

Entry	Identifier	Compound Name	Ref
1	HAWBIS	catena-((μ_6 -benzene-1,3,5-tricarboxylato)-(μ_3 -hydroxido)-(μ_3 -oxido)-hexakis(μ -pyrazolato-N,N'))-hexa-copper(ii)	30
2	QUSMIB	(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-tris(1H-pyrazole)-tri-copper(ii) (μ_3 -oxido)-tris(μ -pyrazolato-N,N')-tris(1H-pyrazole)-tri-copper(ii)bis(trifluoromethanesulfonato) trifluoromethanesulfonate	31
3	KEWRAG	bis(triphenylphosphine)iminium bis(μ_3 -oxido)-tris(μ -3,5-diphenylpyrazolato-N,N')-hexakis(μ -pyrazolato-N,N')-hexa-copper(ii)	32
4	NESQOS	tetra-n-butylammonium (μ_3 -oxido)-tris(μ -pyrazolato-N,N')-(benzoato-O)-tri-copper(ii)	33
5	XOBCEW01	bis(bis(triphenylphosphine)iminium) (μ_3 -oxido)-tris(μ -pyrazolato-N,N')-trichlorido-tri-copper(ii)	34
6	RUYGIB	tetra-n-butylammonium (μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-trichlorido-tri-copper(ii)	34
7	RUYHEY	triethylammonium (μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-(1H-pyrazole)-trichlorido-tri-copper(ii)	34
8	LUDZIV	bis(tetra-n-butylammonium) octakis(μ -hydroxido)-octadecakis(μ -pyrazolato-N,N')-pentadeca-copper diphosphate bromobenzene nitrobenzene solvate	35
9	LUDZOB	bis(tetra-n-butylammonium) octakis(μ -hydroxido)-octadecakis(μ -pyrazolato-N,N')-pentadeca-copper diarsenate bromobenzene nitrobenzene solvate	35
10	MAFBOL	bis(tetrabutylammonium) bis((μ_3 -hydroxido)-(μ -acetato-O,O)-bis(acetato-O)-tris(μ -pyrazolato-N,N')-tri-copper(ii)) hexahydrate	36
11	XOKWUQ	bis(tetra-n-butylammonium) bis(μ_3 -hydroxido)-hexakis(μ -pyrazolato-N,N')-bis(μ -thiocyanato-N,S)-tetrakis(isothiocyanato)-hexa-copper(ii)	37
12	XEMYEV	bis(triethylammonium) bis(μ_3 -hydroxido)-bis(μ -acetato-O)-hexakis(μ -pyrazolato-N,N')-tetrakis(acetato-O)-hexa-copper(ii) benzene solvate	38
13	RUYGEX	bis(triphenylphosphine)iminium (μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-trichlorido-tri-copper(ii) tetrahydrofuran dichloromethane solvate	34
14	MAFBEB	bis(triphenylphosphino)iminium (μ_3 -hydroxido)-tris((μ -pyrazolato-N,N')-(isocyanato))-tri-copper(ii)	36
15	MAFBIF	bis(bis(triphenylphosphino)iminium) bis((μ_3 -hydroxido)-(μ -acetato-O,O)-aqua-bis(acetato-O)-tris(μ -pyrazolato-N,N')-tri-copper(ii)) dihydrate	36
16	DIBXES	bis(μ_3 -hydroxido)-bis(μ -acetato-O,O)-hexakis(μ -pyrazolato-N,N')-tetrakis(1H-pyrazole)-hexa-copper(ii) dichloride dihydrate	39
17	YUYGUW	bis(μ_3 -hydroxido)-hexakis(μ -pyrazolato-N,N')-bis(μ -chloroacetato)-tetrakis(1H-pyrazole)-hexa-copper bis(chloride)	40
18	KEBBUQ	bis(μ_3 -hydroxido)-hexakis(μ -pyrazolato-N,N')-bis(μ -4,4'-bipyridine)-diaqua-tetrakis(4,4'-bipyridine)-bis(formato)-hexa-copper(ii) dihydroxide 4,4'-bipyridine	41
19	KEBCAX	bis(μ_3 -hydroxido)-hexakis(μ -pyrazolato-N,N')-bis(μ -4,4'-bipyridine)-diaqua-tetrakis(4,4'-bipyridine)-bis(formato)-hexa-copper(ii) dihydroxide benzene solvate	41
20	KEBCIF	bis(μ_3 -hydroxido)-hexakis(μ -pyrazolato-N,N')-bis(μ -4,4'-bipyridine)-diaqua-tetrakis(4,4'-bipyridine)-bis(formato)-hexa-copper(ii) dihydroxide hemikis(4,4'-bipyridine) cyclohexane solvate	41
21	KEBCUR	bis(μ_3 -hydroxido)-hexakis(μ -pyrazolato-N,N')-bis(μ -4,4'-bipyridine)-diaqua-tetrakis(4,4'-bipyridine)-bis(formato)-hexa-copper(ii) dihydroxide toluene solvate	41
22	RUGLEM	bis(μ -4,4'-bipyridine)-bis(μ_3 -hydroxido)-hexakis(μ -pyrazolato-N,N')-bis(acetato)-diaqua-tetrakis(4,4'-bipyridine)-hexa-copper 4,4'-bipyridine dihydroxide dihydrate	42
23	RUGLIQ	bis(μ -4,4'-bipyridine)-bis(μ_3 -hydroxido)-hexakis(μ -pyrazolato-N,N')-bis(acetato)-diaqua-tetrakis(4,4'-bipyridine)-hexa-copper 4,4'-bipyridine dihydroxide tetrahydrate	42
24	XOKXAX	(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-tris(pyridine-N)-tri-copper(ii) (trifluoromethanesulfonato) trifluoromethanesulfonate acetone solvate	37
25	MUZRIJ	catena-[bis(μ_3 -hydroxido)-tris(μ -4,4'-bipyridine-N,N')-hexakis(μ -pyrazolato-N,N')-hexa-copper(ii) tetrakis(trifluoromethanesulfonate) hexahydrate]	43
26	VIMYEX	(μ_3 -hydroxido)-(μ -chlorido)-tris(μ -pyrazolato-N,N')-(aqua)-tris(1H-pyrazole)-tri-copper dicyano(nitro)methanide monohydrate	44
27	BOFLEP	(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-tetrakis(1H-pyrazole)-bis(nitrato)-di-copper monohydrate	45
28	BOZBIB	catena-(μ_3 -nitrato-O,O',O'')-(μ_3 -hydroxido)-1-nitrato-1,2:1,3:2,3-tris(μ -pyrazolato-N,N')-2,3-bis(1H-pyrazole)-tri-copper(ii) monohydrate	46
29	MINZIU	(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-(μ -nitrato)-tris(pyridine)-(nitrato)-tri-copper	47
30	ZOQGOB	bis((μ_3 -hydroxido)-(μ_3 -nitrato-O,O')-(μ -nitrato-O,O')-tris(μ -pyrazolato-N,N')-tris(pyrazol-2-yl))-hexa-copper(ii)	48
31	DIBXIW	catena-(bis(μ_3 -chlorido)-bis(μ_3 -hydroxido)-hexakis(μ -pyrazolato-N,N')-diaqua-tetrachlorido-hexakis(1H-pyrazole)-hepta-copper(ii))	39
32	DIBXOC	bis(μ_3 -hydroxido)-bis(μ -chlorido)-hexakis(μ -pyrazolato-N,N')-dichlorido-hexakis(1H-	39

		pyrazole)-hexa-copper(ii) monohydrate	
33	QIMSIQ	(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-bis(1H-pyrazole)-(N,N-dimethylformamide)-dichlorido-tri-copper (μ_3 -hydroxido)-(μ -chlorido)-tris(μ -pyrazolato-N,N')-bis(1H-pyrazole)-chlorido-tri-copper N,N-dimethylformamide solvate	49
34	SIJKOL	(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-(μ -chlorido)-chlorido-bis(pyridyl)-tri-copper(ii) pyridine solvate	50
35	BOLXEH	catena-((μ_3 -hydroxido)-bis(μ -bromido)-tris(μ -pyrazolato-N,N')-tetrahydrofuran-tri-copper tetrahydrofuran solvate)	51
36	QOPJIP	bis(μ_3 -perchlorato-O,O',O'')-bis(μ_3 -hydroxido)-bis(μ -perchlorato-O,O')-hexakis(μ -pyrazolato-N,N')-hexakis(1H-pyrazole)-hexa-copper(ii) ethanol methanol solvate dihydrate	52
37	QUSLOG	bis(μ_3 -hydroxido)-bis(μ_3 -perchlorato-O,O',O'')-bis(μ -perchlorato-O,O')-hexakis(μ -pyrazolato-N,N')-hexakis(1H-pyrazole)-hexa-copper(ii)	31
38	QUSMUN	(μ_3 -hydroxido)-(μ_3 -trifluoromethanesulfonato-O,O',O'')-tris(μ -pyrazolato-N,N')-tris(1H-pyrazole)-(trifluoromethanesulfonato-O)-tri-copper(ii) monohydrate	31
39	MUZQUU	(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-(μ -trifluoromethanesulfonato-O,O')-tripyridine-(trifluoromethanesulfonato-O)-tri-copper(ii) hemihydrate	43
40	MUZRAB	bis(μ_3 -hydroxido)-(μ -4,4'-bipyridine-N,N')-hexakis(μ -pyrazolato-N,N')-tetrapyridine-hexa-copper(ii) tetrakis(trifluoromethanesulfonato)	43
41	MUZREF	catena-[bis(μ_3 -hydroxido)-bis(μ -4,4'-bipyridine-N,N')-hexakis(μ -pyrazolato-N,N')-dipyridine-hexa-copper(ii) tetrakis(trifluoromethanesulfonato) monohydrate]	43
42	QUSLEW	(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-(μ -sulfato-O,O')-tris(1H-pyrazole)-tri-copper(ii) monohydrate	31
43	MINZOA	octakis(μ -4-methylphenyl)phosphonato)-octakis(μ -hydroxido)-dodecakis(μ -pyrazolato-N,N')-diaqua-tetrapyridine-octadeca-copper acetonitrile unknown solvate tetrahydrate	47
44	DOKKAQ	catena-((μ_6 -sulfato)-bis(μ_3 -hydroxido)-hexakis(μ -pyrazolato-N,N)-bis(μ -nitrate)-hexakis(1H-pyrazole)-hexa-copper acetonitrile methanol solvate sesquihydrate)	53
45	KEBBOK	catena-(tetrakis(μ_3 -hydroxido)-dodecakis(μ -pyrazolato-N,N')-(μ -4,4'-bipyridine)-tetrakis(μ -formato)-diaqua-tetrakis(formato)-dodeca-copper(ii) decahydrate)	41
46	KEBDEC	catena-(bis(μ_3 -hydroxido)-hexakis(μ -pyrazolato-N,N')-(μ -4,4'-bipyridine)-bis(μ -formato)-diaqua-bis(4,4'-bipyridine)-bis(formato)-hexa-copper(ii) dihydrate)	41
47	JAVGAP	catena-((μ_3 -hydroxido)-(μ -formato)-tris(μ -pyrazolato-N,N')-formato-bis(1H-pyrazole)-tri-copper(ii) monohydrate)	54
48	RUGKUB	catena-[bis(μ -acetato)-bis(μ -4,4'-bipyridine)-bis(μ_3 -hydroxido)-hexakis(μ -pyrazolato-N,N')-bis(acetato)-hexa-copper methanol solvate monohydrate]	42
49	RUGLAI	catena-[bis(μ -4,4'-bipyridine)-(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-bis(acetato)-aqua-tri-copper 4,4'-bipyridine methanol solvate tetrahydrate]	42
50	LAHYUP	catena-[(μ_3 -acetato)-(μ_3 -hydroxido)-(μ -acetato)-tris(μ -pyrazolato-N,N')-(1H-pyrazole)-tri-copper(ii)]	55
51	QUSMEX	(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-(μ -trifluoroacetato-O,O')-bis(1H-pyrazole)-(trifluoroacetato-O)-tri-copper(ii)	31
52	JEWWEO	(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-aqua-bis(propionato)-tri-copper(ii) monohydrate	7
53	JEWWIS	(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-aqua-bis(propionato)-tri-copper(ii)	7
54	RUGLUC	catena-[bis(μ -4,4'-bipyridine)-bis(μ_3 -hydroxido)-bis(μ -propanoato)-hexakis(μ -pyrazolato-N,N')-bis(propanoato)-hexa-copper dihydrate]	42
55	JAVGET	catena-((μ_3 -hydroxido)-(μ -propionato-O,O)-(μ -propionato-O,O')-tris(μ -pyrazolato-N,N')-ethanol-tri-copper(ii))	54
56	JAVGIX	bis((μ_3 -hydroxido)-(μ -butyrato)-tris(μ -pyrazolato-N,N')-aqua-butyrate-methanol-tri-copper(ii))	54
57	HUTZED	catena-[(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-(μ -4,4'-bipyridine)-(μ -valerato)-(valerato)-methanol-tri-copper]	56
58	HUTZON	catena-[(μ_3 -hydroxido)-(μ -4,4'-bipyridine)-tris(μ -pyrazolato-N,N')-(μ -hexanoato)-(hexanoato)-aqua-tri-copper]	56
59	FUPYOG	catena-[bis(μ_3 -hydroxido)-bis(μ -heptanoato)-(4,4'-bipyridine)-hexakis(μ -pyrazolato-N,N')-bis(heptanoato)-hexa-copper]	56
60	RUGMEN	catena-[(μ -4,4'-bipyridine)-(μ_3 -hydroxido)-(μ -acrylato)-tris(μ -pyrazolato-N,N')-(acrylato)-aqua-tri-copper]	42
61	RUGMOX	catena-[(μ -4,4'-bipyridine)-(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-(acrylato-O)-(acrylato-O,O')-(4,4'-bipyridine)-(1H-pyrazole)-tri-copper dihydrate]	42
62	XUCRET	bis(μ_3 -hydroxido)-bis(μ -acrylato-O,O)-hexakis(μ -pyrazolato-N,N')-bis(acrylato-O,O')-tetra-aqua-bis(1H-pyrazole)-hexa-copper(ii)	57
63	XUCRIX	catena-((μ_3 -hydroxido)-(μ -acrylato-O,O')-(μ -acrylato-O,O)-tris(μ -pyrazolato-N,N')-methanol-tri-copper(ii))	57

64	XUCROD	catena-((μ_3 -hydroxido)-bis(μ -methacrylato-O,O'))-tris(μ -pyrazolato-N,N')-tri-copper(ii)	57
65 ^a	1454767	(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-bis(pivalato)-(1H-pyrazole)-bis(pivalic acid)-tri-copper(ii)	58
66 ^a	1454763	catena-((μ_3 -hydroxido)-bis(μ -phenylacetato-O,O'))-tris(μ -pyrazolato-N,N')-tri-copper(ii)	58
67 ^a	1454764	catena-((μ_3 -hydroxido)-(μ_3 -vinylacetato)-(μ -vinylacetato))-tris(μ -pyrazolato-N,N')-tri-copper(ii)	58
68 ^a	1454765	bis((μ_3 -hydroxido)-(μ_3 -phenylpropanoato)-(μ -phenylpropanoato))-tris(μ -pyrazolato-N,N')-tri-copper(ii)-bis((μ_3 -hydroxido)-(μ_3 -phenylpropanoato)-(μ -phenylpropanoato))-tris(μ -pyrazolato-N,N')-diaqua-tri-copper(ii)	58
69 ^a	1454766	catena-((μ_3 -hydroxido)-bis(μ -cyclohexylcarboxylato-O,O'))-tris(μ -pyrazolato-N,N')-tri-copper(ii)	58
70	DEGBAU	bis(μ_3 -hydroxido)-tetrakis(μ -hydroxido)-hexadecakis(μ -pyrazolato-N,N')-bis(isocyanato)-dodeca-copper methanol solvate	59
71	TAZWOI	catena-[(μ_3 -fumarato)-(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-(1H-pyrazole)-tri-copper(ii)]	60
72	TAZWUO	catena-[(μ_3 -2-methylfumarato)-(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-(1H-pyrazole)-tri-copper(ii)]	60
73	CENJIQ	catena-((μ_3 -succinato)-(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-aqua-(methanol)-tri-copper monohydrate unknown solvate)	61
74	CENKAJ	catena-((μ_3 -succinato)-(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-triaqua-tri-copper hemihydrate unknown solvate)	61
75	CENKEN	catena-((μ_4 -succinato)-(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-tri-copper)	61
76 ^b	QOJZEW01	catena-[(μ -2-hydroxynaphthalene-1,4-dicarboxylato)-(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-tri-copper N,N-dimethylformamide methanol solvate monohydrate]	62
77 ^b	QOJZIA01	catena-[(μ -biphenyl-4,4'-dicarboxylato)-(μ_3 -hydroxido)-tris(μ -pyrazolato-N,N')-diaqua-tri-copper]	62
78 ^b	QOKCOK01	catena-((μ_3 -oxido)-(μ_3 -pyridine-3,4-dicarboxylato))-tris(μ -pyrazolato-N,N')-diaqua-methanol-tri-copper unknown solvate)	62
79	HUXWUU	tris(μ -3,5-diphenylpyrazolato-N,N')-(μ_6 -fluoro)-bis(μ_3 -hydroxido)-hexakis(μ -pyrazolato-N,N')-hexa-copper(ii) unknown solvate	63
80	KEBBEA	catena-((μ_3 -methoxido)-tris(μ -pyrazolato-N,N')-(μ -4,4'-bipyridine)-(μ -formato)-(formato)-tri-copper(ii) methanol solvate)	41
81	FUPYIA	catena-[bis(μ -methoxido)-bis(μ -butanoato)-hexakis(μ -pyrazolato-N,N')-bis(μ -4,4'-bipyridine)-bis(butyrate)-hexa-copper]	56
82	HUTZIH	catena-[bis(μ_3 -methoxido)-bis(μ -4,4'-bipyridine)-bis(μ -hexanoato)-hexakis(μ -pyrazolato-N,N')-bis(hexanoato)-hexa-copper]	56

^a For compounds **65-69** reported in ref. 58 the CCDC deposit numbers are indicated. ^b Atomic coordinates of compounds **76-78** (QOJZEW01, QOJZIA01 and QOKCOK01) (ref. 62) can be retrieved from the corresponding QOJZEW, QOJZIA and QOKCOK files, reported in in the CCDC database as Personal Communication.