
								80.1(3)[e]	
								88.6(3, 8.5)	
							N_{ax},O_{ax}	164.6(2)	
							O_{eq},O_{ax}	90.0(3)	
				CuN_4O_2	N_{eq}	2.051(7, 63)	N_{eq},N_{eq}	93.2(3, 1.2)	
					O_{eq}	2.106(5)		172.2(4)	
					bpyN_{eq}	2.012(5)	N_{eq},N_{ax}	78.2(3)[e]	
					bpyN_{ax}	2.203(5)		96.7(3, 6)	
					O_{ax}	2.262(4)	N_{eq},O_{ax}	77.6(3)[e]	
								92.8(3, 1.4)	
							N_{eq},O_{eq}	79.8(3)[e]	
								94.4(3)	
								170.9(3)	
							N_{ax},O_{ax}	169.6(3)	
							O_{eq},N_{ax}	89.6(3)	
							O_{eq},O_{ax}	98.2(7)	
$Cu(esop)_2(phen)$	tr	12.414(2)	112.55(2)	CuN_4O_2	N_{eq}	2.017(4)	N_{eq},N_{ax}	81.5(1)[e]	360
(green)	P-1	12.882(2)	92.58(1)		phenN_{eq}	2.021(4)		89.6(1, 3.5)	
	2	11.371(2)	83.96(1)		O_{eq}	2.304(4, 1)	N_{eq},N_{eq}	168.5(1)	
					N_{ax}	2.061(3)	N_{eq},O_{eq}	78.0(1)[e]	
					phenN_{ax}	2.031(4)		94.5(2, 1.5)	
							N_{ax},N_{ax}	174.6(2)	
							O_{eq},N_{ax}	76.9(1)[e]	
								94.4(1, 4.5)	
							O_{eq},O_{eq}	164.8(1)	
$Cu(dien)(im)(ClO_4)_2$	or	14.043(2)		CuN_4O_2	imN_{eq}	1.970(5)	N_{eq},N_{eq}	83.6(3)[e]	361
(purple)	Pnma	9.322(2)			N_{eq}	2.009(7, 3)		90.0(3, 6.4)	
	4	12.347(2)			O_3ClO_{ax}	2.667(8, 96)		170.2(3, 4.0)	
							O_{ax},N_{eq}	90.1(3, 11.8)	
							O_{ax},O_{ax}	177.6(3)	
$Cu(dien)(1\text{-}Etim)(ClO_4)_2$	m	8.326(2)		CuN_4O_2	imN_{eq}	1.971(7)	N_{eq},N_{eq}	82.9(4, 7)[e]	361
(purple)	$P2_1/c$	14.600(3)	94.88(2)		N_{eq}	2.012(9, 4)		89.7(4, 7.5)	
	4	15.055(3)			O_3ClO_{ax}	2.628(18, 58)		172.0(4, 5.6)	
							N_{eq},O_{ax}	90.0(5, 9.4)	
							O_{ax},O_{ax}	172.0(5)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	*α* [°] *β* [°] *γ* [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
[Cu(pcam)(pyf)(ClO_4)]·H_2O	m	8.443(4)		CuN_4O_2	pcamN_{eq}	2.012(4, 11)	N_{eq},N_{eq}	82.1(2, 1)[e]	362
(dark blue)	$P2_1/n$	27.145(12)	100.40(6)		pyfN_{eq}	1.931(4)		97.9(2, 3)	
	4	9.781(5)			pyfO_{ax}	2.316(3)		170.5(2, 8.5)	
					O_3ClO_{ax}	2.726(3)	N_{eq},O_{ax}	76.1(1)[e]	
								104.9(1)	
								85.10(3, 2.55)	
								95.3(3, 2.0)	
							O_{ax},O_{ax}	170	
Cu(pcam)(pybox)(SO_3CF_3)	m	9.927(4)		CuN_4O_2	pcamN_{eq}	1.991(5, 56)	N_{eq},N_{eq}	82.0(2, 5)[e]	108
(dark blue)	$P2_1/n$	26.727(5)	98.72(2)		pyboxN_{eq}	2.000(4)		98.0(2, 1.2)	
	4	8.594(4)			pyboxO_{ax}	2.381(4)		170.8(2, 7.3)	
					O_{ax}	2.709(6)	N_{eq},O_{ax}	75.5(2)[e]	
								93.9(2, 11.7)	
							O_{ax},O_{ax}	164.8(2)	
Cu(12-aneN_4ac)$_2$	or	9.444(2)		CuN_4O_2	O_{eq}	1.965(5) × 2	N_{eq},N_{eq}	105.0(3)	363
(light blue)	Pccn	15.300(6)			N_{eq}	2.107(5) × 2	N_{eq},N_{ax}	81.1(2)[e]	
	4	13.109(6)			N_{ax}	2.318(6) × 2	N_{ax},N_{ax}	152.6(3)	
							O_{eq},O_{eq}	88.1(2)	
							O_{eq},N_{ax}	104.9(2)	
							N_{eq},O_{eq}	83.8(2)[e]	
[Cu(bcmgly)$_2$]·2H_2O	m	6.845(1)		CuN_4O_2	O_{eq}	1.954(2) × 2	N_{eq},O_{ax}	77.97(9)[e]	364
(pale blue)	$P2_1/c$	14.095(4)	91.95(2)		N_{eq}	2.062(2) × 2		86.11(9)[e]	
	2	9.427(3)			O_{ax}	2.321(2) × 2	O_{eq},O_{ax}	86.8(1)	
							O_{ax},O_{ax}	180	
[Cu(2-Clbquam)$_2$]Cl_2·2H_2O	tr	6.82(1)	95.3(3)	CuN_4O_2	N_{eq}	2.017(–, 25)	N_{eq},N_{eq}	82.5(3)[e]	365
(deep blue)	P1	7.19(1)	103.0(3)		O_{ax}	2.635 × 2			
	1	8.25(1)	110.0(3)						
[Cu(bpykh)$_2$]Cl_2·4H_2O	m	14.504(4)		CuN_4O_2	N_{eq}	2.000(5, 6)	N_{eq},N_{eq}	87.9(2)[d]	366
(not given)	C2/c	12.333(8)	90.92		O_{ax}	2.465(5) × 2	N_{eq},O_{ax}	74.1(2)[e]	
	4	14.630(3)						89.6(2, 15.5)	

$[Cu(bpykh)_2](NO_3)_2\cdot 2H_2O$	m	7.601(5)		CuN_4O_2	N_{eq}	2.013(5, 23)	N_{eq},N_{eq}	87.3(2)[d]	366
(not given)	$P2_1/n$	11.977(4)	93.10(8)		O_{ax}	2.464(4) × 2	N_{eq},O_{ax}	73.8(2, 3)[e]	
	2	14.463(6)							
$[Cu(aenol)_2](NCS)_2$	tr	6.624(2)	62.78(3)	CuN_4O_2	N_{eq}	2.038(7, 16)	N_{eq},N_{eq}	87.3(3)[d]	367
(violet)	P-1	9.050(4)	80.64(3)		O_{ax}	2.441(8) × 2	N_{eq},O_{ax}	83.0(3, 4.6)[e]	
	1	9.532(4)	70.20(3)						
$[Cu(EtenOH)_2](ClO_4)_2$	m	15.914(3)		CuN_4O_2	N_{eq}	2.027(4, 15)	N_{eq},N_{eq}	84.9(2, 1)[e]	368
(dark blue)	$P2_1/n$	12.710(1)	101.39(2)		O_{ax}	2.460(3, 50)		96.9(1, 1.9)	
	4	9.041(2)						165.9(2, 2)	
							N_{eq},O_{ax}	75.7(1, 1)[e]	
								85.2(1, 4.5)	
								95.5(1, 3.2)	
							O_{ax},O_{ax}	154.7(1)	
$[Cu(pslh)(psalh)](ClO_4)\cdot EtOH$	m	21.230(9)		CuN_4O_2	N_{eq}	1.930(4)	N_{eq},N_{eq}	79.0(2)[e]	369
(green)	$P2_1/n$	11.493(5)	100.47(4)			2.062(4, 19)		99.6(1)	
	4	12.091(5)			O_{eq}	2.062(3)	N_{eq},O_{ax}	71.5(2)[e]	
					N_{ax}	2.277(4)		86.1(1)	
					O_{ax}	2.334(4)		101.3(1)	
							O_{eq},N_{eq}	78.2(1)[e]	
								102.8(1)	
							O_{eq},O_{ax}	97.3(1)	
							O_{eq},N_{ax}	93.9(1)	
							N_{eq},N_{ax}	75.3(2)[e]	
								95.7(2)	
								111.9(2)	
$[Cu(EtenOH)_2](suc)_2$	or	9.589(5)		CuN_4O_2	N_{eq}	2.057(4, 24)	N_{eq},N_{eq}	83.5(1)[e]	370
(not given)	Pbcn	14.003(9)			O_{ax}	2.510(2) × 2		92.5(2, 9.0)	
	4	12.596(10)						172.6(1)	
							N_{eq},O_{ax}	77.3(1)[e]	
								89.9(1, 12.6)	
							O_{ax},O_{ax}	158.0(1)	
$[Cu(peme)_2][Ag_2I_4]$	tr	8.5402(14)	110.221(10)	CuN_4O_2	N_{eq}	2.000(3) × 4	N_{eq},N_{eq}	86.9(1)[e]	371
(pale brown)	P-1	10.0286(16)	95.476(10)		O_{ax}	2.393(3) × 2		93.1(1)	
	1	10.584(2)	93.420(12)				O_{ax},O_{ax}	180	
							N_{eq},O_{ax}	75.4(1)[e]	
								105.9(1, 1.3)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
[Cu(peme)$_2$][Cu$_2$I$_4$] (red brown)	tr P-1 1	8.574(2) 9.860(3) 10.441(3)	109.10(2) 95.04(2) 94.54(2)	CuN$_4$O$_2$	N$_{eq}$ O$_{ax}$	2.011(4, 8) 2.380(4) × 2	N$_{eq}$,N$_{eq}$ N$_{eq}$,O$_{ax}$ O$_{ax}$,O$_{ax}$	86.7(1)^d 99.3(1) 180 74.3(1, 1.5)^e 105.8(1, 1.5) 180	372
[Cu(cyclam)(H$_2$O)$_2$]F$_2$·4H$_2$O (purple)	m C2/m 2	8.179(2) 15.854(2) 7.123(3)	 101.98(3)	CuN$_4$O$_2$	N$_{eq}$ H$_2$O$_{ax}$	2.012(5) × 4 2.484(6) × 2	N$_{eq}$,O$_{ax}$ N$_{eq}$,N$_{eq}$	90.0(2, 1.3) 94.4(3)^d 85.6(3)^e	285
[Cu(tim)(H$_2$O)$_2$](NO$_3$)$_2$ (red violet)	or Cmca 4	12.007(2) 15.690(4) 10.869(5)		CuN$_4$O$_2$	N$_{eq}$ H$_2$O$_{ax}$	1.969(2) × 4 2.556(5) × 2	N$_{eq}$,N$_{eq}$ N$_{eq}$,O$_{ax}$	90.0(1, 8.9)^e 86.5(1)	373
[Cu(Mecyclam)(H$_2$O)$_2$](ClO$_4$)$_2$ (red)	m P2$_1$/c 2	8.201(1) 16.082(3) 10.432(1)	 103.30(1)	CuN$_4$O$_2$	N$_{eq}$ H$_2$O$_{ax}$	2.033(4, 2) 2.815(5) × 2	N$_{eq}$,N$_{eq}$ N$_{eq}$,O$_{ax}$	94.5(1)^d 85.5(1)^e 80.1(1, 2.3)	374
[Cu(tpy)(H$_2$O)(NO$_3$)]NO$_3$·H$_2$O (not given)	tr P-1 2	13.472(1) 10.861(8) 7.863(3)	98.7 78.6 103.6	CuN$_4$O$_2$	N$_{eq}$ H$_2$O$_{ax}$ O$_2$NO$_{ax}$	1.996(−, 44) 2.286(3) 2.695(3)	N$_{eq}$,N$_{eq}$ N$_{eq}$,O$_{ax}$ O$_{ax}$,O$_{ax}$	80.0(−, 2)^e 119.4 90.1(1, 7.1) 172.5(6)	375
Cu(trioc)(ClO$_4$)$_2$^{c} (red)	tr P-1 2	8.572(2) 8.499(3) 15.204(3)	80.42(5) 73.57(3) 69.82(4)	CuN$_4$O$_2$	N$_{eq}$ O$_3$ClO$_{ax}$	2.020(14, 35) 2.757(13) × 2	N$_{eq}$,N$_{eq}$ N$_{eq}$,O$_{ax}$	87.7(6)^e 92.3(6)^d 90.0(5, 1.3)	376
				CuN$_4$O$_2$	N$_{eq}$ O$_3$ClO$_{ax}$	2.018(11, 22) 2.660(19) × 2	N$_{eq}$,N$_{eq}$ N$_{eq}$,O$_{ax}$	85.6(5)^e 94.4(5)^d 90.0(5, 1.4)	
Cu(EtMecyclam)(ClO$_4$)$_2$ (red)	or Pbca 4	14.516(6) 11.674(7) 16.225(9)		CuN$_4$O$_2$	N$_{eq}$ O$_3$ClO$_{ax}$	2.032(6, 2) 2.716(11) × 2	N$_{eq}$,N$_{eq}$	86.3(2)^e 93.7(2)^d	377
Cu(cyclam)(ClO$_4$)$_2$ (not given)	tr P-1 1	8.744(6) 8.022(5) 8.677(6)	118.73(2) 56.94(2) 113.50(2)	CuN$_4$O$_2$	N$_{eq}$ O$_3$ClO$_{ax}$	2.02(4) × 4 2.57(4) × 2	N$_{eq}$,N$_{eq}$	86.0(2)^e 94.0(2)^d	378

$Cu(pyha)(ClO_4)_2$ (blue)	or $P2_12_12_1$ not given	14.295(6) 13.143(6) 9.068(6)		CuN_4O_2	N_{eq} O_3ClO_{ax}	1.99(2, 4) 2.66(2, 15)	N_{eq},N_{eq}	83.7(8, 2.7)[e] 109.5(8) 165.3(7, 4.1)	379
							O_{ax},O_{ax}	172.5(6)	
$Cu(ndap)(ClO_4)_2$ (blue purple)	or $P2_1cn$ 4	9.083(2) 15.198(3) 16.025(3)		CuN_4O_2	N_{eq} O_3ClO_{ax}	1.976(17, 44) 2.726(20, 53)	N_{eq},N_{eq}	83.5(7, 10)[e] 92.5(6)[d] 103.8(1) 165.0(9, 3)	380
$Cu(mmcyclam)(ClO_4)_2$ (not given)	m $P2_1/c$ 4	14.061(1) 8.908(1) 19.710(1)	90.912(5)	CuN_4O_2	N_{eq} O_3ClO_{ax}	2.036(4, 15) 2.677(5, 20)	N_{eq},N_{eq}	85.7(2, 2)[e] 179.7(2, 2) 94.3(2, 3)[d]	381
							N_{eq},O_{ax} O_{ax},O_{ax}	90.0(4, 8.1) 168.2(2)	
$Cu(bpdz)(ClO_4)_2$ (blue violet)	or $Pnm2_1$ 8	13.746(1) 26.388(2) 11.225(1)		CuN_4O_2	N_{eq} O_3ClO_{ax}	2.02(3, 1) 2.67(3, 3)	N_{eq},N_{eq}	83.5(10, 5)[e] 93(1)[d] 98(1, 5) 166.5(10, 25)	382
							N_{eq},O_{ax} O_{ax},O_{ax}	90(1, 15) 171(1)	
$Cu(pydoc)(ClO_4)_2$ (deep blue)	m $C2/c$ 4	14.5156(6) 9.7118(4) 15.8993(6)	111.064(3)	CuN_4O_2	N_{eq} O_3ClO_{ax}	2.016(5, 2) 2.693(4) × 2	N_{eq},N_{eq}	84.6(2)[e] 94.2(2)[d] 92.2(2, 7.6) 157.0(2)	383
							N_{eq},O_{ax}	78.7(2, 1.2) 101.2(2, 4.4)	
$Cu([15]aneN_4)(ClO_4)_2$ (not given)	tr P-1 1	8.663(3) 8.443(3) 7.804(3)	61.27(4) 67.49(3) 69.88(4)	CuN_4O_2	N_{eq} O_3ClO_{ax}	2.035(36, 48) 2.591(4) × 2	N_{eq},N_{eq}	86.1(9, 2.2)[e] 102.0(9) 168.9(8, 7)	384
							N_{eq},O_{ax}	78.7(4) 91.1(6, 1.3)	
$Cu(mmcyclam)(ClO_4)_2$ (red)	m $P2_1/c$ 2	8.47(1) 9.26(1) 16.61(2)	112.3(3)	CuN_4O_2	N_{eq} O_3ClO_{ax}	2.042(3, 20) 2.594(5) × 2	N_{eq},O_{ax} N_{eq},N_{eq}	86.4(1, 3.5) 85.7(1)[e]	385
$Cu(ethc)(ClO_4)_2$ (not given)	m $P2_1/c$ 4	8.968(3) 8.435(3) 32.007(11)	99.18(3)	CuN_4O_2	N_{eq} O_{ax}	2.054(4, 28) 2.31(1, 1)	N_{eq},N_{eq}	72.9(2)[e] 94.6(3, 2.8)[d] 163.2(3, 7)	386
							N_{eq},O_{ax}	96.9(3, 11.1)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
$[Cu(amcyclam)(ClO_4)_2](ClO_4)_2$	m	8.77(2)		CuN_4O_2	N_{eq}	2.024(6, 3)	N_{eq},N_{eq}	94.3(2)[d]	387
$6H_2O$	$P2_1/c$	14.08(1)	107.5(1)		O_3ClO_{ax}	2.523(7) × 2	N_{eq},O_{ax}	91.7(2, 3.8)	
(blue)	2	13.59(2)							
$[Cu(tmte)(NO_3)]NO_3{\cdot}H_2O$	m	13.136(6)		CuN_4O_2	N_{eq}	2.002(6, 4)	N_{eq},N_{ax}	90.6(2, 1.6)[d]	388
(olive green)	$P2_1/c$	17.294(7)	127.66(2)		$(NO_3)O_{eq}$	2.580(8, 77)		151.7(2)	
	4	17.391(4)			N_{ax}	1.961(6, 4)	N_{ax},N_{ax}	175.5(2)	
							O_{eq},N_{eq}	85.1(2, 7.0)	
								125.7(3, 1)	
							O_{eq},O_{eq}	46.5(2)[f]	
							O_{eq},N_{ax}	77.4(2)	
								98.6(2)	
$[Cu(cyclax)(ClO_4)]ClO_4$	m	8.718(3)		CuN_4O_2	N_{eq}	2.016(7, 13)	N_{eq},N_{eq}	93.7(3, 2)[d]	389
(not given)	$P2_1$	13.977(2)	105.93(6)		O_{ax}	2.703(6)		91.2(3, 2)	
	2	9.102(9)			O_3ClO_{ax}	2.582(8)		149.7(3)	
								161.2(3)	
							N_{eq},O_{ax}	73.1(2)[e]	
								92.6(3, 16.6)	
							O_{ax},O_{ax}	164.2(2)	
$[Cu(mntcp)(ClO_4)]ClO_4$	m	8.635(8)		CuN_4O_2	N_{eq}	2.037(6, 56)	N_{eq},N_{eq}	85.7(2, 9)[e]	389
(blue purple)	$P2_1/c$	12.755(3)	105.08(5)		O_{ax}	2.443(5)		94.9(2, 7)[d]	
	4	19.716(8)			O_3ClO_{ax}	2.62(3)		171.9(2, 7)	
							N_{eq},O_{ax}	90.2(7, 16.7)	
								81.4(2)[e]	
								92.6(2, 6.2)	
							O_{ax},O_{ax}	169.6(7, 2.2)	
$[Cu(6\text{-}NO_2cyclam)](EtOH){\cdot}H_2O$	tr	8.537(4)	99.48(5)	CuN_4O_2	O_{eq}	2.005(6, 1)	N_{eq},N_{ax}	86.6(2, 4)[e]	390
(blue)	P-1	8.684(6)	98.69(5)		N_{eq}	2.005(6, 11)		93.4(2)[d]	
	2	21.614(15)	90.51(5)		N_{ax}	2.398(6, 31)	N_{eq},N_{eq}	179.4(3)	
							N_{ax},O_{eq}	91.4(2, 2.1)	
							N_{ax},N_{ax}	179.3(2)	

Ba[Cu(cyclamac)]·$6H_2O$[c] (blue)	tr P-1 2	8.928(3) 10.893(4) 15.889(2)	91.98(2) 101.96(1) 117.28(3)	CuN_4O_2	N_{eq} O_{ax}	2.104(6, 81) 2.302(5) × 2	N_{eq},O_{eq} O_{eq},O_{eq} N_{eq},N_{eq} N_{eq},O_{ax}	90.6(2, 2.8) 85.4(2)[e] 178.0(2) 86.7(2)[e] 83.6(2, 3.1)[e]	391
				CuN_4O_2	N_{eq} O_{ax}	2.097(7, 56) 2.278(6) × 2	N_{eq},N_{eq} N_{eq},O_{ax}	87.2(3)[e] 83.5(2, 3.8)[e]	
$[Cu(en)_2(H_2O)Cl]Cl$ (purple)	m $P2_1/n$ 4	6.18(2) 15.16(4) 11.80(3)	99.0(1)	CuN_4OCl	enN_{eq} H_2O_{ax} Cl_{ax}	2.00(−, 2) 2.62 2.81	N_{eq},N_{eq}	85.2(−, 1)[e]	392
$[Cu(C_{20}H_{28}N_4S)(H_2O](ClO_4)_2$ (not given)	or $P2_12_12_1$ 4	16.793(3) 14.530(2) 10.393(2)		CuN_4OS	N_{eq} S_{ax} H_2O_{ax}	2.050(11, 15) 2.525(4) 2.638(9)		not given	393
Cu(1-viim)$_4Cl_2$ (not given)	m $P2_1/c$ 2	7.40 14.70 11.26	112.1	CuN_4Cl_2	N_{eq} Cl_{ax}	2.04(−, 1) 2.80 × 2	N_{eq},N_{eq} N_{eq},Cl_{ax}	93(2) 90(2)	394
$[Cu(mic)_4Cl_2]\cdot 2H_2O$ (blue)	tr P-1 1	8.888(8) 15.196(9) 15.297(4)	95.59(3) 102.42(2) 93.20(4)	CuN_4Cl_2	N_{eq} Cl_{ax}	2.025(10, 5) 3.060(4) × 2	N_{eq},N_{eq}	89.6(5)	395
Cu(nphyr)$_2Cl_2$ (green)	m C/2c 4	13.786(1) 8.192(1) 16.396(1)	122.5(1)	CuN_4Cl_2	N_{eq} Cl_{eq} N_{ax}	2.028(3) × 2 2.253(1) × 2 2.764(3) × 2	N_{eq},N_{eq} N_{eq},Cl_{ax} Cl_{eq},Cl_{eq}	87.0(2) 90.4(1) 94.6(1)	396
Cu(OH-1,3-pn)$_2Cl_2$ (not given)	tr P-1 1	7.196(2) 7.585(2) 5.864(2)	98.51(2) 102.99(2) 92.97(3)	CuN_4Cl_2	N_{eq} Cl_{ax}	2.038(4, 17) 2.953(1) × 2	N_{eq},N_{eq} N_{eq},Cl_{ax}	87.4(2)[d] 84.6(1, 4.2)	397
Cu(dafone)$_2Cl_2$ (blue)	m $P2_1/n$ 2	6.5911(6) 13.0712(5) 11.4813(9)	95.575(4)	CuN_4Cl_2	N_{eq} Cl_{eq} N_{ax}	1.978(4) × 2 2.292(1) × 2 2.773(4) × 2	N_{eq},Cl_{eq} N_{eq},N_{ax} Cl_{eq},N_{ax}	91.3(1) 76.6(1)[e] 93.11(9)	398
Cu(EtenOH)$_2Cl_2$ (not given)	tr P1 1	6.569(3) 9.472(5) 6.158(3)	98.07(3) 101.57(3) 80.76(4)	CuN_4Cl_2	N_{eq} Cl_{ax}	2.039(5, 21) 2.831(2) × 2	N_{eq},N_{eq} N_{eq},Cl_{ax}	86.3(2)[e] 93.4(2, 3.7)	399
$[Cu(2Me\text{-}1,2\text{-}pn)_2Cl_2]\cdot 0.5MeOH$ (not given)	tg P4/nmm 8	11.827(2) 11.827(1) 21.361(7)		CuN_4Cl_2		not given			308

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
$[Cu(12\text{-}aneN_4)Cl_2]\cdot H_2O$	or	13.452(2)		CuN_4Cl_2	N_{eq}	2.067(1, 22)	N_{eq},N_{eq}	78.86(5)	400
(light green)	Pbca	14.9319(6)			Cl_{eq}	2.292(1, 9)	N_{eq},N_{ax}	77.64(6, 78)[e]	
	8	18.2366(14)			N_{ax}	2.348(2, 15)	N_{ax},N_{ax}	147.81(5)	
							Cl_{eq},N_{ax}	100.77(4, 1.25)	
							Cl_{eq},N_{eq}	92.67(4, 1.66)	
							Cl_{eq},Cl_{eq}	95.81(2)	
$Cu(OH\text{-}1,3\text{-}pn)_2(NCS)_2$	or	8.612(3)		CuN_4S_2	N_{eq}	2.040(6, 18)	N_{eq},N_{eq}	90.3(2)[d]	401
(red)	Pbca	10.926(3)			NCS_{ax}	2.971(2) × 2	N_{eq},S_{ax}	87.8(2, 3.6)	
	4	15.725(5)							
$Cu(1,3\text{-}pn)_2(NCS)_2$	m	13.01(1)		CuN_4S_2	N_{eq}	2.017(5, 12)	N_{eq},N_{eq}	86.5(2)[d]	402
(not given)	C2/c	6.89(1)	92.3(2)		NCS_{ax}	3.154(2) × 2	N_{eq},S_{ax}	94.9(2, 4.5)	
	4	16.12(1)							
$Cu(hd)_2(tu)_2$	m	15.065(4)		CuN_4S_2	hdN_{eq}	2.951(1, 1)	N_{eq},N_{eq}	99.8(1)	403
(dark brown)	C2/c	10.216(3)	103.86(2)		tuS_{ax}	2.941(1) × 2			
	4	15.513(4)							
$Cu(en)_2(Et_2sp)_2$	m	13.597(4)		CuN_4S_2	enN_{eq}	2.03(3, 3)	N_{eq},N_{eq}	83.5(–, 3.3)[e]	404
(dark violet)	$P2_1$	6.945(1)	121.22(1)		S_{ax}	2.97(2, 7)			
	2	16.071(1)							
$[Cu(Meimthp)_2](BF_4)_2\cdot 2EtOH$	m	8.262(2)		CuN_4S_2	N_{eq}	2.01(2, 2)	N_{eq},N_{eq}	90.0(9, 1.5)	405
(not given)	$P2_1/c$	9.609(3)	100.04(2)		S_{ax}	2.790(8) × 2	N_{eq},S_{ax}	80.4(7, 6)[e]	
	2	22.582(5)						99.7(7, 6)	
$[Cu(Meimthb)_2]Cl_2\cdot 2H_2O$	m	7.742(1)		CuN_4S_2	N_{eq}	2.026(3, 8)	N_{eq},N_{eq}	90.5(2)	406
(purple)	$P2_1/c$	14.845(4)	104.80(2)		S_{ax}	2.774(2) × 2	N_{eq},S_{ax}	81.1(2, 1.8)[e]	
	2	9.936(2)							
$[Cu(Phimthp)_2](ClO_4)_2\cdot 5MeOH$	m	12.08(2)		CuN_4S_2	N_{eq}	2.020(9, 1)	N_{eq},N_{eq}	89.0(3)	407
(orange brown)	$P2_1/c$	11.98(2)	96.19(4)		S_{ax}	2.824(5) × 2	N_{eq},S_{ax}	78.6(3, 4)[e]	
	2	18.93(3)							
$[Cu(9\text{-}aneN_2S)_2](NO_3)_2$	or	14.50(1)		CuN_4S_2	N_{eq}	2.077(3, 20)	N_{eq},N_{eq}	84.1(1)[e]	408
(purple)	Pbca	10.34(1)			S_{ax}	2.707(1) × 2		95.9(1)	
	4	12.95(1)					N_{eq},S_{ax}	82.0(1, 2.2)[e]	
								98.0(1, 2.2)	

$[Cu(daes)_2]\cdot(NO_3)_2$[c]	tr	10.50(1)	90.34(5)	CuN_4S_2	N_{eq}	2.058(4, 12)	N_{eq},N_{eq}	90.0(2, 1.2)	408
(dark blue)	P-1	9.96(1)	99.67(5)		S_{ax}	2.745(1) × 2	N_{eq},S_{ax}	81.3(1, 8)[e]	
	2	8.55(1)	89.24(5)					98.7(1, 8)	
				CuN_4S_2	N_{eq}	2.057(4, 4)	N_{eq},N_{eq}	90.0(2, 1.6)	
					S_{ax}	2.772(1) × 2	N_{eq},S_{ax}	81.5(1, 1.2)[e]	
								98.6(1, 1.2)	
$Cu(cyclam)(F_5Sph)_2$	tr	7.140(4)	75.02(3)	CuN_4S_2	N_{eq}	2.008(3, 3)	N_{eq},N_{eq}	85.2(1)[e]	409
(red)	P-1	8.320(5)	88.97(4)		S_{ax}	2.940(1) × 2		94.8(1)	
	1	12.033(9)	71.07(5)					180	
							N_{eq},S_{ax}	90.0(1, 7.1)	
							S_{ax},S_{ax}	180	
$[Cu(2Me\text{-}1,2\text{-}pn)_2Br_2]\cdot 0.6H_2O$	tg	12.171(2)		CuN_4Br_2		not given			308
(not given)	I4cm	12.171(2)							
	8	21.435(9)							
$Cu(dmpr)_2(NCSe)_2$	or	8.852(4)		CuN_4Se_2	N_{eq}	2.033(10, 13)	N_{eq},N_{eq}	90.2(4)[d]	410
(not given)	Pbca	10.888(6)			$NCSe_{ax}$	3.109(2) × 2	N_{eq},Se_{ax}	87.4(3, 3.9)	
	4	15.947(8)							
$Cu(2Me\text{-}1,2\text{-}pn)_2I_2$	m	12.815(8)		CuN_4I_2		not given			308
(not given)	Pc;P2/c	12.215(5)	104.36(6)						
	8	20.777(12)							
$(cbq)_2[CuCl_4(H_2O)_2]$	m	6.522(3)		$CuCl_4O_2$	H_2O_{eq}	1.992(3)	O_{eq},Cl_{eq}	81.57(8)	411
(not given)	$P2_1/c$	11.218(3)	110.66(3)		Cl_{eq}	2.305(1)	O_{eq},Cl_{ax}	89.46(8)	
	2	11.790(3)			Cl_{ax}	2.791(1)	Cl_{eq},Cl_{ax}	88.07(3)	
$(NH_4)_2[Cu(NH_3)_2Cl_4]$	c	3.91(1)		$CuCl_4N_2$	H_3N	1.96(1)		not given	412
(not given)	Pm3				Cl	2.76(1)			
	1/4								
$[Cu(acth)_2Cl_4]\cdot H_2O$	m	15.153(14)		$CuCl_4N_2$	N_{eq}	2.049(3) × 2	N_{eq},Cl_{eq}	97.2(1)	413
(olive green)	C2/c	6.962(14)	121.47(6)		Cl_{eq}	2.258(2) × 2	N_{eq},Cl_{ax}	88.9(1)	
	4	18.274(16)			Cl_{ax}	2.967(2) × 2	Cl_{eq},Cl_{ax}	90.0(1)	
$[Cu(dsco)_2](ClO_4)_2$	m	6.811(3)		CuS_4O_2	S	2.334(1, 1)	S,S	91.0(1)[d]	414
(purple)	$P2_1/c$	9.225(4)	90.54(3)		O	2.350(1) × 2	S,O	80.7(1, 1.0)[e]	
	2	16.575(5)							
$[Cu(14\text{-}aneS_4)(ClO_4)_2]$	m	7.904(3)		CuS_4O_2	S_{eq}	2.303(1, 6)	S_{eq},S_{eq}	89.9(4)[e]	415
(blue)	$P2_1/c$	8.830(4)	126.33(2)		O_3ClO_{ax}	2.652(4) × 2		90.1(4)[d]	
	2	16.840(6)					S_{eq},O_{ax}	92.4(2, 5.4)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
Cu(15-ane-S_4)$(ClO_4)_2$	m	7.994(1)		CuS_4O_2	S_{eq}	2.318(3, 5)	S_{eq},S_{eq}	90.3(1)[d]	416
(not given)	$P2_1/c$	9.167(3)	100.96(5)		O_3ClO_{ax}	2.53(1) × 2	S_{eq},O_{ax}	89.2(2, 3.9)	
	2	13.978(3)							
Cu(16-aneS_4)$(ClO_4)_2$	m	7.931(3)		CuS_4O_2	S_{eq}	2.359(1, 28)	S_{eq},S_{eq}	90.37(5)[d]	416
(not given)	$P2_1/c$	9.613(5)	110.71(3)		O_3ClO_{ax}	2.482(5) × 2	S_{eq},O_{ax}	88.8(2, 2.9)	
	2	14.885(5)							
[Cu(18-aneS_4N_2)]ClO_4·H_2O	or	12.020(8)		CuS_4N_2	S_{eq}	2.543(5, 56)	S_{eq},S_{eq}	86.11(16)[f]	417
(not given)	Pcab	17.733(17)			N_{ax}	2.022(13, 15)		84.23(17)[e]	
	8	21.999(23)						95.77(16, 54)	
								169.57(17, 11)	
							N_{ax},S_{eq}	84.83(4, 1.23)[e]	
								95.03(5, 37)	
							N_{ax},N_{ax}	178.8(6)	
$(NH_4)_2$[Cu$(NH_3)_2Br_4$]	c	4.070(1)		$CuBr_4N_2$	N	2.035(1) × 2		not given	418
(not given)	Pm3				Br	2.878(1) × 4			
	1/4								
Cu$(prtac)_2(qu)_3$	tr	11.55(1)	100.32(5)	CuO_3N_3	O	1.990(7, 30)	O,O	55.1(2)[f]	419a
(blue)	P-1	16.912(6)	109.96(13)			2.642(10)		178.8(2)	
	2	9.729(9)	79.50(5)		N	2.047(9, 3)	N,N	98.1(3, 3.9)	
						2.359(11)		163.7(3)	
							O,N	89.9(3, 2.2)	
[Cu(pmca)$(H_2O)_3$]NO_3·$2H_2O$	tr	13.626(3)	101.48(1)	CuO_3N_3	N_{eq}	2.000(17, 62)	N_{eq},N_{eq}	81.79(7, 22)[e]	419b
(blue)	P-1	6.512(1)	109.32(1)		H_2O_{eq}	1.976(2)		163.50(9)	
	2	10.497(2)	94.83(1)		H_2O_{ax}	2.011(2, 9)	N_{eq},O_{eq}	98.25(7, 2.48)	
								173.78(8)	
							N_{eq},O_{ax}	92.04(7, 7.79)	
							O_{eq},O_{ax}	79.90(7)	
							O_{ax},O_{ax}	165.54(8)	
[Cu(azcm)$(H_2O)_2$·(SO_4)]·$3H_2O$	m	13.652(1)		CuO_3N_3	H_2O_{eq}	1.968(−, 19)	N_{eq},O_{ax}	93.50(6, 5.47)	420
(deep green)	Cc	14.630(1)	95.34(8)		N_{eq}	1.966(−, 6)	N_{ax},N_{eq}	87.11(6)[e]	

	4	6.795(1)			N_{ax}	2.793		89.35(6)	
					O_3SO_{ax}	2.500	N_{ax},O_{ax}	172.90(5)	
							N_{eq},N_{eq}	80.56(7)[e]	
							N_{eq},O_{eq}	95.58(7, 4)	
								171.77(8, 3.73)	
							O_{eq},O_{eq}	88.65(8)	
							O_{eq},O_{ax}	91.28(7, 91)	
							O_{eq},N_{ax}	87.11(7, 5.62)	
Cu(amdza)(H_2O)(ClO_4)$_2$	m	12.661(3)		CuO_3N_3	N_{eq}	2.003(5, 4)	N_{eq},N_{eq}	85.5(2, 6)[e]	387
(not given)	$P2_1/c$	13.660(7)	130.03(2)		H_2O_{eq}	1.968(5)		164.7(2)	
	4	16.403(4)			O_3ClO_{ax}	2.729(5, 92)	N_{eq},O_{eq}	94.8(2, 9)	
							N_{eq},O_{ax}	72.9(1)	
								84.6(1, 2.4)	
								97.1(2, 1.1)	
								120.3(1)	
							O_{eq},O_{ax}	83.4(2, 1.2)	
							O_{ax},O_{ax}	150.3(2)	
[Cu(terpy)(fm)(H_2O)]·(ClO_4)	m	7.341(3)		CuO_3N_3	H_2O_{eq}	2.247(3)	O_{eq},O_{ax}	51.9(1)[f]	421
(blue)	$P2_1/c$	13.919(2)	101.68(3)		terpyN_{eq}	2.011(4, 64)		88.4(1)	
	4	18.081(3)			fmO_{eq}	1.935(3)	O_{ax},O_{ax}	140.0(1)	
					fmO_{ax}	2.815(4)	N_{eq},O_{ax}	94.7(1, 6.0)	
								120.5(1)	
							N_{eq},O_{eq}	99.4(1, 6)	
								172.4(1)	
							N_{eq},N_{eq}	80.0(2, 1)[e]	
								158.5(1)	
[Cu(croc)(terpy)(H_2O)][Cu(croc)-(terpy)]·$4H_2O$[c]	tr	15.204(3)	84.18(2)	CuO_3N_3	terpyN_{eq}	1.987(9.67)	O_{eq},O_{ax}	80.4(2)[e]	422
(blue)	P-1	12.825(2)	110.18(2)		crocO_{eq}	1.962(7)		90.1(3)	
	2	11.006(2)	105.22(2)		crocO_{ax}	2.393(6)	N_{eq},O_{eq}	100.2(3, 6)	
					H_2O_{ax}	2.420(7)		172.4(2)	
							N_{eq},O_{ax}	92.2(3, 5.1)	
							N_{eq},N_{eq}	79.1(3)[e]	
								80.6(4)	
								159.7(3)	
							O_{ax},O_{ax}	170.5(3)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
				CuN_3O_2	terpyN_{eq}	2.043(7, 97)	N_{eq},N_{eq}	80.1(3, 2)	
					crocO_{eq}	2.318(7)	N_{eq},O_{eq}	99.1(3, 2)	
					crocO_{ax}	1.940(7)		172.4(4)	
							N_{eq},O_{ax}	89.1(3)	
								106.0(3, 4)	
							O_{eq},O_{ax}	81.9(3)	
[Cu(terpy)(H_2O)(ox)]·4H_2O	tr	10.192(2)	86.65(3)	CuO_3N_3	terpyN_{eq}	2.023(2, 95)	O_{eq},O_{ax}	79.64(9)[e]	423
(green)	P-1	12.319(2)	96.80(3)		oxO_{eq}	1.928(2)		88.39(10)	
	2	8.397(3)	106.14(1)		oxO_{ax}	2.249(2)	N_{eq},O_{ax}	96.66(10, 10.14)	
					H_2O_{ax}	2.559(3)	N_{eq},N_{eq}	79.58(10, 7)[e]	
								158.89(1)	
							O_{ax},O_{ax}	167.41(9)	
							O_{eq},N_{eq}	100.43(10, 50)	
								179.24(10)	
Cu(hist)(thr))(H_2O)	m	5.843(10)		CuO_3N_3	thrN_{eq}	2.00	N_{eq},O_{ax}	68.3[e]	424
(blue)	$P2_1$	12.249(10)	102.46		thrO_{eq}	1.97			
	2	11.049(10)			histN_{eq}	1.98(–, 3)			
					histO_{ax}	2.58			
Cu(ibpca)(ac)(H_2O)	m	7.130(2)		CuO_3N_3	N_{eq}	1.981(5, 59)	O_{eq},O_{ax}	54.1(2)[f]	425
(green)	$P2_1/c$	10.918(3)	105.59(2)		acO_{eq}	1.987(4)		103.8(2)	
	4	21.686(7)			acO_{ax}	2.636(5)	O_{ax},O_{ax}	157.7(1)	
					H_2O_{ax}	2.518(4)	N_{eq},O_{ax}	93.9(2, 11.1)	
							N_{eq},O_{eq}	93.6(2, 4.9)	
								159.1(2)	
							N_{eq},N_{eq}	81.5(2)[e]	
								94.1(2)[d]	
								170.3(2)	
Cu(asp)(hist)(H_2O)	m	12.654(4)		CuO_3N_3	aspN_{eq}	2.019(8)	N_{eq},O_{ax}	74.3(3)[e]	426
(light blue)	$P2_1$	11.623(4)	100.47(3)		aspO_{eq}	1.972(6)		91.8(3, 8.1)	
	2	5.931(2)			histN_{eq}	1.980(7, 26)	O_{eq},O_{ax}	100.2(3)	
					histO_{ax}	2.366(7)	O_{ax},O_{ax}	87.7(2)	

					H_2O_{ax}	2.642(7)		170.8(2)	
							N_{eq},N_{eq}	92.8(3)[d]	
								93.6(3, 8)	
							N_{eq},O_{eq}	172.1(3, 9)	
								91.4(3)	
								82.2(3)[e]	
[Cu(ptcbx)(bpy)(H_2O)]·3H_2O	m	7.046(1)		CuO_3N_3	H_2O_{eq}	1.972(3)	N_{eq},N_{eq}	81.1(1)[e]	427
(not given)	$P2_1/n$	26.459(3)	102.90(1)		bpyN_{eq}	1.999(3, 6)		97.0(1)	
	4	11.001(2)			N_{eq}	2.013(3)		177.1(1)	
					O_{ax}	2.445(3, 54)	N_{eq},O_{ax}	85.8(1, 2.8)	
								106.2(1, 1.8)	
								74.3(1)[e]	
							N_{eq},O_{eq}	73.1(1)[e]	
								93.0(1)	
								171.1(2)	
							O_{ax},O_{ax}	146.7(1)	
							O_{eq},O_{ax}	92.8(1, 8)	
[Cu(salen)(cyt)(NO_3)]·H_2O	m	7.453(3)		CuO_3N_3	salN_{eq}	1.993(1, 55)	N_{eq},N_{eq}	83.4(1)[e]	428
(deep blue)	$P2_1/c$	12.555(2)	110.07(3)		salO_{eq}	1.922(1)		94.4(1)	
	4	20.36(7)			cytN_{eq}	2.008(1)		174.6(1)	
					cytO_{ax}	2.772(1)	N_{eq},O_{eq}	90.9(1, 2.3)	
					O_2NO_{ax}	2.806(1)		88.6(1)[d]	
								175.5(1)	
Cu(phepy)(NO_3)$_2$	m	11.1956(2)		CuO_3N_3	N_{eq}	1.998(3, 85)	N_{eq},N_{eq}	79.2(1)[e]	429
(dark green)	$P2_1/c$	14.3477(12)	123.36(1)		(NO_3)O_{eq}	1.968(3)		80.0(1)	
	4	16.2180(15)			O_2NO_{ax}	2.213(4)		158.8(1)	
					(NO_3)O_{ax}	2.533(5)	N_{eq},O_{eq}	98.5(1)	
								161.2(2)	
							N_{eq},O_{ax}	97.1(2, 9.5)	
							O_{eq},O_{ax}	55.9(1)[f]	
								92.1(1)	
							O_{ax},O_{ax}	147.9(1)	
[Cu(bimpa)(NO_3)(MeOH)]NO_3	or	16.136(5)		CuO_3N_3	N_{eq}	1.949(5, 4)	N_{eq},N_{eq}	82.5(2, 2)[e]	430
(not given)	Pbca	15.316(5)				2.102(5)		164.6(2)	
	8	18.901(3)			(NO_3)O_{eq}	1.982(4)	N_{eq},O_{ax}	89.6(2, 3.6)	
					(NO_3)O_{ax}	2.602(5)		109.3(2, 9.2)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
					$MeHO_{ax}$	2.390(5)	N_{eq},O_{eq}	97.7(2, 7)	
								172.7(2)	
							O_{eq},O_{ax}	54.3(2)[f]	
								89.3(2)	
							O_{ax},O_{ax}	143.4(2)	
$[Cu(bimpa)(NO_3)\cdot(MeOH)]NO_3$	or	16.635(3)		CuO_3N_3	N_{eq}	1.924(6, 8)	N_{eq},N_{eq}	82.4(2, 3)[e]	430
(not given)	Pbca	18.768(4)				2.138(6)		163.4(2)	
	8	15.548(5)			$(NO_3)O_{eq}$	1.998(4)	N_{eq},O_{ax}	90.3(2, 7.1)	
					$(NO_3)O_{ax}$	2.637(5)		104.8(2, 7)	
					$MeHO_{ax}$	2.266(6)	N_{eq},O_{eq}	99.2(2)	
								157.2(2)	
							O_{eq},O_{ax}	53.3(2)[f]	
								97.2(2)	
							O_{ax},O_{ax}	147.5(2)	
$[Cu(bzibza)(NO_3)(MeOH)]NO_3$	m	10.409(4)		CuO_3N_3	N_{eq}	1.941(6, 1)	N_{eq},N_{eq}	82.4(2, 4)[e]	431
(blue)	$P2_1/n$	16.237(5)	103.82(3)			2.109(6)		163.4(2)	
	4	15.828(5)			$(NO_3)O_{eq}$	1.998(4)	N_{eq},O_{ax}	85.3(2, 5)	
					$(NO_3)O_{ax}$	2.637(5)		104.6(2, 8)	
					$MeHO_{ax}$	2.266(6)	N_{eq},O_{eq}	96.6(2, 3.4)	
								157.2(2)	
							O_{eq},O_{ax}	53.3(2)[b]	
								97.2(2)	
							O_{ax},O_{ax}	147.5(2)	
$[Cu(terpy)(NO_3)(MeOH)]ClO_4$	tr	9.105(2)	78.21(2)	CuO_3N_3	N_{eq}	1.969(3, 48)	N_{eq},N_{eq}	80.4(1, 1)[e]	432
(blue)	P-1	9.588(2)	80.45(2)		$(NO_3)O_{eq}$	1.975(2)		160.8(1)	
	2	11.753(3)	69.72(1)		$(NO_3)O_{ax}$	2.634(3)	O_{eq},N_{eq}	99.5(1, 1.5)	
					$MeHO_{ax}$	2.284(3)		165.5(1)	
							N_{eq},O_{ax}	86.2(1, 2.3)	
								103.7(1, 1.0)	
								112.4(1)	
							O_{eq},O_{ax}	53.8(1)[b]	
								91.8(1)	
							O_{ax},O_{ax}	142.1(1)	

$[Cu(asp)(phen)(H_2O)]\cdot 4H_2O$	or	23.852(2)		CuO_3N_3	phenN_{eq}	2.002(−, 18)	N_{eq},N_{eq}	176.4(1)	433
(blue)	$P2_12_12_1$	11.731(1)			aspN_{eq}	1.989		100.3(1)	
	4	6.969(1)			aspO_{ax}	2.560		82.0(1)[e]	
					H_2O_{ax}	2.446	N_{eq},O_{eq}	84.1(1)[e]	
								93.8(1)	
								174.3(1)	
							N_{eq},O_{ax}	78.2(1)[e]	
								93.4(1, 11.1)	
							O_{eq},O_{ax}	87.9(1, 4.2)	
							O_{ax},O_{ax}	169.2(1)	
$[Cu(terpy)(odac)]\cdot 2H_2O$	m	10.681(6)		CuO_3N_3	terpyN_{eq}	2.004(4, 62)	N_{eq},N_{eq}	80.0(1, 0)[e]	434
(green)	$P2_1/c$	22.44(1)	136.1(2)		odacO_{eq}	2.070(5)	O_{eq},O_{ax}	73.4(2, 1.0)[e]	
	4	11.534(6)			odacO_{ax}	2.257(5, 55)	O_{ax},O_{ax}	146.6(1)	
							N_{eq},O_{ax}	97.5(2, 18.3)	
							N_{eq},O_{eq}	99.9(4, 3)	
								170.0(2)	
$[Cu(opai)(ClO_4)_2]\cdot 0.5H_2O$	m	32.777(8)		CuO_3N_3	N_{eq}	2.003(3, 27)	N_{eq},N_{eq}	88.6(1)	435
(deep blue)	C2/c	9.395(2)	111.97(2)		O_{eq}	2.008(3)		176.9(1)	
	8	14.14(6)					N_{eq},O_{eq}	83.7(1)	
								174.5(1)	
$[Cu(ac)(C_6H_{21}N_4O_2)]\cdot 0.5H_2O$[c]	tr	15.873(15)	93.080(8)	CuO_3N_3	acO	1.979(3)	O,O	52.48(10)[f]	436
(green)	P-1	9.693(9)	93.378(8)			2.765(3)		94.6	
	4	13.104(22)	95.29(7)		O	2.527(3)		146.9	
					N	1.998(3, 39)	N,N	82.04(14)[e]	
								94.88(13)	
								168.28(14)	
							O,N	78.67(11)[e]	
								97.1(1, 17.1)[f]	
				CuO_3N_3	acO	1.969(3)	O,O	55.74(10)[f]	
						2.612(3)		94.8	
					O	2.707(3)		150.5	
					N	1.996(3, 41)	N,N	82.68(13)[e]	
								96.41(13)	
								165.43(13)	
							O,N	77.27(11)[e]	
								96.5(1, 14.9)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
$[Cu(17\text{-}aneN_3O_2)(H_2O)](ClO_4)_2$	m	12.350(27)		CuO_3N_3	H_2O_{eq}	2.02(5)	O_{ax},O_{ax}	145.4(1)	437
(not given)	$P2_1/n$	13.879(16)	101.16(16)		N_{eq}	2.01(5, 2)	O_{ax},O_{eq}	94.0(2, 3.6)	
	4	15.954(30)			O_{ax}	2.49(4, 19)	N_{eq},O_{ax}	73.4(2, 2.8)[e]	
								85.1(2, 3.6)[d]	
								98.2(2)	
								125.4(2)	
							N_{eq},O_{eq}	87.3(2, 5)	
								161.9(2)	
							N_{eq},N_{eq}	84.8(2)[e]	
								104.5(2)	
								163.1(2)	
$Cu(dacac)(N_3)$	or	32.289(4)		CuO_3N_3	$(N_3)N_{eq}$	1.950(4)	N_{eq},O_{ax}	76.09(10, 89)[e]	438
(violet blue)	Pccn	13.187(2)			N_{eq}	2.057(3, 25)		100.08(10, 5.12)	
	8	8.679(1)			O_{eq}	1.925(3)	N_{eq},N_{eq}	94.6(1, 4.5)	
					O_{ax}	2.779(2, 3)		170.1(1)	
							N_{eq},O_{eq}	85.4(1, 1.1)[d]	
								174.4(1)	
							O_{eq},O_{ax}	82.39(9, 2)[d]	
							O_{ax},O_{ax}	164.73(8)	
$[Cu(dtpa)]\cdot H_2O$	tr	6.443(2)	101.20(4)	CuO_3N_3	N_{eq}	2.049(2, 7)	N_{eq},N_{eq}	85.40(8, 2.05)[e]	439
(blue)	P-1	9.524(4)	93.89(4)		O_{eq}	1.974(2, 2)	N_{eq},O_{eq}	81.97(7)[e]	
	2	16.308(8)	104.51(3)		O_{ax}	2.518(2)		166.55(6, 27)	
					N_{ax}	2.336(2)	N_{eq},O_{ax}	72.76(7)[e]	
							O_{eq},N_{ax}	76.79(7)[e]	
							O_{ax},N_{ax}	144.28(4)	
$[Cu(ottd)]\cdot 5H_2O$	m	11.19(3)		CuO_3N_3	O_{eq}	1.973(6)	N_{eq},N_{eq}	94.7(3, 1.9)[d]	440
(blue)	$P2_1/c$	12.19(2)	110.16(9)		N_{eq}	2.150(7, 44)		153.4(2)	
	4	16.22(6)				1.983(7)	N_{eq},O_{ax}	76.7(3, 2.6)[e]	
					O_{ax}	2.414(6)		96.1(3, 8)	
						2.171(6)		127.8(3)	
							O_{eq},N_{eq}	81.7(3)[e]	
								89.3(3)	
								174.1(2)	

							O_{eq},O_{ax}	85.4(3, 6)	
							O_{ax},O_{ax}	149.5(1)	
Cu(dacac)Cl	or	12.734(2)		CuO_3N_2Cl	O_{eq}	1.929(3)	N_{eq},Cl_{eq}	94.2(1, 9)	441
(dark blue)	Pbca	11.965(2)			N_{eq}	2.044(3, 22)	Cl_{eq},O_{eq}	177.6(1)	
	8	23.252(3)			Cl_{eq}	2.261(1)	N_{eq},O_{ax}	76.3(1, 1)[e]	
					O_{ax}	2.760(3, 7)		102.7(1, 2)	
							N_{eq},N_{eq}	171.6(1)	
							O_{ax},O_{ax}	164.7(1)	
							O_{eq},O_{ax}	82.4(1, 3)	
							N_{eq},O_{eq}	85.8(1, 1.2)	
							Cl_{eq},O_{ax}	97.6(7, 1.7)	
[Cu(pith)(H_2O)(ClO_4)$_2$]·H_2O	m	9.212(7)		CuO_3N_2S	N_{eq}	1.972(3, 29)	S_{eq},O_{eq}	97.05(8)	442
(deep green)	$P2_1/c$	14.439(6)	95.60(6)		S_{eq}	2.320(1)	N_{eq},O_{ax}	91.43(10, 9.53)	
	4	15.117(9)			H_2O_{eq}	1.931(2)	S_{eq},O_{ax}	89.78(8, 4.16)	
					O_3ClO_{ax}	2.525(4, 35)	S_{eq},N_{eq}	84.70(8)[e]	
								163.01(8)	
							N_{eq},N_{eq}	82.56(10)[e]	
							N_{eq},O_{eq}	96.54(10)	
								175.29(11)	
							O_{eq},O_{ax}	87.90(12, 4.34)	
							O_{ax},O_{ax}	175.68(11)	
[Cu(fpsem)(H_2O)(ClO_4)$_2$]·2H_2O	m	12.9615(5)		CuO_3N_2S	N_{eq}	1.975(3, 42)	N_{eq},N_{eq}	80.5(1)[e]	443
(green black)	$P2_1/c$	9.7638(4)	111.580(4)		S_{eq}	2.278(1)	N_{eq},S_{eq}	85.2(1)[e]	
	4	14.9964(8)			H_2O_{eq}	1.935(2)		165.7(1)	
					O_3ClO_{ax}	2.652(5, 58)	N_{eq},O_{eq}	96.2(1)	
								175.9(2)	
							N_{eq},O_{ax}	82.1(1, 6.7)	
							S_{eq},O_{eq}	98.1(1)	
							S_{eq},O_{ax}	101.1(1, 2.2)	
							O_{eq},O_{ax}	93.4(2, 5)	
							O_{ax},O_{ax}	155.9(2)	
[Cu(bpy)(tdac)(H_2O)]·4H_2O	m	11.136(7)		CuO_3N_2S	bpyN_{eq}	2.022(4, 3)	N_{eq},O_{eq}	93.2(2, 1.5)	444
(light blue)	$P2_1/c$	21.13(1)	113.2(2)		tdacO_{eq}	1.975(4, 2)		172.3(2, 4)	
	4	8.999(6)			tdacS_{ax}	2.697(1)	S_{ax},O_{eq}	80.2(1, 4)[e]	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
					H_2O_{ax}	2.353(3)	N_{eq},S_{ax}	102.5(1, 4.1)	
							O_{eq},O_{eq}	93.1(2)	
							O_{eq},O_{ax}	87.8(1, 4.7)	
							N_{eq},N_{eq}	80.9(2)[e]	
							N_{eq},O_{ax}	91.1(2, 1)	
							O_{ax},S_{ax}	161.0(1)	
[Cu(Me-pyrpy)Cl]ClO_4	or	11.057(1)		CuN_3O_2Cl	N_{eq}	2.106(5, 7)	N_{eq},Cl_{eq}	100.23(14, 21)	445
(blue)	$P2_12_12_1$	12.643(1)				1.930(4)		179.00(14)	
	4	16.799(3)			Cl_{eq}	2.2248(14)	Cl_{eq},O_{ax}	91.32(14, 1.62)	
					O_{ax}	2.494(5, 28)	N_{eq},N_{eq}	79.73(23, 29)[e]	
								159.55(18)	
							N_{eq},O_{ax}	78.24(20, 57)[e]	
								94.98(21, 8.91)	
							O_{ax},O_{ax}	176.81(17)	
[Cu(OH-pyrpy)Cl]$ClO_4 \cdot H_2O$	or	11.207(1)		CuN_3O_2Cl	N_{eq}	2.118(6, 12)	Cl_{eq},N_{eq}	100.24(18, 24)	445
(blue)	$P2_12_12_1$	11.628(1)				1.939(5)		178.53(17)	
	4	17.174(2)			Cl_{eq}	2.2205(18)	Cl_{eq},O_{ax}	93.28(20, 8)	
					O_{ax}	2.468(6, 15)	N_{eq},N_{eq}	79.73(23, 29)[e]	
								159.39(24)	
							N_{eq},O_{ax}	78.18(22, 49)[e]	
								93.93(25, 9.45)	
							O_{ax},O_{ax}	172.68(24)	
[Cu(bz-pyrpy)Cl]ClO_4[c]	or	11.724(1)		CuN_3O_2Cl	N_{eq}	2.110(10, 3)	Cl_{eq},N_{eq}	100.7(3, 5)	445
(blue)	$P2_12_12_1$	30.346(5)				1.938(9)		175.0(3)	
	8	17.871(2)			Cl_{eq}	2.204(3)	Cl_{eq},O_{ax}	87.9(2, 5)	
					O_{ax}	2.563(8)	N_{eq},N_{eq}	79.5(4, 8)[e]	
						2.664(8)		158.6(4)	
							N_{eq},O_{ax}	77.1(3, 1.4)[e]	
								97.9(3, 10.1)	
							O_{ax},O_{ax}	173.5(3)	
				CuN_3O_2Cl	N_{eq}	2.122(11, 2)	Cl_{eq},N_{eq}	99.5(3, 3)	
						1.928(10)		177.7(4)	

					Cl_{eq}	2.196(4)	Cl_{eq},O_{ax}	90.9(3, 2.5)	
					O_{ax}	2.609(11, 77)	N_{eq},N_{eq}	80.6(4, 1.2)[e]	
								161.1(4)	
							N_{eq},O_{ax}	77.2(4, 4)[e]	
								95.8(4, 7.7)	
							O_{ax},O_{ax}	178.3(4)	
[Cu(pdto)(1-Meim)(ClO_4)]ClO_4	m	8.996(2)		CuN_3S_2O	imN_{eq}	2.011(5)	N_{eq},S_{eq}	85.0(1)[e]	446
(deep blue)	$P2_1/c$	18.435(4)	116.84(1)		N_{eq}	1.996(5, 2)		91.8(2)	
	4	13.687(3)			S_{eq}	2.414(2)	N_{eq},N_{eq}	90.7(2, 6)	
					S_{ax}	2.560(2)	S_{eq},S_{ax}	86.1(3)[e]	
					O_3ClO_{ax}	2.845(2)	N_{eq},S_{ax}	84.1(2)[e]	
								105.5(2, 3.2)	
							S_{ax},O_{ax}	157.0(1)	
Cu(imdth)(NO_3)(NCS)	m	9.641(2)		CuN_3S_2O	SCN_{eq}	1.968(9)	S_{eq},S_{ax}	84.0(1)[e]	447
(green)	$P2_1/n$	8.040(3)	92.56(2)		N_{eq}	1.969(9, 1)	N_{eq},S_{ax}	99.2(3, 1.6)	
	4	25.480(6)			S_{eq}	2.370(4)		80.1(3)[e]	
					S_{ax}	2.746(4)	S_{eq},O_{ax}	88.6(2)	
					O_2NO_{ax}	2.70(1)	N_{eq},O_{ax}	89.5(4, 3.7)	
							S_{eq},N_{eq}	83.0(3)[e]	
								89.0(3)	
								174.6(3)	
							N_{eq},N_{eq}	94.1(4, 2)	
								171.9(4)	
							S_{ax},O_{ax}	166.1(2)	
[Cu(dtun)Br]Br·H_2O	m	5.559(7)		CuS_3N_2Br	N_{eq}	2.03(2) × 2	N_{eq},S_{eq}	85.1(5)[e]	448
(not given)	$P2_1/m$	10.009(11)	90.0(1)		S_{eq}	2.340(6) × 2		170.6(5)	
	2	14.720(13)			S_{ax}	2.576(9)	N_{eq},S_{ax}	102.2(5)	
					Br_{ax}	3.130(5)	N_{eq},Br_{ax}	80.6(5)	
							N_{eq},N_{eq}	95.4(5)	
							S_{eq},S_{ax}	86.8(2)[e]	
							S_{eq},Br_{ax}	90.3(2)	
							S_{eq},S_{eq}	92.9(2)	
							S_{ax},Br_{ax}	175.7(2)	
[Cu(nc)$_2$(H_2O)$_2$$F_2$]·4$H_2O$	tr	8.895(1)	110.57(1)	$CuF_2O_2N_2$	N_{eq}	2.009(3) × 2	N_{eq},F_{eq}	90.7(5)	449
(blue)	P-1	8.008(1)	103.11(1)		F_{eq}	1.911(3) × 2	O_{ax},N_{eq}	87.1(5)	
	1	7.222(1)	90.36(1)		H_2O_{ax}	2.560(4) × 2	F_{eq},O_{ax}	90.4(5)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* Z	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
$[Cu(nc)_2(H_2O)_2(BF_4)_2]\cdot 2H_2O$	tr	6.773(0)	98.114(2)	$CuF_2O_2N_2$	N_{eq}	1.99(1) × 2	O_{eq},N_{eq}	87.9(5)	450
(blue)	F-1	16.483(1)	92.973(2)		H_2O_{eq}	1.99(1) × 2	O_{eq},F_{ax}	88.8(5)	
	4	19.340(2)	92.539(2)		F_{ax}	2.48(1) × 2	N_{eq},F_{ax}	88.9(5)	
$Cu(bzph)_2(BF_4)_2$	m	13.540(3)		$CuF_2O_2N_2$	N_{eq}	1.984(4) × 2	O_{eq},N_{eq}	86.9(1)[d]	451
(green brown)	$P2_1/c$	7.772(1)	109.00(2)		O_{eq}	1.956(2) × 2	N_{eq},F_{ax}	81.6(1)	
	2	12.858(2)			F_{ax}	2.468(4) × 2	O_{eq},F_{ax}	96.8(1)	
$Cu(mesim)_2(BF_4)_2$	m	13.844(4)		$CuF_2N_2S_2$	N_{eq}	1.930(6) × 2	S_{eq},N_{eq}	84.2(2)[e]	452
(not given)	C2/c	11.251(1)	111.39(2)		S_{eq}	2.413(2) × 2		95.8(2)	
	4	15.753(4)			F_{ax}	2.551(5) × 2	S_{eq},F_{ax}	90.0(1, 7.3)	
							S_{eq},S_{eq}	180	
							N_{eq},F_{ax}	90.0(2, 1.1)	
							N_{eq},N_{eq}	180	
							F_{ax},F_{ax}	180	
$Cu(dcam)_2(H_2O)_2Cl_2$	tr	5.42(1)	74.5(2)	$CuO_2N_2Cl_2$	H_2O_{eq}	2.00 × 2		not given	453
(blue green)	P-1	6.45(1)	80.4(3)		N_{eq}	1.92 × 2			
	1	9.31(1)	84.7(3)		Cl_{ax}	2.87 × 2			
$[Cu(9\text{-}Meop)_2(H_2O)_2Cl_2]\cdot H_2O$	m	16.858(4)		$CuO_2N_2Cl_2$	N_{eq}	2.055(2) × 2	N_{eq},Cl_{ax}	88.46(5)	454
(deep blue)	C2/c	8.541(4)	91.02(5)		H_2O_{eq}	1.972(2) × 2	O_{eq},Cl_{ax}	86.67(5)	
	4	14.293(11)			Cl_{ax}	2.787(1) × 2	N_{eq},O_{eq}	87.27(5)	
$Cu(hemq)_2(H_2O)_2Cl_2$	m	19.416(2)		$CuO_2N_2Cl_2$	N_{eq}	2.029(2) × 2	O_{eq},Cl_{ax}	92.0	455
(green)	C2/c	10.086(1)	111.17(1)		H_2O_{eq}	1.983(2) × 2	N_{eq},O_{eq}	90.8(1)	
	4	13.524(2)			Cl_{ax}	2.883(1) × 2	N_{eq},Cl_{ax}	84.5(1)	
$[Cu(actr)_2Cl_2]\cdot 2H_2O$	tr	6.915(3)	100.55(4)	$CuO_2N_2Cl_2$	Cl_{eq}	2.300(1) × 2	N_{eq},Cl_{eq}	90.8(1)	131
(not given)	P-1	8.765(5)	108.50(4)		N_{eq}	1.970(2) × 2	N_{eq},O_{ax}	73.1(1)[e]	
	1	6.845(3)	106.58(5)		O_{ax}	2.647(2) × 2	Cl_{eq},O_{ax}	89.2(1)	
$Cu(mnim)_2Cl_2$	m	7.685(2)		$CuO_2N_2Cl_2$	Cl_{eq}	2.307(2) × 2	Cl_{eq},N_{ax}	90.0(2, 4)	456
(deep blue)	$P2_1/a$	13.587(4)	114.80(2)		N_{eq}	1.985(5) × 2	N_{ax},N_{ax}	180	
	2	7.796(2)			O_{ax}	2.600(5) × 2	Cl_{eq},Cl_{eq}	180	

$Cu(cyt)_2Cl_2$	m	8.359(2)		$CuO_2N_2Cl_2$	Cl_{eq}	2.287(−, 20)	N_{eq},O_{ax}	52.9(6, 9)[f]	457
(light blue)	$P2_1/c$	13.744(5)	128.00(1)		N_{eq}	1.96(1, 1)		107.6(6)	
	4	13.660(4)			O_{ax}	2.81(−, 7)		146.6(6)	
							Cl_{eq},O_{ax}	91.0(4, 9.3)	
							N_{eq},Cl_{eq}	91.9(5, 9)	
							N_{eq},N_{eq}	90.5(5, 1.9)	
							Cl_{eq},Cl_{eq}	165.7(3)	
$Cu(sim)_2Cl_2$	or	19.530(4)		$CuO_2N_2Cl_2$	Cl_{eq}	2.29(2) × 2	Cl_{eq},Cl_{eq}	125.0(1.1)	458
(brownish yellow)	Pbcn	8.040(1)			O_{eq}	2.78(2) × 2	Cl_{eq},N_{ax}	97.0(1, 1.2)	
	4	16.006(5)			N_{ax}	2.00(2) × 2	N_{ax},N_{ax}	152.0(1.1)	
$Cu(atr)_2Cl_2$	m	23.465(3)		$CuO_2N_2Cl_2$	Cl_{eq}	2.28(2) × 2	Cl_{eq},Cl_{eq}	124.0(1.1)	458
(brownish yellow)	C2/c	8.059(1)	106.19(1)		O_{eq}	2.75(2) × 2	Cl_{eq},N_{ax}	98.0(1.1,2)	
	4	15.427(1)			N_{ax}	2.00(2) × 2	N_{ax},N_{ax}	148.0(1.1)	
$[Cu(pmtrz)_2Cl_2](pmtrz)$	tr	12.190(3)	111.45(2)	$CuO_2N_2Cl_2$	Cl_{eq}	2.268(5, 12)	Cl_{eq},Cl_{eq}	157.5(1)	459
(not given)	P-1	15.970(3)	101.88(3)		O_{eq}	2.917(9)	Cl_{eq},N_{ax}	91.4(3, 3.2)	
	2	12.092(3)	95.93(3)			2.757(9)	N_{ax},N_{ax}	165.4(4)	
					N_{ax}	2.013(11, 3)			
$[Cu(lys)_2Cl_2]\cdot 2H_2O$	m	5.189(1)		$CuO_2N_2Cl_2$	N_{eq}	1.989(10, 14)	O_{eq},Cl_{ax}	90.1(4, 4.0)	460
(blue)	$P2_1$	16.988(3)	93.57(1)		O_{eq}	1.949(9, 5)	N_{eq},Cl_{ax}	90.0(4, 8.8)	
	2	11.482(2)			Cl_{ax}	2.823(6) × 2	N_{eq},O_{eq}	84.8(4, 1)[d]	
								94.9(4, 5)	
							O_{eq},O_{eq}	176.1(4)	
							N_{eq},N_{eq}	169.0(4)	
$[Cy(orn)_2Cl_2]\cdot 2H_2O$	m	5.218(3)		$CuO_2N_2Cl_2$	O_{eq}	1.958(4, 12)	O_{eq},N_{eq}	85.0(11, 4)[e]	461
(royal blue)	$P2_1$	15.636(2)	93.37(2)		N_{eq}	1.976(5, 13)		95.2(11, 9)	
	2	12.058(4)			Cl_{ax}	2.906(2, 11)	O_{eq},Cl_{ax}	90.0(10, 1.5)	
							N_{eq},Cl_{ax}	90.0(10, 3.7)	
							O_{eq},O_{eq}	177.6(12)	
							Cl_{ax},Cl_{ax}	178.9(3)	
							N_{eq},N_{eq}	176.1(15)	
$[Cu(orn)_2Cl_2]\cdot 2H_2O$	m	5.18		$CuO_2N_2Cl_2$	O_{eq}	1.976(5) × 2	O_{eq},N_{eq}	87.7[e]	462
(deep blue)	$P2_1/c$	15.57	93.3		N_{eq}	1.992(6) × 2			
	2	11.90			Cl_{ax}	2.89(2) × 2			
$Cu(sc)_2Cl_2$	or	6.90		$CuO_2N_2Cl_2$	O_{eq}	1.97 × 2	N_{eq},O_{eq}	83.0[e]	463
(blue)	$Pn2_1a$	10.22			N_{eq}	1.99 × 2	O_{eq},Cl_{ax}	89.1	
	4	8.26			Cl_{ax}	2.84 × 2	N_{eq},Cl_{ax}	86.5	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	*α* [°] *β* [°] *γ* [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
Cu(2,4,6-Cl_3ph)$_2$(py)$_2$	tr	9.576(6)	125.61(8)	$CuO_2N_2Cl_2$	pyN_{eq}	2.036(4) × 2	O_{eq},N_{eq}	89.0(1)	187
(reddish brown)	P-1	9.017(7)	101.73(4)		O_{eq}	1.911(2) × 2	N_{eq},Cl_{ax}	89.0(2)	
	1	9.129(7)	94.02(6)		Cl_{ax}	2.916(4) × 2	O_{eq},Cl_{ax}	77.0(1)^e	
Cu(2,4,6-Cl_3ph)$_2$(py)$_2$	tr	8.292(2)	85.91(2)	$CuO_2N_2Cl_2$	pyN_{eq}	2.036(3) × 2	O_{eq},N_{eq}	90.8(1)	464
(brown)	P-1	9.002(2)	72.44(2)		O_{eq}	1.909(2) × 2			
	1	9.587(2)	63.48(2)		Cl_{ax}	2.912(1) × 2			
[Cu(2,4,6-Cl_3ph)$_2$(im)$_2$]·H_2O	or	11.711(5)		$CuO_2N_2Cl_2$	imN_{eq}	1.98(1) × 2	N_{eq},O_{eq}	89.7(6)	465
(yellow brown)	Pbnb	24.829(6)			O_{eq}	1.97(1) × 2	O_{eq},Cl_{ax}	75.1(6)^e	
	4	8.257(4)			Cl_{ax}	2.83(1) × 2	N_{eq},Cl_{ax}	88.2(6)	
Cu(18-aneO_4N_2)Cl_2	m	12.209(19)		$CuO_2N_2Cl_2$	Cl_{eq}	2.311(2, 27)	N_{eq},O_{eq}	76.2(2, 1)^e	466
(not given)	P2$_1$/c	10.813(16)	93°39′(8′)		N_{eq}	2.035(6, 5)		103.3(2, 1.8)	
	4	12.588(5)			O_{ax}	2.732(5, 23)	N_{eq},Cl_{eq}	90.0(2, 2.3)	
							O_{eq},Cl_{ax}	90.0(1, 8.1)	
							O_{eq},O_{eq}	164.4(2)	
							N_{eq},N_{eq}	175.6(2)	
							Cl_{ax},Cl_{ax}	179.4(8)	
[Cu(9-aneN_2Sac)Cl]·ClO_4	m	13.808(2)		CuO_2N_2ClS	N_{eq}	2.031(5, 21)	Cl_{eq},S_{ax}	96.97(7)	467
(blue)	P2$_1$	8.195(2)	104.68(2)		O_{eq}	2.058(4)	Cl_{eq},N_{eq}	97.2(2)	
	2	8.702(2)			Cl_{eq}	2.241(2)		174.0(1)	
					O_{ax}	2.554(4)	Cl_{eq},O_{ax}	94.2(2)	
					S_{ax}	2.635(2)	Cl_{eq},O_{eq}	92.5(1)	
							N_{eq},S_{ax}	82.9(1)^e	
								86.6(1)	
							S_{ax},O_{ax}	155.9(1)	
							O_{eq},S_{ax}	110.0(1)	
							N_{eq},N_{eq}	88.0(2)	
							N_{eq},O_{ax}	74.6(2)^e	
								84.1(2)	
							N_{eq},O_{eq}	162.8(2)	
								81.7(2)^e	
							O_{eq},O_{ax}	90.6(2)	

$[Cu(mesim)_2(H_2O)_2]\cdot(NO_3)_2$	m	10.451(3)		$CuO_2N_2S_2$	N_{eq}	1.934(2) × 2	N_{eq},S_{eq}	84.11(7)[e]	468
(dark green)	$P2_1/n$	13.430(5)	109.24(3)		S_{eq}	2.449(1) × 2		95.89(7)	
	2	8.757(4)			H_2O_{ax}	2.440(2) × 2	S_{eq},O_{ax}	90.0(5, 5.8)	
							N_{eq},O_{ax}	90.0(8, 9)	
$Cu(mceam)_2(ClO_4)_2$	m	5.756(2)		$CuO_2N_2S_2$	N_{eq}	1.977(2) × 2	S_{eq},N_{eq}	86.8(1)[e]	469
(purple)	$P2_1/c$	16.353(4)	93.31(3)		S_{eq}	2.366(1) × 2	O_{ax},N_{eq}	84.8(1)	
	2	8.592(3)			O_3ClO_{ax}	2.599(2) × 2	S_{eq},O_{ax}	100.7(1)	
$Cu(prcpy)_2(ClO_4)_2$	tr	8.955(1)	104.37(1)	$CuO_2N_2S_2$	N_{eq}	2.015(3) × 2	S_{eq},N_{eq}	83.8(1)[e]	470
(not given)	P-1	8.794(1)	109.723(8)		S_{eq}	2.366(1) × 2	S_{eq},O_{ax}	85.3(1)	
	1	8.517(1)	78.86(1)		O_3ClO_{ax}	2.501(3) × 2	N_{eq},O_{ax}	85.7(1)	
$Cu(prcim)_2(ClO_4)_2$	m	10.131(1)		$CuO_2N_2S_2$	N_{eq}	1.940(6) × 2	S_{eq},N_{eq}	84.1(2)[e]	471
(brown)	$P2_1/n$	8.229(1)	90.40(1)		S_{eq}	2.397(2) × 2	S_{eq},O_{ax}	100.1(1)	
	2	13.663(1)			O_3ClO_{ax}	2.594(6) × 2	N_{eq},O_{ax}	95.0(2)	
$Cu(sbzh)_2(NO_3)_2$	m	22.056(4)		$CuO_2N_2S_2$	N_{eq}	1.978(6) × 2	S_{eq},N_{eq}	86.1(1)[e]	472
(not given)	$P2_1/a$	5.774(2)	88.28(2)		S_{eq}	2.293(2) × 2			
	2	7.756(3)			$(NO_3)O_{ax}$	2.617(5) × 2			
$Cu(acatr)_2(SCN)_2$	tr	9.057(3)	75.79(2)	$CuO_2N_2S_2$	N_{eq}	1.932(3) × 2	N_{eq},O_{eq}	89.1(1)[d]	304
(brownish green)	P-I	6.442(2)	73.16(2)		O_{eq}	2.019(3) × 2	N_{eq},S_{ax}	90.0(1)	
	1	7.602(3)	77.82(2)		NCS_{ax}	2.864(2) × 2	O_{eq},S_{ax}	90.3(1)	
$Cu(bhdhx)(NO_3)_2$	or	14.351(5)		$CuO_2N_2S_2$	O_2NO_{eq}	2.280(3) × 2	S_{eq},S_{ax}	83.6(1)[e]	473
(green)	Pbcn	8.554(3)			S_{eq}	2.495(1) × 2		90.6(1)	
	4	13.057(4)			N_{ax}	1.933(4) × 2	S_{eq},O_{eq}	99.41(9)	
								169.38(8)	
							S_{eq},S_{eq}	89.88(6)[e]	
							O_{eq},N_{ax}	93.3(1, 2.2)	
							N_{ax},N_{ax}	171.8(2)	
							O_{eq},O_{eq}	71.9(2)	
$Cu(14\text{-}aneS_2N_2)(ClO_4)_2$	m	15.008(5)		$CuO_2N_2S_2$	N_{eq}	2.024(6, 7)	N_{eq},N_{eq}	95.1(2)[d]	474
(dark purple)	$P2_1/n$	8.606(3)	113.79(2)		S_{eq}	2.296(2, 2)	N_{eq},S_{eq}	87.7(2, 1)[e]	
	4	17.967(4)			O_3ClO_{ax}	2.459(7)		175.1(2, 2)	
						2.697(12)	S_{eq},S_{eq}	89.28(7)[d]	
$[Cu(qusp)(NO_3)(H_2O)]NO_3$	m	6.480(3)		$CuO_2N_2S_2$	H_2O_{eq}	2.030(6)	S_{eq},S_{ax}	103.5(2)[d]	475
(green)	$P2_1/n$	17.430(5)	97.81(3)		N_{eq}	1.990(7, 4)	N_{eq},S_{ax}	83.5(3)[e]	
	4	21.248(5)			S_{eq}	2.343(3)		100.2(3)	
					S_{ax}	2.507(3)	S_{eq},O_{eq}	160.3(2)	

TABLE I (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	α [°] β [°] γ [°]	*Chromophore*		Cu-L [Å]		L-Cu-L [°]	*Ref.*
					O_2NO_{ax}	2.677(7)	S_{eq},O_{ax} O_{eq},O_{ax} N_{eq},S_{eq} O_{eq},N_{eq} O_{eq},S_{ax} N_{eq},O_{ax} S_{ax},O_{ax} N_{eq},N_{eq}	80.9(2) 79.4(2) 85.3(2)^{c} 92.9(2) 90.7(3, 7) 96.3(2) 88.3(3, 5.0) 174.6(2) 176.1(3)	
[Cu(pyos)(ClO_4)]ClO_4 (green)	m $P2_1/c$ 4	14.388(2) 9.990(5) 16.076(3)	 107.919(12)	$CuO_2N_2S_2$	N_{eq} S_{eq} O_{ax} O_3ClO_{ax}	2.014(6, 7) 2.375(3, 2) 2.469(10) 2.413(5)	N_{eq},N_{eq} S_{eq},S_{eq} O_{ax},O_{ax} N_{eq},S_{eq} N_{eq},O_{ax} S_{eq},O_{ax}	173.3(3) 159.07(10) 169.6(3) 85.6(2)^{c} 95.6(2, 1) 90.0(2, 5.4) 79.5(1, 4)^{c} 100.5(3, 10.0)	476
Cu(eiphim) (brown red)	m $P2_1/c$ 4	8.887(3) 28.825(1) 10.168(4)	 106.51(2)	$CuO_2N_2S_2$	S_{eq} O_{eq} N_{ax}	2.548(3, 60) 2,098(5, 54) 1.955(5, 14)	S_{eq},S_{eq} S_{eq},O_{eq} S_{eq},N_{ax} O_{eq},O_{eq} O_{eq},N_{ax} N_{ax},N_{ax}	84.0(1)^{c} 90.7(2, 1.1) 168.3(1, 3.2) 83.0(2, 6)^{c} 93.8(2, 1.0) 95.9(2) 92.2(2, 2.7)^{d} 94.4(2) 175.6(2)	477
Cu(bzpy)$_2$$Br_2$ (dark green)	m $P2_1/n$ 2	7.401(3) 20.690(7) 7.403(3)	 105.29(3)	$CuO_2N_2Br_2$	O_{eq} N_{eq} Br_{ax}	2.407(4) × 2 1.970(4) × 2 2.468(1) × 2	N_{eq},O_{eq} O_{eq},Br_{ax} N_{eq},Br_{ax}	74.6(2)^{c} 105.4(2) 90.0(1, 2.2) 90.0(1, 6)	303

$[Cu(gly)_2Br_2][Li_2(gly)_2]\cdot 2H_2O$	m	9.011(1)		$CuO_2N_2Br_2$	O_{eq}	1.984(3) × 2	N_{eq},O_{eq}	97.1(2)[d]	478
(royal blue)	$P2_1/n$	5.061(1)	91.54(5)		N_{eq}	1.956(4) × 2	N_{eq},Br_{ax}	90.5(1)	
	2	20.659(3)			Br_{ax}	2.987(1) × 2	O_{eq},Br_{ax}	91.4(1)	
$Cu(bzimox)Br_2$	or	8.940(1)		$CuO_2N_2Br_2$	N_{eq}	1.987(7) × 2	N_{eq},Br_{ax}	89.5(2, 1.3)	479
(not given)	Pccn	10.634(1)			O_{eq}	2.743(6) × 2	O_{eq},Br_{ax}	95.2(1, 4.4)	
	4	20.455(2)			Br_{ax}	2.465(1) × 2	N_{eq},O_{eq}	67.2(3)[e]	
								123.8(3)	
							Br_{ax},Br_{ax}	168.2(1)	
							N_{eq},N_{eq}	168.9(5)	
							O_{eq},O_{eq}	57.6(3)[e]	
$Cu(18\text{-ane}O_4N_2)Br_2$	m	15.895(6)		$CuO_2N_2Br_2$	O_{eq}	2.772(8) × 2	N_{eq},O_{eq}	75.5[e]	480
(not given)	C2/c	10.593(17)	98°37′(6′)		N_{eq}	2.008(9) × 2		103.9(3)	
	4	10.336(20)			Br_{ax}	2.476(3, 38)	O_{eq},Br_{ax}	90.0(2, 8.6)	
							N_{eq},Br_{ax}	90.0(2, 2.0)	
$Cu(esbim)_2Cl_2$	m	9.707(1)		$CuN_2Cl_2S_2$	Cl_{eq}	2.322(2) × 2	Cl_{eq},S_{eq}	85.70(6)	481
(blue green)	$P2_1/c$	14.977(2)	112.03(1)		S_{eq}	3.001(2) × 2	Cl_{eq},N_{ax}	91.2(2)	
	2	8.525(1)			N_{ax}	2.000(5) × 2	S_{eq},N_{ax}	76.2(1)[e]	
$Cu(10\text{-ane}N_2S_2)Cl_2$	or	12.927(3)		$CuN_2Cl_2S_2$	Cl_{eq}	2.395(1)	Cl_{eq},S_{eq}	86.31(3, 69)	482
(brown)	Pbca	18.933(5)				2.457(1)		159.99(4, 1.13)	
	8	14.469(2)			S_{eq}	2.886(1)	N_{ax},N_{ax}	168.6(1)	
						2.970(1)	Cl_{eq},Cl_{eq}	112.08(3)	
					N_{ax}	1.952(2, 3)	S_{eq},S_{eq}	76.81(3)[d]	
							Cl_{eq},N_{ax}	92.5(1, 1.8)	
							S_{eq},N_{ax}	76.3(1, 4)[e]	
								94.5(1, 1)	
							Cl_{eq},N_{eq}	93.9(1, 15)	
$Cu(mindth)Cl_2$	or	17.917(2)		$CuN_2Cl_2S_2$	Cl_{eq}	2.475(3, 87)	Cl_{eq},Cl_{eq}	108.03(8)	483
(green)	Pbca	14.502(4)			S_{eq}	2.714(3, 91)	Cl_{eq},S_{eq}	86.3(1, 1.6)	
	8	12.905(2)			N_{ax}	1.971(7, 9)		165.1(1, 1.7)	
							Cl_{eq},N_{ax}	93.4(2, 2.0)	
							S_{eq},S_{eq}	79.6(1)[e]	
							S_{eq},N_{ax}	80.2(3.7)[e]	
								90.9(2, 4)	
							N_{ax},N_{ax}	168.5(3)	

TABLE I (*Continued*)

Compound	Cryst. Cl. Space G. Z	a [Å] b [Å] c [Å]	α [°] β [°] γ [°]	Chromophore		Cu-L [Å]		L-Cu-L [°]	Ref.
$Cu(bhdhx)Cl_2$	or	12.738(3)		$CuN_2Cl_2S_2$	Cl_{eq}	2.589(1)	Cl_{eq},N_{ax}	93.7(1, 1.1)	484
(not given)	Pbca	17.218(4)				2.371(1)	S_{eq},N_{ax}	79.8(1, 2.1)[e]	
	8	13.894(7)			S_{eq}	2.523(1)		91.3(1, 2.0)	
						2.845(1)	S_{eq},S_{eq}	81.2(1)[e]	
					N_{ax}	1.961(3, 1)	S_{eq},Cl_{eq}	89.0(1, 1.5)	
							Cl_{eq},Cl_{eq}	101.5(1)	
							N_{ax},N_{ax}	168.2(1)	
$[Cu(18\text{-}aneN_2S_2)Cl_2]\cdot 0.5tol$[c]	tr	12.828(6)	93.15(2)	$CuN_2Cl_2S_2$	N_{eq}	2.165(10, 95)	S_{eq},S_{eq}	176.6(2)	485
(light green)	P-1	21.963(4)	109.35(2)		S_{eq}	2.293(6, 93)	S_{eq},N_{eq}	90.15(3)[d]	
	4	10.872(3)	82.32(2)		Cl_{ax}	2.594(5)	S_{eq},Cl_{ax}	90.0(2, 2.3)	
						2.951(6)	N_{eq},N_{eq}	164.4(4)	
							Cl_{ax},Cl_{ax}	178.8(2)	
							Cl_{ax},N_{eq}	89.98(3, 7.78)	
				$CuN_2Cl_2S_2$	N_{eq}	2.185(10, 75)	S_{eq},S_{eq}	176.1(2)	
					S_{eq}	2.402(6, 7)	S_{eq},Cl_{ax}	90.0(2, 2.6)	
					Cl_{ax}	2.547(5)	S_{eq},N_{eq}	89.83(40, 48)[d]	
						2.932(5)	Cl_{ax},Cl_{ax}	179.1(1)	
							Cl_{ax},N_{eq}	90.0(4, 5.4)	
							N_{eq},N_{eq}	169.2(5)	
$[Cu(imdth)(BF_4)Cl]$	m	13.975(5)		CuN_2S_2FCl	N_{eq}	1.946(3, 7)	Cl_{eq},S_{ax}	97.1(1)	447
(green)	$P2_1/n$	8.347(3)	116.34(2)		S_{eq}	2.436(1)	Cl_{eq},S_{eq}	176.7(1)	
	4	17.156(6)			Cl_{eq}	2.299(1)	Cl_{eq},N_{eq}	93.9(1, 1)	
					S_{ax}	2.747(1)	Cl_{eq},F_{ax}	98.5(1)	
					F_{ax}	2.592(2)	S_{eq},S_{ax}	83.9(1)	
							N_{eq},S_{ax}	81.3(1)[e]	
								100.3(1)	

S_{ax},F_{ax}	163.0(1)
S_{eq},N_{eq}	82.8(1)[e]
	89.4(1)
S_{eq},F_{ax}	80.9(1)
N_{eq},N_{eq}	171.8(1)
N_{eq},F_{ax}	88.1(1, 2.6)

[a] Where more than one chemically equivalent distance or angle is present, the mean value is tabulated. The first number in parenthesis is e.s.d., 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 two crystallographically independent molecules. [d] Six-membered metallocyclic ring. [e] Five-membered metallocyclic ring. [f] Four-membered metallocyclic ring. [g] There are three crystallographically independent molecules. [h] Eight-membered metallocyclic ring. [i] Seven-membered metallocyclic ring.

The ligands used range from unidentate to hexadentate, accounting for the variations in distortion about the Cu(II) atoms. The mean $Cu-L_{eq}$ bond distances for the unidentate ligands increases in the sequence: 1.915 Å(F) < 1.99 Å(OL) < 2.02 Å(NL) < 2.31 Å(Cl) < 2.41 Å(Br), which follows the covalent radius of the coordinated atom. The mean $Cu-L_{ax}$ bond distances are somewhat longer than those of the $Cu-L_{eq}$ bond distances and increases in the order: 2.265 Å(H) < 2.46 Å(H_2O) < 2.47 Å(NL) < 2.56 Å(OL) < 2.56 Å(F) < 2.73 Å(Br) < 2.85 Å(Cl) < 2.97 Å(SL). For bidentate ligands, $Cu-L_{eq}$ *vs.* $Cu-L_{ax}$ bond distances are: 2.05 *vs.* 2.32 Å(N) < 2.06 *vs.* 2.45 Å(O). For tridentate ligands the values are: 2.00 *vs.* 2.325 Å(O), 2.065 *vs.* 2.31 Å(N) and 2.44 *vs.* 2.44 Å(S). The most common donor atoms are O and N.

In Table IA are summarized Cu–L bond distances for the trigonal-bipyramidal, square-pyramidal and tetragonal-bipyramidal configuration about Cu(II) atoms. In the series of trigonal-bipyramidal configuration, the $Cu-L_{eq}$ bond distances are somewhat longer than those of $Cu-L_{ax}$ bond distances; in the remaining two configurations (square-pyramidal and tetragonal-bipyramidal) the opposite is observed, $Cu-L_{eq}$ bond distances are somewhat shorter than those of $Cu-L_{ax}$. The mean $Cu-L_{eq}$ bond distance increases in the sequence: square-pyramidal < tetragonal-bipyramidal < trigonal-bipyramidal and $Cu-L_{ax}$: trigonal-bipyramidal < square-pyramidal < tetragonal-bipyramidal.

Other than the ligand donor atoms of the same type, a wide range of hetero-donors also exist. There are bidentates: O+N; O+S; N+S and even O+Cl; tridentates: 2O+N; 2O+S; O+2N; 2N+S and O+2S; tetradentates: 3O+N; 2O+2N; O+3N and 2N+2S; pentadentates: 3O+2N; 2O+3N; O+4N; 4N+S; 2N+3S; 2O+2N+S; O+2N+2S; and hexadentates: 4O+2N; 3O+3N; 2O+4N; 2N+4S and 2O+2N+2S donor atoms.

TABLE IA Summary of the mean $Cu-L_{eq}$ *vs.* $Cu-L_{ax}$ bond distances

Coord. atom	*Trigonal-Bipyramid* (*ref.* 2)	*Square-Pyramid* (*ref.* 2)	*Tetragonal-Bipyramid*
O	2.13 *vs.* 1.96	1.97 *vs.* 2.33	1.99 *vs.* 2.51
	2.23 *vs.* 2.01	2.01 *vs.* 2.32	2.06 *vs.* 2.45[a]
N	2.04 *vs.* 2.00	1.97 *vs.* 2.26	2.02 *vs.* 2.47
	2.12 *vs.* 1.995	2.015 *vs.* 2.22	2.05 *vs.* 2.32[a]
	2.06 *vs.* 2.01	2.005 *vs.* 2.25	2.065 *vs.* 2.31[b]
F		1.89 *vs.* 2.50	1.915 *vs.* 2.565
Cl	2.32 *vs.* 2.25	2.285 *vs.* 2.51	2.31 *vs.* 2.85
Br	2.50 *vs.* 2.43	2.41 *vs.* 2.63	2.41 *vs.* 2.73

[a]Bidentate ligands. [b]Tridentate ligands.

An interesting feature of the chelate rings is that the bite angle (the angles formed by two donor atoms and the central Cu(II) atom) may vary widely. The effect of both electronic and steric hindrances of the ligands can be seen in the opening of the L–Cu–L angles of the respective metallocyclic rings. The metallocyclic intra-ligand O–Cu–O ring angle opens with increasing size of the ring, for example: 54.0(7.5; 3.5)° (four-membered) < 77.5(6.0; 8.0)° (five-membered) < 89.8(4.8; 3.3)° (six-membered) < 90.5° (seven-membered). The first number in parenthesis is the mean minus the smallest value and the second is the largest value minus the mean. The N–Cu–N rings follow this trend: 78.0(5.0; 2.5)° (five-membered, unsaturated ligands) < 84.5(4.5; 5.5)° (five-membered, saturated ligands) < 90.2(4.8; 6.3)° (six-membered) < 98.0° (seven-membered). The values for S–Cu–S rings are: 86.0(6.4; 3.9)° (five-membered) < 90.5(13.7; 13.0)° (six-membered) and for O–Cu–N rings: 52.0(1.5)° (four-membered) < 76.0(8.8; 3.5)° (five-membered, unsaturated ligands) < 84.0(4.0; 6.0)° (five-membered, saturated ligands) < 90.0(6.0; 5.2)° (six-membered) < 99.6° (seven-membered) < 101.8° (eight-membered).

Table IB summarizes L–Cu–L bond angles of the metallocyclic rings for tetra-, penta-, hexa- and hepta-coordinate Cu(II) derivatives. It can be see that the L–Cu–L bond angles of the respective metallocyclic rings increase

TABLE IB Summary of the L–Cu–L angles[°] of the metallocyclic rings[a]

Metallocyclic ring	*4-Coordination*[2]	*5-Coordination*[2]	*6-Coordination*	*7-Coordination*
4-membered				
O–Cu–O	64.3	57.6	54.0	51.0
O–Cu–N	—	56.9	52.1	
N–Cu–N	67.4	62.0	—	
5-membered				
O–Cu–O	85.0	84.0	77.5	72.0
O–Cu–N	—	83.0	76.0	
N–Cu–N	79.5[b]	80.0[b]	77.5[b]	69[b]
	85.5[c]	84.5[c]	84.0[c]	80[c]
S–Cu–S	92.0	88.5	85.0	
S–Cu–O	—	82.5	80.0	
S–Cu–N	—	85.5	82.5	
6-membered				
O–Cu–O	93.0	92.0	90.0	
O–Cu–N	—	92.0	90.0	
N–Cu–N	93.3	95.0	90.5	
N–Cu–S	—	91.0	91.5	
7-membered				
N–Cu–N	96.0	98.0	98.0	

[a]The mean values are tabulated. [b]Unsaturated ligands. [c]Saturated ligands.

with increasing covalent radius of the donor atoms and consequently decreasing with coordination number about Cu(II). In general, the mean Cu–L bond distance increases with coordination number, which means that, at greater Cu–L bond lengths, the angle must be smaller, and at shorter it must be larger. The data given in Table IA and IB follow this trend.

Some hexa-coordinate Cu(II) compounds were studied at two different temperatures, $Rb_2[Cu(H_2O)_6](SO_4)_2$,[5] $[Cu(H_2O)_6]SiF_6$,[12] $K_2Pt[Cu(NO_2)_6]$,[71] $[Cu(en)_3]SO_4$,[85,86] $[Cu(dien)_2](NO_3)_2$[94] and $Cu(debt)(NCS)_2$.[109] The mean Cu–L bond distances decrease with decreasing temperature. Notably, $[Cu(en)_3]SO_4$ is hexagonal at 295K[85] but at 120K is triclinic.[86]

There are several examples which contain two monomeric forms $[Cu(ahmi)_6][Cu(ahmiCl_3]_2$ with CuO_6 and $CuCl_3O$ chromophores; $[Cu(H_2O)_6][Cu(C_8H_8O_5)_2]$[85,86] with CuO_6, $[Cu(C_{22}H_{34}N_6][CuCl_4]$[11] with CuN_6 and $CuCl_4$ chromophores, $[Cu(F_3ac)_2(py)_2][Cu(py)_4](F_3ac)_2]$[137,150] with CuO_4N_2 and CuN_4O_2 chromophores; $[Cu(croc)(terpy(H_2O)]$-$[Cu(croc)(terpy)]\cdot 4H_2O$[422] with the CuO_3N_3 and CuN_3O_2 chromophores.

Some hexacoordinate Cu(II) compounds exist in two isomeric forms differing mostly by degree of distortion involving both Cu–L distances and L–Cu–L angles. For example, $Cu(NO_3)_2(apy)_2$ exists in monoclinic[51] and triclinic[52] crystal classes, with the ratios of $(Cu-L_{eq})/(Cu-L_{ax})$ (degree of tetragonality) at 0.78 and 0.81, respectively. Two monoclinic forms of $[Cu(phen)_3](ClO_4)_2$[90] differ by unit cell dimensions (Cu–N distances and N–Cu–N angles are not given). Another two monoclinic forms, α- and β-$Cu(pipc)_2(H_2O)_2$[156] differ mostly by unit cell dimensions and by the ratio of $(Cu-L_{eq})/(Cu-L_{ax})$ with values of 0.835 and 0.76, respectively. The ratio in orthorombic[216] and monoclinic forms of $Cu(Clac)_2(Me_4en)$ are equal to 0.76. For the $Cu(NO_3)_2(Et_2en)$ complexes which also exist in monoclinic[224] and orthorombic[225] forms, the ratio is 0.82 and 0.84, respectively. In another pair, monoclinic[227] and orthorombic[228] forms of $Cu(NO_3)_2(Me_4en)$, the ratio is 0.82 and 0.77, respectively. A somewhat higher degree of tetragonality (0.80) was found for the triclinic brown complex than for the monoclinic green complex (0.83) of $[Cu(papt)_2(H_2O)_2](BF_4)_4$.[300] For the Cu(1,3-bn)$_2(ClO_4)_2$ complex,[317] which exists in two monoclinic forms, red violet and blue violet, the degree of tetragonality is 0.76 and 0.79, respectively.

Two crystallographically independent molecules differing by degree of distortion and coexisting in the same crystal have been found in several species.[15,16,43,50,67,72,112,141,187,201,208,216,220b,236,240,280,359,376,391,408,445,485] In blue $[Cu(en)_3]Cl_2\cdot 0.75en$[86] three such independent molecules are present.

Almost all Cu(II) complexes are blue or green. Exceptions are generally caused by strong ultraviolet charge-transfer bands tailing off into the blue end of the visible spectrum and causing the substances to appear red or brown. There are examples, which are red[102,173,222,249,261,266,277,301,317,337,359,372,374,376,377,385,401,409] as well as brown.[91,112,113,187,213,220a,257,300,371,403,407,458,465,471,477,482] There are three examples[17,64,68] which are colourless, and even two[83,250] which are black.

Mononuclear hexacoordinate Cu(II) compounds "prefer" the monoclinic crystal class, then triclinic and orthorombic.

HEPTACOORDINATE Cu(II) COMPOUNDS

Crystallographic and structural data for mononuclear Cu(II) compounds with coordination number seven are collected in Table II. The structures are tabulated by the increasing number of different coordinated atoms (ligands). There are eleven examples[486–495] in which Cu(II) atoms are surrounded by seven donor atoms. There are only three types of donor atoms: O, N and Cl, which form a pentagonal bipyramidal geometry about Cu(II). There are no examples with unidentate ligands. The most prevalent structure involves Cu(II) surrounded by three ligands (one pentadentate and two unidentate) in the form of a distorted pentagonal bipyramid, the equatorial plane of which consists of a pentadentate ligand and apical positions are occupied by unidentate ligands.[486,487,490–492,494,495] In $[Cu(shb)]^{2+}$, the heptadentate N-donor ligand sbh creates a distorted pentagonal bipyramid about the Cu(II) atom.[488] In $[Cu(NO_3)_3]^{2-}$, the Cu(II) is surrounded by four ligands (three bidentate and one unidentate) again in the form of a distorted pentagonal bipyramid.[489] Finally, in $Cu(NO_3)_2py_3$ a distorted pentagonal bipyramid is formed by two bidentate NO_3 groups and three unidentate pyridine molecules.[493]

Inspection of the data in Table II reveals that $Cu-L_{ax}$ bond distances except $[Cu(dapsc)(H_2O)Cl]^+$ (see Ref. 495) are shorter than the $Cu-L_{eq}$ bond distances, consistent with the two apical sites of a pentagonal bipyramid being less sterically hindered than the five equatorial sites. The mean $Cu-L_{ax}$ *vs.* $Cu-L_{eq}$ bond distances are: 2.06 *vs.* 1.98 Å(NL); 2.40 *vs.* 2.21 Å(bidentate O donors); 2.43 *vs.* 1.995 Å(heptadentate N donors); 2.35 *vs.* 2.40 Å(Cl). The mean $Cu-OH_{2(ax)}$ bond distance is 1.93 Å and $Cu-O_{eq}$ bond distance (pentadentate) is 2.25 Å.

Another factor of interest is the sum of all interatomic distances around Cu(II), the observed values ranging from 14.96 to 15.97 Å with an average value 15.5 Å. The sum increasing from 15.0 Å in CuO_7, through 15.1 Å in CuO_5N_2 to 15.9 Å in CuO_5Cl_2, which corresponds well with the increasing size of the atoms of the coordinated ligands.

TABLE II Structural data for seven- and eight-coordinated Cu(II) compounds[a]

Compound	Cryst. Cl. Space G. Z	a [Å] b [Å] c [Å]	α [°] β [°] γ [°]	Chromophore	Cu–L [Å]		L–Cu–L [°]		Ref.
$[Cu(C_{14}H_{20}O_5)(H_2O)_2](ClO_4)_2\cdot$	m	16.142(5)		CuO_7	O_{eq}[b]	2.232(2, 35)	O_{eq},O_{eq}[b]	72.4(1, 3.5)[c]	486
$3H_2O$	$P2_1/a$	20.233(4)	95.53(3)		H_2O_{ax}	1.915(2, 4)	O_{ax},O_{ax}	175.11(8)	
(brown)	4	7.622(3)							
$[Cu(C_{10}H_{20}O_5)(H_2O)_2](NO_3)_2$[d]	m	14.758(5)		CuO_7	O_{eq}	2.248(5, 128)		not given	487
(colourless)	Pc	13.978(4)	102.19(3)		H_2O_{ax}	1.914(7, 18)			
	20	43.914(13)							
				CuO_7	O_{eq}	2.242(6, 118)			
					H_2O_{ax}	1.907(5, 2)			
				CuO_7	O_{eq}	2.253(6, 99)			
					H_2O_{ax}	1.894(6, 1)			
				CuO_7	O_{eq}	2.254(6, 123)			
					H_2O_{ax}	1.956(7, 6)			
				CuO_7	O_{eq}	2.249(6, 135)			
					H_2O_{ax}	1.922(7, 36)			
				CuO_7	O_{eq}	2.283(7, 142)			
					H_2O_{ax}	1.924(5, 18)			
				CuO_7	O_{eq}	2.250(7, 135)			
					H_2O_{ax}	1.945(6, 46)			
				CuO_7	O_{eq}	2.236(5, 93)			
					H_2O_{ax}	1.917(6, 52)			
				CuO_7	O_{eq}	2.218(6, 97)			
					H_2O_{ax}	1.937(8, 32)			
				CuO_7	O_{eq}	2.224(6, 112)			
					H_2O_{ax}	1.956(7, 29)			
$[Cu(sbh)](ClO_4)_2$	m	12.18(1)		CuN_7	N_{eq}	2.303(26,95)	N_{eq},N_{eq}	68.8(8, 5.0)[c]	488
(not given)	$P2_1/n$	13.78(1)	98.3(1)			2.565(24)		88.5(8)	
	4	14.92(1)			N_{ax}	1.995(20,2)		142.5(8, 14.6)	
							N_{eq},N_{ax}	80.0(8, 1.4)[c]	
								92.7(8, 7.6)	
							N_{ax},N_{ax}	175.3(8)	

$(lc)_2[Cu(NO_3)_3Cl]$	m	10.554(2)		CuO_6Cl	O_{eq}	2.231(12,70)	O_{eq},O_{eq}	53.9(4)[e]	489
(not given)	$P2_1/n$	24.402(7)	100.02(2)			2.474(10)	O_{eq},Cl_{eq}	152.9(3)	
	4	14.124(3)			Cl_{eq}	2.3538(24)	O_{eq},O_{ax}	48.2(5, 4.2)[e]	
					O_{ax}	2.123(7, 18)		86.5(4, 3.2)	
							O_{ax},Cl_{ax}	96.1(2, 1.1)	
							O_{ax},O_{ax}	165.1(3)	
$[Cu(15\text{-crown-}5)(MeCN)_2][Cu_3Cl_8]$	tr	9.762(2)	95.02(2)	CuO_5N_2	O_{eq}	2.24(2, 10)	O_{eq},O_{eq}	72.3(7, 1.7)[c]	490
(orange)	P-1	9.644(2)	97.80(2)		$MeCN_{ax}$	1.95(1) × 2		143.5(7, 2.9)	
	1	9.353(2)	122.53(2)						
							O_{eq},N_{ax}	90.0(6, 5.7)	
							N_{ax},N_{ax}	180.0	
$[Cu(15\text{-crown-}5)(MeCN)Cl]_2 \cdot$	m	14.732(5)		CuO_5NCl	O_{eq}	2.261(3, 99)	O_{eq},O_{eq}	72.2(2, 2.2)[c]	490
$[Cu_2Cl_6]$	$P2_1/a$	11.357(4)			$MeCN_{ax}$	1.981(4)		142.8(3, 3.5)	
(orange)	4	13.520(3)	112.25(2)		Cl_{ax}	2.209(2)	O_{eq},N_{ax}	86.5(3, 5.8)	
							O_{eq},Cl_{ax}	93.5(3, 5.5)	
							N_{ax},Cl_{ax}	179.2(2)	
$[Cu(15\text{-crown-}5)(MeCN)Cl] \cdot$	m	11.367(6)		CuO_5NCl	O_{eq}	2.261(5, 90)	O_{eq},O_{eq}	72.2(2, 1.9)[c]	491
$[CuCl_3]$	$P2_1/c$	13.521(7)	112.40(4)		N_{ax}	1.987(5)		143.0(2, 3.0)	
(red)	4	14.751(9)			Cl_{ax}	2.212(2)	O_{eq},N_{ax}	86.5(2, 6.4)	
							O_{eq},Cl_{ax}	93.5(1, 5.2)	
							N_{ax},Cl_{ax}	178.5(1)	
				$CuCl_4$	Cl	2.185(2, 4)	Cl_{ax},Cl_{ax}	96.7(1, 6.0)	
					μCl	2.318(2, 10)	$Cl,\mu Cl$	99.4(1, 1.3)	
								136.3(1, 6)	
							$\mu Cl,\mu Cl$	89.32(8)	
$[Cu(C_{14}H_{20}O_5)Cl_2] \cdot CHCl_3$	m	14.650(5)		CuO_5Cl_2	O_{eq}	2.285(5, 52)	O_{eq},O_{eq}	72.3(6, 4.2)[c]	492
(red)	$P2_1/c$	11.268(7)	106.94(3)		Cl_{ax}	2.248(2, 6)			
	4	13.623(4)							
$Cu(NO_3)_2(py)_3$	m	12.783(6)	CuO_4N_3		O_{eq}	2.154(7) × 2	O_{eq},O_{eq}	50.0(3)[e]	493
(not given)	C2/c	9.199(5)	108.35(3)			2.732(9) × 2		91.4(3)	
	4	16.055(8)			pyN_{eq}	2.064(9)		141.3(3)	
					pyN_{ax}	2.018(8, 2)	O_{eq},N_{eq}	84.4(2)	
								134.2(2)	
							O_{eq},N_{ax}	89.4(3, 4.2)	
							N_{eq},N_{ax}	92.0(2)	
							N_{ax},N_{ax}	176.0(3)	

TABLE II (*Continued*)

Compound	*Cryst. Cl.* *Space G.* *Z*	*a* [Å] *b* [Å] *c* [Å]	*α* [°] *β* [°] *γ* [°]	*Chromophore*		Cu–L [Å]		L–Cu–L [°]	*Ref.*
$[Cu(dapsc)(H_2O)_2]\cdot(NO_3)_2\cdot H_2O$ (not given)	m Pc(P2/c) 2	10.977(4) 13.930(3) 6.977(3)	 104.55(3)	CuO_4N_3	O_{eq} N_{eq} H_2O_{ax}	2.350(4) × 2 2.260(6, 5) 1.922(3) × 2		not given	494
$[Cu(dapsc)(H_2O)Cl]Cl\cdot 2H_2O$ (pale yellow)	tr P-1 2	7.903(4) 7.768(3) 18.477(12)	86.37(4) 84.90(5) 67.00(4)	CuO_3N_3Cl	O_{eq} N_{eq} H_2O_{ax} Cl_{ax}	2.341(4, 11) 2.051(5, 73) 2.269(5) 2.701(2)		not given	495
$[Cu(dapsc)(H_2O)_{2-x}Cl_x]Cl_{2-x}\cdot$ $(x+1)H_2O$ (golden yellow)	m I2/a 4	17.980(5) 13.192(2) 7.956(4)	 99.95(3)	CuO_3N_3Cl	O_{eq} N_{eq} H_2O_{ax} Cl_{ax}	2.269(3) 2.172(5, 24) 1.976(8) 2.625(3)		not given	495
$(AsPh_4)_2[Cu(NO_3)_4]\cdot 10CH_2Cl_2$ (not given)	m $P2_1/n$ 2	10.714 16.753 14.082	 92.58	CuO_8	O	1.946(8, 27) × 4 2.733(9, 60) × 4		not given	496
$[Cu(6\text{-}am)_4](ClO_4)_2$ (not given)	tg P-4 1	10.60 7.72		CuO_8	O	1.97 × 4 2.79 × 4		not given	497
$[Cu(bet]\cdot(NO_3)_2$ (blue violet)	tg I4-2m 2	11.443(2) 11.672(2)		CuO_8	O	1.948(3) × 4 2.833(4) × 4	O,O	51.3(3)[e] 84.1 90.2(4) 173.2(4)	498
$Cu(prometone)_2(NO_3)_2$ (green)	or Pbcn 4	23.809(5) 8.855(2) 14.978(5)		CuO_6N_2	O N $(NO_3)O$	2.75 × 2 2.00 × 2 1.99 × 2 2.65 × 2		not given	499

[a] Where more than one chemically equivalent distance or angle is present, the mean value is tabulated. The first number in parenthesis is e.s.d., the second is a maximum deviation from the mean value. [b] The chemical identity of coordinated atom/ligand is specified in these columns. [c] The five-membered metallocyclic ring. [d] There are ten crystallographically independent molecules. [e] The four-membered metallocyclic ring.

One of the important shape characteristics for describing a pentagonal bipyramidal geometry is the ratio of bond distances (M–L_{ax})/(M–L_{eq}). The ratio ranges from 0.84 to 0.93 for the series in which the mean Cu–L_{eq} bond distance is longer than that of Cu–L_{ax}; but in $[Cu(dapsc)(H_2O)Cl]^+$ where Cu–L_{eq} < Cu–L_{ax} the ratios are 1.04 and 1.15.

However, we also note that any distortions from ideal geometry will be reflected in the value of the bond angles: L_{ax}–M–L_{eq}; L_{ax}–M–L_{ax}; L_{eq}–M–L_{eq}. In the ideal pentagonal bipyramid, the values of these angles are: L_{ax}–M–L_{eq} 90°, L_{ax}–M–L_{ax} 180° and L_{eq}–M–L_{eq} 72 and 144°, respectively.

Inspection of the data in Table II reveals that L_{eq}–Cu–L_{eq} angles in the pentagonal base differ from the ideal pentagonal angles of 72 and 144° respectively, by twenty degrees for the former and by ten degrees for the latter, the observed values ranging from 50.0 to 91.4° with an average value of 72.5°, and from 134.2 to 152.9° with an average value of 143°, respectively. Smaller L_{eq}–Cu–L_{eq} angles occur between the intraligand coordinated atoms while the larger ones involve interligand bonded atoms. The L_{ax}–Cu–L_{eq} bond angles ranging from 44 to 99° with an average value of 86°. The average value of 176° for L_{ax}–Cu–L_{ax} angles (range from 165 to 180°) is again smaller than in the ideal pentagonal bipyramid (180°). These smaller/larger angles reflect significant deviation from ideal pentagonal biyramidal geometry.

The metallocyclic intraligand O–Cu–O ring angle opens with increasing size of the ring: 51°(four-membered) < 72° (five-membered). For five-membered metallocyclic rings, N–Cu–N angles are 69° (for unsaturated ligand) and 80° (for saturated). One would expect that at the greater size of the chelate ring, the M–L bond lengths would be somewhat shorter. The data presented in Table II, show this trend. For example, the mean Cu–O bond distance of 2.37 Å for four-membered chelate rings is about 0.11 Å longer than the mean Cu–O bond distance (2.26 Å) for a five-membered chelate ring. The mean values of L–Cu–L bond angles of the metallocyclic rings found for seven-coordinate Cu(II) derivatives are smaller that those of six-, five- and four-coordinated (Table IB).

It is well known, that coordination number seven is unusual for Cu(II), but there is an example, $[Cu(C_{10}H_{20}O_5)(H_2O)](NO_3)_2$,[487] which contains ten crystallographically independent molecules differing by degree of distortion in the same crystal, a rarity in the complex chemistry of Cu(II).

There are two examples, which contain two non-equivalent forms, the [Cu(15-crown-5)(MeCN)$_2$[Cu_3Cl_8][490] a monomeric cation with the CuO_5N_2 chromophore and a trimeric complex $[Cu_3Cl_8]^{2-}$ anion in which each

Cu(II) is a tetrahedral coordinated by four chlorine atoms and [Cu(15-crown-5)(MeCN)Cl]·$[CuCl_3]$[490,491] consists of complex cation, where Cu(II) is surrounded by seven donor atoms (CuO_5NCl) and a dimeric complex $[CuCl_3]^-$ anion, with a *pseudo*-tetrahedrally coordinated Cu(II) atom. Hepta-coordinate Cu(II) compounds are mostly red (orange) and by far "prefer" a monoclinic crystal class (Table II).

OCTACOORDINATE Cu(II) COMPOUNDS

Coordination number eight is rare for transition elements and especially for Cu(II). There are four examples[496–499] for which crystallographic and structural data are given in Table II. There are two principal ways in which a cube may become distorted, square antiprism (symmetry D_{4d}) and dodecahedron (symmetry D_{2h}). The second distortion (all four examples belong to this class) can be best understood by recognizing that the cube is composed of two interpenetrating tetrahedra. The distortion occurs when the vertices of one of these tetrahedra are displaced so as to decrease the two vertical angles, that is, to elongate the tetrahedron, while the vertices of the other one are displaced to produce a flattened tetrahedron. It is important to note that its vertices (symmetry D_{2h}), are not all equivalent but are divided into two bisphenoidal sets, those within each set being equivalent; Table II shows this for Cu(II) examples. All examples[496–498] contain bidentate ligands in which the two coordinated atoms are very close together. In these, the close pairs of ligand atoms lie on the m edges of the dodecahedron; these edges are the very short. The mean values of the two sets of Cu–O bond distances are 1.96 and 2.75 Å, respectively.

CONCLUSIONS

This review has classified almost six hundred six-, seven- and eight-coordinate Cu(II) coordination compounds which have been characterized by X-ray (neutron) diffraction. There are five hundred and fifty examples which are six-coordinate, and from the three principal forms of distortion of the octahedron, all occur in the chemistry of Cu(II) in varying degrees. The tetragonal distortion most commonly involves an elongation of one C_4 axis. In the series of heptacoordinate Cu(II) compounds only a pentagonal bipyramidal geometry around Cu(II) is observed. For Cu(II) octacoordinate complexes only a dodecahedral configuration is found.

The ligands in these complexes are homo- and hetero-donors. The former are uni-, bi-, tri-, tetra-, penta-, hexa- and even heptadentate; the latter are bi-, tri-, tetra-, penta- and hexadentate. The O- and N-donor ligands are most prevalent along with chloride. In general, the mean $Cu-L_{eq}$ bond distance is shorter than that for $Cu-L_{ax}$ in the series of six-coordinate complexes, but for seven-coordinate complexes and for some six-coordinate complexes the opposite is observed. In both series, there are some exceptions, which were discussed in the respective sections, and will not be repeated here.

We compared six-coordinate with five-coordinate Cu(II) compounds[2] and found that the mean $Cu-L_{eq}$ bond distance increases as follows with configuration around Cu(II): square-pyramidal < tetragonal-bipyramidal < trigonal-bipyramidal; and $Cu-L_{ax}$ bond distance: trigonal-bipyramidal < square-pyramidal < tetragonal-bipyramidal. In general, distortion around Cu(II) increases in the order: trigonal-bipyramidal < pentagonal-bipyramidal; and square-pyramidal < tetragonal-bipyramidal.

The effect of both electronic and steric hindrance of the ligands can be seen in the opening of the L–Cu–L angles of the respective metallocyclic rings. There is an impressive correlation between the Cu–L bond length and bite angle, at greater Cu–L bond lengths the angle is smaller and vice versa. The four- and five-membered rings are relatively rigid; however six- and higher-membered rings show more flexibility. In general, the mean values of the L–Cu–L bond angles of the respective metallocyclic rings, open with a decrease of coordination number about Cu(II) and with an increase of covalent radius of the donor atom/ligand.

There are several examples[20,21,51,52,90,156,216,217,224,225,227,228,300,317] which exist in two isomeric forms, differing mostly by degree of distortion. Two crystallographically independent molecules differing by degree of distortion and coexisting in the same crystal have been found in several species.[15,16,43,50,67,72,112,141,187,201,208,216,220b,236,240,280,359,376,391,408,445,485] In $[Cu(en)_3]Cl_2 \cdot 0.75en$[86] three such molecules are present and in $[Cu(C_{10}H_{20}O_5)(H_2O)_2](NO_3)_2$[487] ten exist. The coexistence of two or even more species differing only by degree of distortion within the same crystal is typical of distortion isomerism.[500]

The influence of temperature on degree of distortion of structures has been reported for some compounds.[5,12,71,85,94,109] There are examples[18,19,30,111,137,150,422] which contain two non-equivalent monomeric species. In $[Cu(15\text{-crown-}5)(MeCN)_2][Cu_3Cl_8]$[490] the monomeric complex cation contains about the Cu(II) a pentagonal bipyramid (CuO_5N_2) and the trimeric complex anion has a tetrahedral ($CuCl_4$) arrangement. In

$[Cu(15\text{-crown-5})(MeCN)Cl][Cu_2Cl_6]$[490,491] besides the monomeric complex cation (CuO_5N_2), there is also the dimeric complex anion ($CuCl_4$).

Cu(II) compounds are mostly blue or green; there are also examples of red and brown. The majority have a monoclinic crystal class, but triclinic and orthorhombic are also observed.

Relationships between the various structural parameters have been discussed within each section.

This review, together with its precursor for four- and five-coordinate mononuclear Cu(II) compounds,[2] represents the first overview of structural data for over one thousand eight hundred mononuclear Cu(II) derivatives. In collecting and organizing the data it has become clear that despite the increasing availability of data retrieval systems, the tracing of relevant material is not always a straightforward task. One of the problems appears to be associated with the choice of keywords for indices, resulting in the effective invisibility of some material from a particular point of view. Some of the data is only available as supplementary material, and this can lead to overlooking of relevant structural features for comparative purposes. In view of the limitations inherent in information retrieval, we believe that such reviews will continue to serve a useful function by crystallizing available material, and delineating areas of both interest and weakness. Related reviews on the dimeric, as well as oligomeric and polymeric derivatives of Cu(II) are currently in progress.

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