Supplementary data F for [Cu<sub>6(</sub>phen)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>(μ-O<sub>2</sub>CC<sub>2</sub>H<sub>5</sub>)<sub>12</sub>]<sub>n</sub> [Cu<sub>2</sub>(μ-O<sub>2</sub>CC<sub>2</sub>H<sub>5</sub>)<sub>4</sub>(H<sub>2</sub>O)<sub>2</sub>]<sub>2n</sub>(H<sub>2</sub>O)<sub>0.5n</sub> (VI)

**Table F1**Atomic Coordinates  $[x \ 10^4]$  and equivalent isotropic displacement<br/>parameters  $[Å^2 x \ 10^3]$  for complex VI. U(eq) is defined as one third of<br/>the trace of the orthogonalized U<sub>ij</sub> tensor

	X	У	Z	U(eq)
C(1)	2167(4)	12090(2)	1380.7(19)	68(1)
C(2)	1473(5)	12276(2)	948(2)	94(1)
C(3)	0240(5)	12458(2)	1095(2)	92(1)
C(4)	-311(4)	12487.4(19)	1665(2)	65(1)
C(5)	468(4)	12300.9(16)	2062.3(18)	47(1)
C(6)	4(4)	12330.7(16)	2644.3(19)	49(1)
C(7)	-1564(5)	12690(2)	1856(2)	86(1)
C(8)	-2011(4)	12719(2)	2406(3)	86(1)
C(9)	-1223(4)	12549.1(19)	2816(2)	68(1)
C(10)	-1600(5)	12573(2)	3390(3)	96(1)
C(11)	-790(5)	12393(3)	3748(2)	111(1)
C(12)	0418(5)	12171(2)	3544(2)	84(1)
C(13)	4380(4)	11038.4(16)	2167.9(16)	41(1)
C(14)	5736(12)	10932(5)	1854(4)	55(1)
C(15)	6638(13)	1113(5)	2360(7)	111(1)
C(16)	2769(5)	9126(2)	1644(2)	66(1)
C(17)	2510(18)	9254(7)	1074(8)	132(1)
C(18)	1639(16)	9730(5)	880(7)	152(1)
C(19)	979(4)	91719(19)	3016.1(18)	55(1)
C(20)	-405(13)	9229(5)	3283(5)	71(1)
C(21)	-1212(19)	9461(11)	2796(7)	152(1)
C(22)	3892(4)	8970(2)	3584(2)	64(1)
C(23)	414(2)	8766(11)	4276(9)	217(1)
C(24)	5070(2)	9139(8)	4157(8)	235(1)
C(25)	5689(4)	8979(2)	2122(2)	63(1)
C(26)	7165(9)	8971(6)	1761(5)	61(1)
C(27)	7022(17)	9034(11)	1159(7)	253(1)
C(28)	2814(4)	7097.6(18)	3259.6(18)	47(1)

**Table F1**Atomic Coordinates  $[x \ 10^4]$  and equivalent isotropic displacement<br/>parameters  $[Å^2 x \ 10^3]$  for complex VI. U(eq) is defined as one third of<br/>the trace of the orthogonalized U<sub>ij</sub> tensor (cont.)

	X	У	Z	U(eq)
C(29)	1472(9)	7052(6)	3717(6)	81(1)
C(30)	1429(13)	6604(6)	4226(6)	133(1)
C(31)	3459(4)	60337(17)	2167.2(16)	41(1)
C(32)	2404(9)	5935(4)	1832(3)	43(1)
C(33)	1126(10)	5866(5)	2406(5)	95(1)
C(34)	6002(4)	4182(2)	3013.3(18)	55(1)
C(35)	7228(16)	4279(8)	3261(7)	73(1)
C(36)	8390(2)	4457(11)	2805(9)	157(1)
C(37)	5588(5)	4129(2)	1646(2)	68(1)
C(38)	6478(18)	4204(8)	1019(5)	105(1)
C(39)	7716(14)	4448(6)	1078(7)	148(1)
C(40)	2186(4)	3973(2)	2120.3(19)	63(1)
C(41)	1000(9)	4003(5)	1792(6)	78(1)
C(42)	1826(16)	4019(9)	1168(6)	201(1)
C(43)	2531(4)	3970(2)	3587(2)	65(1)
C(44)	1563(15)	4013(6)	4174(6)	91(1)
C(45)	1130(3)	3558(11)	4365(10)	42.1(1)
C(46)	3922(4)	2096.3(18)	3263.5(17)	48(1)
C(47)	4786(13)	2089(10)	3720(8)	123(1)
C(49)	8360(4)	3293.8(19)	9780(2)	63(1)
C(48)	3907(12)	1892(6)	4287(6)	116(1)
C(50)	9617(16)	3797(6)	9520(9)	166(1)
C(51)	9963(13)	3879(6)	9932(6)	162(1)
C(52)	8139(4)	1708.8(19)	10221(2)	62(1)
C(53)	8647(18)	949(12)	10453(8)	26.2(1)
C(54)	9915(13)	1101(6)	10061(6)	158(1)
C(55)	4856(4)	1665(2)	10188(2)	66(1)
C(56)	3816(12)	1212(4)	10256(4)	98(1)

**Table F1**Atomic Coordinates  $[x \ 10^4]$  and equivalent isotropic displacement<br/>parameters  $[Å^2 x \ 10^3]$  for complex VI. U(eq) is defined as one third of<br/>the trace of the orthogonalized U<sub>ij</sub> tensor (cont.)

	X	У	Z	U(eq)
C(57)	4856(18)	583(7)	10457(8)	27.4(1)
C(58)	5041(4)	3333(2)	9811(2)	71(1)
C(59)	4154(16)	3803(5)	9733(6)	99(1)
C(60)	3394(15)	4040(7)	1.0188(6)	189(1)
C(61)	1437(5)	96178(19)	5693(2)	60(1)
C(62)	2361(9)	9408(4)	6061(4)	43(1)
C(63)	3635(14)	9598(8)	5914(8)	201(1)
C(64)	64(5)	8987.7(19)	4754(2)	62(1)
C(65)	310(2)	8340(7)	4598(9)	134(1)
C(66)	-709(19)	7992(10)	4769(9)	223(1)
C(67)	5187(4)	3984.4(19)	4758(2)	62(1)
C(68)	5050(3)	3326(9)	4606(10)	12(1)
C(69)	5970(2)	2924(9)	4785(9)	157(1)
C(71)	8379(5)	5631(3)	3898(3)	111(1)
C(70)	7131(4)	5379.4(19)	4304(2)	6(1)
C(72)	9424(8)	5509(5)	4104(4)	29.7(1)
C(74)	6443(4)	7086(2)	1380(18)	68(1)
C(75)	7583(5)	7277(2)	949(2)	95(1)
C(76)	8667(5)	7456(2)	1089(2)	93(1)
C(77)	8644(4)	7484.8(19)	1664(2)	67(1)
C(79)	7350(4)	7330.9(16)	2639.9(19)	52(1)
C(78)	7466(4)	7303.2(16)	2060.6(18)	47(1)
C(80)	9709(4)	7691(2)	1854(3)	88(1)
C(81)	9597(5)	7719(2)	2401(3)	90(1)
C(82)	8412(4)	7548.3(19)	2819(2)	69(1)
C(83)	8202(5)	7575(2)	3395(2)	97(1)
C(84)	7043(5)	7384(3)	3751(2)	108(1)
C(85)	6039(5)	7168(2)	3547(2)	82(1)

**Table F1**Atomic Coordinates  $[x \ 10^4]$  and equivalent isotropic displacement<br/>parameters  $[Å^2 x \ 10^3]$  for complex VI. U(eq) is defined as one third of<br/>the trace of the orthogonalized U<sub>ij</sub> tensor (cont.)

	X	У	Z	U(eq)
Cu(1)	2443.2(5)	11794.4(2)	2606.0(2)	42(1)
Cu(2)	3561.2(5)	9647.5(2)	2497.6(2)	54(1)
Cu(3)	3173.8(5)	8475.1(2)	2714.7(2)	49(1)
Cu(4)	4950.8(5)	6794.7(2)	2606.1(2)	42(1)
Cu(5)	3941.1(5)	4648.1(2)	2497.8(2)	54(1)
Cu(6)	4111.3(5)	3475.1(2)	2714.8(2)	49(1)
Cu(7)	6278.3(5)	2530.2(2)	10546.5(2)	48(1)
Cu(8)	6825.1(5)	2469.9(2)	9453.4(2)	48(1)
Cu(9)	10238(5)	196.7(2)	4580.1(2)	53(1)
Cu(10)	4396.1(5)	5196.9(2)	4580.0(2)	54(1)
O(1)	1058(3)	10926.1(13)	2877.6(15)	61(1)
O(2)	3176(2)	11642.0(10)	3299.7(10)	46(1)
O(3)	4047(2)	11576.9(10)	2145.0(10)	44(1)
O(4)	3606(3)	10602.1(11)	2392.8(13)	69(1)
O(5)	3077(3)	96035(12)	1772.9(12)	80(1)
O(6)	2769(3)	8604.2(11)	1948.8(11)	60(1)
O(7)	1709(3)	9644.9(12)	2839.8(13)	69(1)
O(8)	1347(3)	8650.7(11)	3023.6(12)	58(1)
O(9)	3904(3)	9491.2(13)	3279.1(13)	73(1)
O(10)	3608(3)	8494.1(12)	3452.3(12)	67(1)
O(11)	5337(3)	9491.4(12)	2163.3(15)	83(1)
O(12)	5037(3)	8495.5(12)	2342.2(13)	67(1)
O(13)	3049(3)	7520.7(11)	2837.2(12)	58(1)
O(14)	3527(2)	6640.5(10)	3296.3(10)	45(1)
O(15)	6067(3)	5923.4(12)	2881.9(14)	58(1)
O(16)	3805(2)	6577.2(10)	2144.1(10)	44(1)
O(17)	3999(3)	5600.6(11)	2392.4(13)	69(1)
O(18)	5457(3)	4648.2(12)	2836.8(13)	67(1)

**Table F1**Atomic Coordinates  $[x \ 10^4]$  and equivalent isotropic displacement<br/>parameters  $[Å^2 x \ 10^3]$  for complex VI. U(eq) is defined as one third of<br/>the trace of the orthogonalized U<sub>ij</sub> tensor (cont.)

	X	У	Z	U(eq)
O(19)	5637(3)	3649.8(11)	3023.7(12)	57(1)
O(20)	5150(3)	4604.5(12)	1774.6(13)	81(1)
O(21)	5282(3)	3607.3(11)	1949.1(12)	62(1)
O(22)	2494(3)	4491.8(12)	2163.7(14)	80(1)
O(23)	2621(3)	3496.3(12)	2343.1(13)	65(1)
O(24)	2813(3)	4490.7(13)	3278.1(13)	74(1)
O(25)	2939(3)	3493.6(12)	3451.9(12)	67(1)
O(26)	4118(3)	2522.1(11)	2836.8(11)	57(1)
O(27)	7756(3)	3133.5(12)	10294.1(13)	68(1)
O(28)	8174(3)	3090.1(12)	9371.1(12)	67(1)
O(29)	7544(3)	1911.5(13)	10630.2(12)	67(1)
O(30)	8051(3)	1865.7(13)	9708.6(13)	68(1)
O(31)	4961(3)	1896.4(13)	10599.4(12)	72(1)
O(32)	5447(3)	1838.5(13)	9679.5(13)	71(1)
O(33)	5129(3)	3162.2(13)	10320.7(13)	74(1)
O(34)	5563(3)	3105.7(13)	9398.3(13)	73(1)
O(35)	5654(3)	2557.3(12)	11446.2(14)	55(1)
O(36)	7095(4)	2443.7(13)	8555.5(13)	55(1)
O(37)	2752(3)	10421.5(12)	3898.0(14)	65(1)
O(38)	822(3)	10964.2(12)	4828.5(13)	70(1)
O(39)	1953(3)	9880.0(14)	5186.5(13)	76(1)
O(40)	891(3)	9385.3(12)	4448.5(12)	69(1)
O(41)	-241(3)	10462.8(12)	4099.4(12)	62(1)
O(42)	3347(4)	5424.2(12)	3904.6(15)	67(1)
O(43)	2864(3)	4874.9(14)	5187.4(13)	76(1)
O(45)	4664(3)	4379.6(12)	4450.9(12)	70(1)
O(46)	6137(3)	5462.2(12)	4094.6(12)	63(1)
O(47)	8899(15)	9296(5)	8337(6)	104(1)

**Table F1**Atomic Coordinates  $[x \ 10^4]$  and equivalent isotropic displacement<br/>parameters  $[Å^2 x \ 10^3]$  for complex VI. U(eq) is defined as one third of<br/>the trace of the orthogonalized U<sub>ij</sub> tensor (cont.)

	X	У	Z	U(eq)
O(48)	7202(14)	5694(5)	1666(6)	103(1)
O(44)	4346(3)	5962.7(12)	4828.8(12)	69(1)
N(1)	1676(3)	12094.9(13)	1921.2(13)	46(1)
N(2)	814(3)	12146.7(14)	2998.2(14)	50(1)
N(3)	6401(3)	7097.0(14)	1920.3(13)	48(1)
N(4)	6176(3)	7147.2(14)	3001.9(14)	52(1)

### Table F2Bond lengths [Å] for $[Cu_{6}(phen)_{2}(H_{2}O)_{2}(\mu-O_{2}CC_{2}H_{5})_{12}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{4}(H_{2}O)_{2}]_{2n}(H_{2}O)_{0.5n}$ VI

C(56)-C(55)	1.460(11)	Cu(2)-O(11)	1.930(3)
C(56)-C(57)	1.84(2)	Cu(2)-O(7)	1.941(3)
C(45)-C(44)	1.10(2)	Cu(2)-O(9)	1.970(3)
C(51)-C(50)	1.19(2)	Cu(2)-O(4)	2.132(2)
C(48)-C(47)	1.47(2)	Cu(5)-O(22)	1.934(3)
C(27)-C(26)	1.48(2)	Cu(5)-O(18)	1.940(3)
C(39)-C(38)	1.46(2)	Cu(5)-O(20)	1.960(3)
C(42)-C(41)	1.574(19)	Cu(5)-O(24)	1.971(3)
C(66)-C(65)	1.27(3)	Cu(5)-O(17)	2.127(3)
C(24)-C(23)	1.24(3)	Cu(7)-O(33)	1.938(3)
C(21)-C(20)	1.60(2)	Cu(7)-O(29)	1.941(3)
C(36)-C(35)	1.45(3)	Cu(7)-O(31)	1.963(3)
C(33)-C(32)	1.697(14)	Cu(7)-O(27)	1.973(3)
C(72)-C(71)	1.303(9)	Cu(10)-O(43)	1.955(3)
C(69)-C(68)	1.40(3)	Cu(10)-O(44)	1.963(3)
C(53)-C(54)	1.45(2)	Cu(10)-O(45)	1.963(3)
C(53)-C(52)	1.82(2)	Cu(10)-O(46)	1.965(3)
C(20)-C(19)	1.474(14)	Cu(10)-Cu(10)	2.6268(11)
C(44)-C(43)	1.590(14)	O(16)-C(31)	1.276(4)
C(14)-C(13)	1.509(13)	O(14)-C(28)	1.279(4)
C(60)-C(59)	1.427(16)	O(2)-C(46)	1.274(4)
C(59)-C(58)	1.425(10)	O(3)-C(13)	1.267(4)
C(50)-C(49)	1.668(18)	O(23)-C(40)	1.237(4)
C(38)-C(37)	1.586(15)	O13)-C(28)	1.229(4)
C(41)-C(40)	1.609(11)	O(4)-C(13)	1.234(4)
C(71)-C(70)	1.490(6)	O(17)-C(31)	1.220(4)
C(62)-C(63)	1.352(15)	O(46)-C(70)	1.250(5)
C(62)-C(61)	1.465(10)	O(36)-H(10)	0.66(3)
C(65)-C(64)	1.610(15)	O(36)-H(20)	0.69(3)

# Table F2Bond lengths [Å] for $[Cu_{6}(phen)_{2}(H_{2}O)_{2}(\mu-O_{2}CC_{2}H_{5})_{12}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{4}(H_{2}O)_{2}]_{2n}(H_{2}O)_{0.5n}$ VI (cont.)

C(68)-C(67)	1.633(19)	O(37)-H(80)	0.56(3)
C(32)-C(31)	1.551(10)	O(31)-C(55)	1.252(5)
C(61)-O(41)	1.245(5)	N(3)-C(74)	1.313(5)
C(61)-O(39)	1.253(5)	N(3)-C(78)	1.348(4)
C(19)-O(8)	1.245(4)	O(21)-C(37)	1.256(5)
C(19)-O(7)	1.262(4)	$O(40)-C(64)^{j}$	1.249(5)
O(5)-C(16)	1.256(5)	$O(45)-C(67)^k$	1.245(4)
O(5)-Cu(2)	1.961(3)	O(12)-C(25)	1.247(5)
C(16)-O(6)	1.257(4)	O(19)-C(34)	1.266(4)
C(16)-C(17)	1.441(17)	$O(41)-C(61)^{j}$	1.245(5)
C(23)-C(22)	1.728(19)	N(1)-C(1)	1.310(5)
C(30)-C(29)	1.417(16)	N(1)-C(5)	1.349(4)
C(26)-C(25)	1.609(11)	O(34)-C(58)	1.252(5)
C(46)-O(26)	1.239(4)	O(1)-H(90)	0.76(4)
C(46)-O(2)	1.274(4)	O(1)-H(100)	0.66(4)
C(46)-C(47)	1.574(18)	O(9)-C(22)	1.255(5)
C(29)-C(28)	1.584(12)	O(32)-C(55)	1.240(5)
C(35)-C(34)	1.565(15)	O(25)-C(43)	1.249(4)
Cu(9)-O(39)	1.949(3)	O(30)-C(52)	1.245(5)
Cu(9)-O(40)	1.952(3)	O(18)-C(34)	1.242(4)
Cu(9)-O(41)	1.961(3)	O(20)-C(37)	1.251(5)
Cu(9)-O(38)	1.967(3)	O(11)-C(25)	1.242(4)
Cu(9)-O(37)	2.156(3)	O(38)-C(64)	1.245(5)
Cu(9)-Cu(9)	2.6320(11)	O(10)-C(22)	1.248(4)
O(15)-Cu(4)	2.346(3)	O(44)-C(67)	1.238(5)
O(15)-H(120)	0.77(4)	O(24)-C(43)	1.256(5)
O(15)-H(110)	0.98(6)	O(22)-C(40)	1.257(4)
O(42)-Cu(10)	2.141(3)	O(33)-C(58)	1.241(5)
O(42)-H(60)	0.59(3)	O(29)-C(52)	1.236(5)

# Table F2Bond lengths [Å] for $[Cu_{6}(phen)_{2}(H_{2}O)_{2}(\mu-O_{2}CC_{2}H_{5})_{12}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{4}(H_{2}O)_{2}]_{2n}(H_{2}O)_{0.5n}$ VI (cont.)

O(42)-H(50)	0.76(4)	C(6)-N(2)	1.340(4)
C(49)-O(28)	1.236(5)	C(6)-C(9)	1.389(5)
C(49)-O(27)	1.252(5)	C(6)-C(5)	1.414(5)
O(35)-Cu(7)	2.164(3)	N(2)-C(12)	1.319(5)
O(35)-H(40)	0.66(3)	N(4)-C(85)	1.317(5)
O(35)-H(30)	0.69(3)	N(4)-C(79)	1.358(5)
Cu(4)-O(16)	1.942(2)	C(5)-C(4)	1.393(5)
Cu(4)-O(14)	1.962(2)	C(79)-C(82)	1.405(5)
Cu(4)-N(3)	1.999(3)	C(79)-C(78)	1.406(5)
Cu(4)-N(4)	2.022(3)	C(78)-C(77)	1.395(5)
Cu(1)-O(3)	1.939(2)	C(64)-O(38)	1.245(5)
Cu(1)-O(2)	1.966(2)	C(70)-O(43)	1.251(5)
Cu(1)-N(1)	1.993(3)	O(43)-C(70)	1.251(5)
Cu(1)-N(2)	2.025(3)	C(67)-O(44)	1.238(5)
Cu(1)-O(1)	2.342(3)	C(10)-C(11)	1.344(7)
Cu(3)-O(10)	1.955(3)	C(10)-C(9)	1.383(6)
Cu(3)-O(6)	1.962(3)	C(83)-C(84)	1.342(6)
Cu(3)-O(12)	1.965(3)	C(83)-C(82)	1.390(6)
Cu(3)-O(8)	1.975(3)	C(9)-C(8)	1.419(6)
Cu(3)-O(13)	2.129(2)	C(76)-C(75)	1.341(6)
Cu(3)-Cu(2)	2.6212(9)	C(76)-C(77)	1.410(6)
Cu(6)-O(25) <sup>i</sup>	1.956(3)	C(1)-C(2)	1.398(6)
Cu(6)-O(23) <sup>i</sup>	1.961(3)	C(77)-C(80)	1.413(6)
Cu(6)-O(21) <sup>i</sup>	1.964(3)	C(82)-C(81)	1.421(6)
Cu(6)-O(19) <sup>i</sup>	1.981(3)	C(4)-C(3)	1.401(6)
Cu(6)-O(26)	2.126(2)	C(4)-C(7)	1.408(6)
Cu(6)-Cu(5)	2.6214(9)	C(85)-C(84)	1.388(6)
Cu(8)-O(32)	1.944(3)	C(74)-C(75)	1.409(6)
Cu(8)-O(28)	1.948(3)	C(3)-C(2)	1.353(6)

Table F2	Bond lengths [Å] for $[Cu_{6}(phen)_{2}(H_{2}O)_{2}(\mu-O_{2}CC_{2}H_{5})_{12}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{n}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{n}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{n}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{n}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{n}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{n}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{n}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{n}]_{n}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{n}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{n}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{n}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{n}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{n}]_{n}]_{n}[Cu_{2$
	$O_2CC_2H_5)_4(H_2O)_2]_{2n}(H_2O)_{0.5n}$ VI (cont.)

Cu(8)-O(34)	1.961(3)	C(12)-C(11)	1.393(6)
Cu(8)-O(30)	1.973(3)	C(7)-C(8)	1.336(6)
Cu(8)-O(36)	2.159(3)	C(80)-C(81)	1.328(6)
Cu(8)-Cu(7)	2.6356(9)	$O(46)-C(70)^{k}$	1.2501

<sup>i</sup> [x,1+y,z]; <sup>j</sup> [2-x,-y,1-z]; <sup>k</sup> [1-x,1-y,1-z]

C(55)-C(56)-C(57)	92.8(8)	C(13)-O(4)-Cu(2)	138.8(3)
C(54)-C(53)-C(52)	90.4(15)	C(31)-O(17)-Cu(5)	138.8(3)
C(19)-C(20)-C(21)	110.2(10)	C(46)-O(26)-Cu(6)	134.6(3)
C(45)-C(44)-C(43)	105.8(13)	C(19)-O(8)-Cu(3)	122.8(3)
C(58)-C(59)-C(60)	124.4(10)	C(70)-O(46)-Cu(10)	120.1(3)
C(51)-C(50)-C(49)	105.0(17)	Cu(8)-O(36)-H(10)	123(3)
C(39)-C(38)-C(37)	102.8(8)	Cu(8)-O(36)-H(20)	126(3)
C(42)-C(41)-C(40)	98.4(7)	H(10)-O(36)-H(20)	106(4)
C(72)-C(71)-C(70)	114.6(6)	Cu(9)-O(37)-H(80)	127(4)
C(63)-C(62)-C(61)	122.6(8)	C(55)-O(31)-Cu(7)	124.0(3)
C(66)-C(65)-C(64)	112.2(17)	C(46)-O(2)-Cu(1)	107.3(2)
C(69)-C(68)-C(67)	113.5(15)	C(13)-O(3)-Cu(1)	123.5(2)
C(31)-C(32)-C(33)	95.1(6)	C(16)-O(6)-Cu(3)	121.1(3)
O(41)-C(61)-O(39)	125.6(4)	C(40)-O(23)-Cu(6)	122.5(3)
O(41) <sup>j</sup> -C(61)-C(62)	119.4(5)	C(28)-O(13)-Cu(3)	134.8(3)
O(39)-C(61)-C(62)	115.0(5)	C(74)-N(3)-C(78)	119.0(4)
O(8)-C(19)-O(7)	125.4(4)	O(24)-Cu(5)-Cu(6)	83.83(8)
O(8)-C(19)-C(20)	116.4(6)	O(17)-Cu(5)-Cu(6)	172.04(8)
O(7)-C(19)-C(20)	118.0(6)	C(31)-O(16)-Cu(4)	123.2(2)
C(16)-O(5)-Cu(2)	124.8(3)	C(28)-O(14)-Cu(4)	107.2(2)
O(5)-C(16)-O(6)	125.4(4)	O(20)-Cu(5)-Cu(6)	82.88(8)
O(5)-C(16)-C(17)	110.3(7)	O(18)-Cu(5)-Cu(6)	84.99(8)
O(6)-C(16)-C(17)	124.1(7)	C(74)-N(3)-Cu(4)	128.1(3)
C(24)-C(23)-C(22)	91.2(17)	C(78)-N(3)-Cu(4)	112.8(3)
C(27)-C(26)-C(25)	104.0(9)	C(37)-O(21-Cu(6)	121.3(3)
O(26)-C(46)-O(2)	121.6(4)	C(64)-O(40)-Cu(9)	123.9(3)
O(26)-C(46)-C(47)	117.5(8)	C(67)-O(45)-Cu(10)	123.8(3)
O(2)-C(46)-C(47)	120.3(8)	C(25)-O(12)-Cu(3)	122.0(3)
C(30)-C(29)-C(28)	113.5(10)	C(34)-O(19)-Cu(6)	122.0(3)
C(48)-C(47)-C(46)	106.2(10)	C(61)-O(41)-Cu(9)	120.5(3)

C(36)-C(35)-C(34)	111.4(12)	C(1)-N(1)-C(5)	118.7(4)
O(39)-Cu(9)-O(40)	88.97(13)	C(1)-N(1)-Cu(1)	128.6(3)
O(39)-Cu(9)-O(41)	167.93(12)	C(5)-N(1)-Cu(10)	112.6(3)
O(40)-Cu(9)-O(41)	90.05(12)	C(58)-O(34)-Cu(8)	123.8(3)
O(39)-Cu(9)-O(38)	90.67(13)	C(49)-O(27)-Cu(7)	122.7(3)
O(40)-Cu(9)-O(38)	168.33(12)	Cu(1)-O(1)-H(90)	124(3)
O(41)-Cu(9)-O(38)	87.87(12)	Cu(1)-O(1)-H(100)	109(5)
O(39)-Cu(9)-O(37)	95.67(14)	H(90)-O(1)-H(100)	108(5)
O(40)-Cu(9)-O(37)	91.58(12)	C(22)-O(9)-Cu(2)	122.7(3)
O(41)-Cu(9)-O(37)	96.38(13)	C(55)-O(32)-Cu(8)	121.5(3)
O(38)-Cu(9)-O(37)	100.07(12)	C(19)-O(7)-Cu(2)	123.3(3)
O(39)-Cu(9)-Cu(9)	81.88(9)	C(43)-O(25)-Cu(6)	123.1(3)
O(40)-Cu(9)-Cu(9)	82.92(9)	C(52)-O(30)-Cu8)	122.5(3)
O(41)-Cu(9)-Cu(9)	86.06(9)	C(34)-O(18)-Cu(5)	123.1(3)
O(38)-Cu(9)-Cu(9)	85.48(9)	C(37)-O(20)-Cu(5)	124.8(3)
O(37)-Cu(9)-Cu(9)	173.99(8)	C(25)-O(11)-Cu(2)	122.5(3)
Cu(4)-O(15)H(120)	103(4)	C(64)-O(38)-Cu(9)	120.2(3)
Cu(4)-O(15)H(110)	130(3)	C(49)-O(28)-Cu(8)	122.9(3)
H(120)-O(15)-H(110)	100(4)	C(22)-O(10)-Cu(3)	123.0(3)
Cu(10)-O(40)-C(64) <sup>j</sup>	123.90(1)	$Cu(9)-O(45)-C(67)^{k}$	123.74(1)
Cu(10)-O(41)-C(61) <sup>j</sup>	120.49(1)	$Cu(9)-O(46)-C(70)^{k}$	120.05(1)
Cu(10)-O(42)-H(60)	119(3)	C(67)-O(44)-Cu(10)	120.8(3)
Cu(10)-O(42)-H(50)	120(3)	C(43)-O(24)-Cu(5)	123.0(3)
H(60)-O(42)-H(50)	113(4)	C(40)-O(22)-Cu(5)	122.5(3)
O(28)-C(49)-O(27)	126.4(4)	C(58)-O(33)-Cu(7)	121.3(3)
O(28)-C(49)-C(50)	106.8(8)	C(52)-O(29)-Cu(7)	122.8(3)
O(27)-C(49)-C(50)	126.7(8)	N(2)-C(6)-C(9)	124.1(4)
$Cu(6)^{l}-O(19)-C(34)$	121.99(1)	$Cu(6)^{l}-O(21)-C(37)$	121.28(1)
$Cu(6)^{l}-O(23)-C(40)$	122.43(1)	$Cu(6)^{l}-O(25)-C(43)$	123.12(1)
Cu(7)-O(35)-H(40)	124(3)	N(2)-C(6)-C(5)	116.1(4)

Cu(7)-O(35)-H(30)	114(3)	C(9)-C(6)-C(5)	119.8(4)
H(40)-O(35)-H(30)	116(4)	O(17)-C(31)-O(16)	123.1(4)
O(16)-Cu(4)-O(14)	91.42(11)	O(17)-C(31)-C(32)	119.5(5)
O(16)-Cu(4)-N(3)	93.10(12)	O(16)-C(31)-C(32)	117.1(5)
O(14)-Cu(4)-N(3)	170.18(11)	C(12)-N(2)-C(6)	117.9(4)
O(16)-Cu(4)-N(4)	171.13(12)	C(12)-N(2)-Cu(1)	129.4(3)
O(14)-Cu(4)-N(4)	92.96(12)	C(6)-N(2)-Cu(1)	112.5(3)
N(3)-Cu(4)-N(4)	81.44(13)	O(4)-C(13)-O(3)	122.5(4)
O(16)-Cu(4)-O(15)	105.47(10)	O(4)-C(13)-C(14)	118.8(5)
O(14)-Cu(4)-O(15)	96.00(11)	O(3)-C(13)-C(14)	118.3(5)
N(3)-Cu(4)-O(15)	91.19(12)	C(85)-N(4)-C(79)	118.1(4)
N(4)-Cu(4)-O(15)	81.75(11)	C(85)-N(4)-Cu(4)	130.0(3)
O(3)-Cu(1)-O(2)	91.72(11)	C(79)-N(4)-Cu(4)	111.6(3)
O(3)-Cu(1)-N(1)	93.04(12)	N(1)-C(5)-C(4)	123.3(4)
O(2)-Cu(1)-N(1)	170.07(11)	N(1)-C(5)-C(6)	117.0(4)
O(3)-Cu(1)-N(2)	171.06(11)	C(4)-C(5)-C(6)	119.7(4)
O(2)-Cu(1)-N(2)	92.99(12)	C(61)-O(39)-Cu(9)	125.9(3)
N(1)-Cu(1)-N(2)	81.19(13)	O(13)-C(28)-O(14)	121.4(4)
O(3)-Cu(1)-O(1)	105.45(10)	O(13)-C(28)-C(29)	119.9(6)
O(2)-Cu(1)-O(1)	96.22(11)	O(14)-C(28)-C(29)	117.7(6)
N(1)-Cu(1)-O(1)	90.91(13)	N(4)-C(79)-C(82)	123.1(4)
N(2)-Cu(1)-O(1)	81.58(12)	N(4)-C(79)-C(78)	116.7(4)
O(10)-Cu(3)-O(6)	170.36(11)	C(82)-C(79)-C(78)	120.1(4)
O(10)-Cu(3) -O(12)	91.07(13)	N(3)-C(78)-C(77)	123.4(4)
O(6)-Cu(3)-O(12)	88.37(12)	N(3)-C(78)-C(79)	116.7(4)
O(10)-Cu(3)-O(8)	89.98(12)	C(77)-C(78)-C(79)	119.9(4)
O(6)-Cu(3) -O(8)	88.47(12)	O(18)-C(34)-O(19)	126.2(4)
O(12)-Cu(3)-O(8)	167.23(11)	O(18)-C(34)-C(35)	115.3(7)
O(10)-Cu(3)-O(13)	96.67(11)	O(19)-C(34)-C(35)	118.5(8)
O(6)-Cu(3)-O(13)	92.97(11)	O(23)-C(40)-O(22)	126.1(4)

$O(21)^{i}$ -Cu(6)-O(23)^{i}	88.60(1)	$O(21)^{i}$ -Cu(6)-O(25)^{i}	170.20(1)
O(12)-Cu(3)-O(13)	90.74(11)	O(23)-C(40)-C(41)	123.4(5)
O(8)-Cu(3)-O(13)	101.78(11)	O(22)-C(40)-C(41)	110.1(5)
O(10)-Cu(3)-Cu(2)	84.51(8)	O(20)-C(37)-O(21)	125.4(4)
O(6)-Cu(3)-Cu(2)	85.86(8)	O(20)-C(37)-C(38)	115.5(8)
O(12)-Cu(3)-Cu(2)	83.58(8)	O(21)-C(37)-C(38)	118.8(8)
O(8)-Cu(3)-Cu(2)	83.85(7)	O(38)-C(64)-O(40) <sup>j</sup>	127.5(4)
O(13)-Cu(3)-Cu(2)	174.22(8)	O(38)-C(64)-C(65)	119.6(9)
O(25)-Cu(6)-O(23)	90.88(13)	O(40)-C(64)-C(65)	112.7(9)
O(25)-Cu(6)-O(21)	170.20(11)	O(46)-C(70)-O(43)	125.4(4)
O(23)-Cu(6)-O(21)	88.58(12)	O(46) <sup>k</sup> -C(70)-C(71)	114.7(5)
O(25)-Cu(6)-O(19)	90.25(12)	O(43)-C(70)-C(71)	119.9(5)
O(43)-C(70)-O(46)	125.49(1)	C(70)-O(43)-Cu(10)	126.3(3)
O(23)-Cu(6)-O(19)	167.26(11)	O(25)-C(43)-O(24)	125.4(4)
O(21)-Cu(6)-O(19)	88.16(12)	O(25)-C(43)-C(44)	125.4(6)
O(25) <sup>i</sup> -Cu(6)-O(26)	96.60(11)	O(24)-C(43)-C(44)	109.2(6)
O(23) <sup>i</sup> -Cu(6)-O(26)	90.68(11)	$O(44)-C(67)-O(45)^{k}$	127.2(4)
O(21) <sup>i</sup> -Cu(6)-O(26)	93.20(10)	O(44)-C(67)-C(68)	120.7(9)
O(19) <sup>i</sup> -Cu(6)-O(26)	101.80(10)	O(45)-C(67)-C(68)	111.8(9)
O(25)-Cu(6)-Cu(5)	84.63(8)	C(11)-C(10)-C(9)	120.0(5)
O(23)-Cu(6)-Cu(5)	83.75(8)	C(11)-C(10)-H(10)	120
O(21)-Cu(6)-Cu(5)	85.58(8)	C(9)-C(10)-H(10)	120
O(19)-Cu(6)-Cu(5)	83.72(7)	O(29)-C(52)-O(30)	126.9(4)
O(26)-Cu(6)-Cu(5)	174.32(8)	O(29)-C(52)-C(53)	112.0(7)
O(32)-Cu(8)-O(28)	169.96(12)	O(30)-C(52)-C(53)	116.7(7)
O(32)-Cu(8)-O(34)	92.21(14)	O(11)-C(25)-O(12)	126.6(4)
O(28)-Cu(8)-O(34)	88.26(14)	O(11)-C(25)-C(26)	113.5(6)
O(32)-Cu(8)-O(30)	88.98(13)	C(82)-C(81)-H(81)	119(1)

O(28)-Cu(8)-O(30)	88.07(13)	O(12)-C(25)-C(26)	119.8(6)
O(34)-Cu(8)-O(30)	165.36(12)	C(84)-C(83)-C(82)	120.0(5)
O(32)-Cu(8)-O(36)	92.00(12)	C(84)-C(83)-H(83)	120
O(28)-Cu(8)-O(36)	97.98(12)	C(82)-C(83)-H(83)	120
O(34)-Cu(8)-O(36)	93.25(12)	C(10)-C(9)-C(6)	116.4(5)
O(30)-Cu(8)-O(36)	101.30(12)	C(10)-C(9)-C(8)	124.4(5)
O(32)-Cu(8)-Cu(7)	85.57(9)	C(6)-C(9)-C(8)	119.2(5)
O(28)-Cu(8)-Cu(7)	84.56(9)	C(75)-C(76)-C(77)	119.9(5)
O(34)-Cu(8)-Cu(7)	82.30(9)	С(75)-С(76)-Н(76)	120
O(30)-Cu(8)-Cu(7)	83.24(9)	С(77)-С(76)-Н(76)	120
O(36)-Cu(8)-Cu(7)	174.83(9)	O(10)-C(22)-O(9)	125.8(4)
O(11)-Cu(2)-O(7)	169.16(11)	O(10)-C(22)-C(23)	106.3(8)
O(11)-Cu(2)-O(5)	88.93(14)	O(9)-C(22)-C(23)	127.8(8)
O(7)-Cu(2)-O(5)	87.92(14)	N(1)-C(1)-C(2)	122.4(4)
O(11)-Cu(2) -O(9)	92.22(14)	N(1)-C(1)-H(1)	118.8
O(7)-Cu(2) -O(9)	88.47(13)	C(2)-C(1)-H(1)	118.8
O(5)-Cu(2)-O(9)	166.52(12)	O(32)-C(55)-O(31)	126.2(4)
O(11)-Cu(2)-O(4)	103.24(11)	O(32)-C(55)-C(56)	112.3(6)
O(7)-Cu(2)-O(4)	87.48(10)	O(31)-C(55)-C(56)	120.8(6)
O(5)-Cu(2)-O(4)	98.37(12)	C(78)-C(77)-C(76)	116.2(4)
O(9)-Cu(2)-O(4)	94.44(12)	C(78)-C(77)-C(80)	119.1(5)
O(11)-Cu(2)-Cu(3)	84.72(8)	C(76)-C(77)-C(80)	124.7(5)
O(7)-Cu(2)-Cu(3)	84.59(8)	C(83)-C(82)-C(79)	116.3(5)
O(5)-Cu(2)-Cu(3)	82.77(8)	C(83)-C(82)-C(81)	125.8(5)
O(9)-Cu(2)-Cu(3)	83.96(8)	C(79)-C(82)-C(81)	117.9(5)
O(4)-Cu(2)-Cu(3)	171.95(8)	C(5)-C(4)-C(3)	115.9(4)
O(33)-Cu(7)-O(29)	170.05(12)	C(5)-C(4)-C(7)	119.0(5)
O(33)-Cu(7)-O(31)	92.20(14)	C(3)-C(4)-C(7)	125.1(5)

### **Table F3**Bond angle [°] for $[Cu_{6}(phen)_{2}(H_{2}O)_{2}(\mu-O_{2}CC_{2}H_{5})_{12}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{4}(H_{2}O)_{2}]_{2n}(H_{2}O)_{0.5n}$ **VI** (cont.)

O(29)-Cu(7)-O(31)	88.45(14)	N(4)-C(85)-C(84)	121.7(5)
O(33)-Cu(7)-O(27)	88.88(14)	N(4)-C(85)-H(85)	119.1
O(29)-Cu(7)-O(27)	88.02(13)	C(84)-C(85)-H(85)	119.1
O(31)-Cu(7)-O(27)	165.44(12)	N(3)-C(74)-C(75)	121.2(5)
O(33)-Cu(7)-O(35)	91.96(12)	N(3)-C(74)-H(74)	119.4
O(29)-Cu(7)-O(35)	97.91(13)	C(75)-C(74)-H(74)	119.4
O(31)-Cu(7)-O(35)	93.38(11)	C(2)-C(3)-C(4)	121.0(5)
O(27)-Cu(7)-O(35)	101.10(12)	C(2)-C(3)-H(3)	119.5
O(33)-Cu(7)-Cu(8)	85.70(9)	C(4)-C(3)-H(3)	119.5
O(29)-Cu(7)-Cu(8)	84.56(9)	C(76)-C(75)-C(74)	120.1(5)
O(31)-Cu(7)-Cu(8)	82.30(8)	C(76)-C(75)-H(75)	119.9
O(27)-Cu(7)-Cu(8)	83.30(9)	C(74)-C(75)-H(75)	119.9
O(35)-Cu(7)-Cu(8)	174.99(9)	N(2)-C(12)-C(11)	121.6(5)
O(39)-C(61)-O(41) <sup>j</sup>	125.68(1)	N(2)-C(12) -H(12)	119.2
O(43)-Cu(10)-O(44)	90.94(13)	C(11)9C(12)-H()	119.2
O(43)-Cu(10)-O(45)	88.46(13)	O(33)-C(58)-O(34)	126.7(4)
O(44)-Cu(10)-O(45)	168.15(12)	O(33)-C(58)-C(59)	112.8(7)
O(43)-Cu(10)-O(46)	168.15(12)	O(34)-C(58)-C(59)	120.4(7)
O(44)-Cu(10)-O(46)	88.10(12)	C(3)-C(2)-C(1)	118.6(5)
O(45)-Cu(10)-O(46)	90.06(12)	C(3)-C(2)-H(2)	120.7
O(43)-Cu(10)-O(42)	95.59(14)	C(1)-C(2)-H(2)	120.7
O(44)-Cu(10)-O(42)	99.82(12)	C(8)-C(7)-C(4)	121.6(5)
O(45)-Cu(10)-O(42)	92.02(12)	C(8)-C(7)-H(7)	119.2
O(46)-Cu(10)-O(420	96.22(14)	C(4)-C(7)-H(7)	119.2
O(43)-Cu(10)-Cu(10)	81.68(9)	C(7)-C(8)-C(9)	120.6(5)
O(44)-Cu(10)-Cu(10)	85.44(9)	C(7)-C(8)-H(8)	119.7
O(45)-Cu(10)-Cu(10)	82.77(9)	C(9)-C(8)-H(8)	119.7
O(46)-Cu(10)-Cu(10)	86.48(9)	C(10)-C(11)-C(12)	120.1(5)
O(42)-Cu(10)-Cu(10)	174.15(8)		

**Table F3**Bond angle [°] for  $[Cu_{6}(phen)_{2}(H_{2}O)_{2}(\mu-O_{2}CC_{2}H_{5})_{12}]_{n}[Cu_{2}(\mu-O_{2}CC_{2}H_{5})_{4}(H_{2}O)_{2}]_{2n}(H_{2}O)_{0.5n}$ **VI** (cont.)

O(22)-Cu(5)-O(18)	169.31(11)	C(10)-C(11)-H(11)	120
O(22)-Cu(5)-O(20)	89.20(14)	C(12)-C(11)-H(11)	120
O(18)-Cu(5)-O(20)	87.55(14)	C(81)-C(80)-C(77)	120.9(5)
O(22)-Cu(5)-O(24)	91.82(14)	C(81)-C(80)-H(80)	119.5
O(18)-Cu(5)-O(24)	89.00(13)	C(77)-C(80)-H(80)	119.5
O(20)-Cu(5)-O(24)	166.51(11)	C(83)-C(84)-C(85)	120.7(5)
O(22)-Cu(5)-O(17)	103.37(11)	C(83)-C(84)-H(84)	119.7
O(18)-Cu(5)-O(17)	87.18(10)	C(85)-C(84)-H(84)	119.7
O(20)-Cu(5)-O(17)	98.21(12)	C(80)-C(81)-C(82)	122.0(5)
O(24)-Cu(5)-O(17)	94.64(12)	C(80)-C(81)-H(81)	119
$O(19)^{i}$ -Cu(6)-O(21)^{i}	88.17	$O(19)^{i}$ -Cu(6)-O(25)^{i}	90.27
$O(19)^{i}$ -Cu(6)-O(23)^{i}	167.27	$O(23)^{i}-Cu(6)-O(25)^{i}$	90.82
O(22)-Cu(5)-Cu(6)	84.51(8)		

<sup>-i</sup> [x,1+y,z]; <sup>j</sup> [2-x,-y,1-z]; <sup>k</sup> [1-x,1-y,1-z]; <sup>1</sup> [x,-1+y,z]

**Table F4**Anisotropic displacement parameters  $[Å^2 \times 10^3]$  for complex VI.The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2 U_{11}+...+2hka^*b^*U_{12}]$ 

	U11	U22	<b>U33</b>	U23	U13	U12
C(56)	151	71	43	-20	46	-55
C(45)	561	272	25	-089	335	-77
C(51)	139	144	157	18	17	-40
C(48)	141	116	99	-35	-35	-24
C(27)	204	405	118	-62	38	130
C(39)	116	161	172	-114	37	-37
C(42)	206	305	119	-61	-77	-44
C(66)	238	232	17	-149	123	-40
C(24)	345	226	133	13	-104	52
C(21)	14	26	69	-50	-35	26
C(36)	103	267	99	-37	-18	-16
C(33)	49	96	126	3	-2	15
C(72)	159	46	17	62	53	-60
C(69)	297	109	85	-15	-92	-14
C(53)	180	522	13	-146	-58	20.9
C(20)	105	38	88	-23	-51	10
C(44)	75	128	65	-16	-10	-42
C(15)	76	96	198	-67	-72	35
C(14)	53	28	68	-9	14	3
C(60)	234	204	139	-74	-26	160
C(59)	181	60	93	-38	-90	97
C(50)	164	70	336	-109	-148	44
C(38)	153	117	26	-27	36	-47
C(41)	55	63	151	-68	-50	16
C(71)	55	151	133	-46	-18	9
C(62)	49	42	29	100	-8	15

**Table F4**Anisotropic displacement parameters  $[Å^2 \times 10^3]$  for complex VI.The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2 U_{11}+...+2hka^*b^*U_{12}]$  (cont.)

	U11	U22	U33	U23	U13	U12
C(65)	222	28	130	-59	49	-31
C(68)	217	57	114	-46	-69	47
C(32)	65	41	24	-2	-15	-4
O(47)	184	59	75	-4	-55	-5
C(61)	72	57	58	-25	-19	15
C(19)	52	56	53	-19	1	1
O(5)	138	39	60	-11	-16	7
C(16)	94	55	51	-21	-10	14
C(17)	199	76	167	-83	-85	54
C(18)	202	88	192	-9	-124	20
C(23)	195	348	227	-223	-141	59
C(30)	145	114	80	4	82	-6
O(48)	152	50	79	-8	28	15
C(26)	31	75	76	-46	24	9
C(46)	52	45	46	-14	-4	7
C(29)	31	131	77	-35	9	-11
C(47)	92	170	95	2	-21	-36
C(35)	45	105	93	-53	-39	5
Cu(9)	62	50	43	-11	1	0
O(15)	71	42	67	-16	-22	4
O(42)	106	41	59	-7	-33	1
C(49)	63	53	73	-16	-11	-6
O(35)	72	41	46	-14	3	-8
Cu(4)	45	42	40	-12	-6	-1
Cu(1)	44	42	40	-12	-5	7
Cu(3)	64	32	52	-15	-5	3

**Table F4**Anisotropic displacement parameters  $[Å^2 \times 10^3]$  for complex VI.The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2 U_{11}+...+2hka^*b^*U_{12}]$  (cont.)

	U11	U22	U33	U23	U13	U12
Cu(6)	66	31	52	-15	-11	5
Cu(8)	54	48	43	-16	-8	6
Cu(2)	61	33	64	-19	6	2
Cu(7)	53	48	43	-16	-5	3
Cu(10)	68	49	44	-10	-13	6
Cu(5)	74	33	65	-19	-27	8
O(16)	58	30	46	-8	-17	1
O(14)	51	37	44	-8	-3	8
O(2)	55	38	43	-5	-9	-1
O(3)	50	27	50	-11	2	8
O(6)	92	38	47	-1	-9	6
O(23)	80	40	82	-13	-30	-1
O(13)	87	31	49	-9	-2	4
O(4)	57	32	106	-22	17	0
O(17)	91	31	105	-24	-58	15
O(26)	90	31	47	-9	-8	1
O(8)	64	39	70	-19	-2	4
O(46)	67	67	49	-10	-6	-1
O(36)	81	43	44	-13	-16	11
O(37)	76	49	53	-1	11	-2
O(31)	72	81	61	-40	14	-21
N(3)	48	53	41	-14	-2	2
O(21)	86	40	52	-12	0	-3
O(40)	89	48	59	-13	9	-1
O(45)	106	49	61	-19	-28	1
O(12)	69	40	85	-14	1	9

**Table F4**Anisotropic displacement parameters  $[Å^2 \times 10^3]$  for complex VI.The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2 U_{11}+...+2hka^*b^*U_{12}]$  (cont.)

	U11	U22	<b>U33</b>	U23	U13	U12
O(19)	68	42	67	-17	-22	12
O(41)	65	67	51	-10	-7	7
N(1)	46	53	41	-17	-3	8
O(34)	94	81	61	-38	-36	42
O(27)	79	65	60	-21	-7	-18
O(1)	65	49	64	-16	3	4
O(9)	99	53	72	-26	-2	-5
O(32)	80	74	60	-30	1	-23
O(7)	60	41	95	-19	10	0
O(25)	83	53	61	-22	3	10
O(30)	78	66	61	-22	-11	28
O(18)	82	39	95	-2	-45	18
O(20)	138	38	59	-12	-2	2
O(11)	67	40	126	-25	23	7
O(38)	83	56	63	-24	11	-14
O(28)	77	66	52	-9	-04	-20
O(10)	94	55	57	-17	-23	0
O(44)	101	55	58	-21	-26	24
O(24)	96	53	71	-26	-3	18
O(22)	101	45	118	-26	-67	10
O(33)	90	84	57	-36	-19	42
O(29)	80	70	48	-11	-8	25
C(6)	41	37	68	-17	-6	6
C(31)	53	37	36	-16	-7	2
N(2)	48	51	52	-18	-6	130
C(13)	46	37	38	-15	1	5

**Table F4**Anisotropic displacement parameters  $[Å^2 \times 10^3]$  for complex VI.The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2 U_{11}+...+2hka^*b^*U_{12}]$  (cont.)

	U11	U22	U33	U23	U13	U12
N(4)	58	56	47	-16	-14	-3
C(5)	40	42	58	-11	-9	-1
O(39)	64	100	55	-5	-8	5
C(28)	51	44	44	-18	2	-2
C(79)	50	38	72	-18	-19	9
C(78)	37	40	61	-9	-6	4
C(34)	56	65	53	-25	-18	11
C(40)	69	58	69	-22	-24	-2
C(37)	85	70	49	-23	-4	-12
C(64)	94	44	50	-18	-14	9
C(70)	53	6	64	-25	7	-2
O(43)	62	102	55	-5	-7	1
C(43)	68	66	62	-25	-6	8
C(67)	81	48	54	-17	-6	8
C(10)	58	108	122	-54	8	30
C(52)	63	54	69	-9	-18	14
C(25)	53	58	73	-19	2	12
C(83)	83	116	119	-57	-48	-8
C(9)	45	60	98	-26	-7	14
C(76)	59	112	81	-7	31	1
C(22)	68	61	64	-25	-8	2
C(1)	62	87	54	-20	-011	9
C(55)	57	61	78	-28	3	-01
C(77)	46	58	87	-14	4	5
C(82)	58	60	98	-28	-26	1
C(4)	60	62	74	-12	-25	2

**Table F4**Anisotropic displacement parameters  $[Å^2 \times 10^3]$  for complex VI.The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2 U_{11}+...+2hka^*b^*U_{12}]$  (cont.)

	U11	U22	U33	U23	U13	U12
C(85)	80	112	62	-38	-14	-9
C(74)	63	91	46	-15	-4	2
C(3)	90	106	89	-7	-57	0
C(75)	82	142	49	-20	12	-2
C(12)	77	117	60	-39	-2	28
C(58)	72	74	83	-36	-32	23
C(2)	91	14	53	-14	-26	6
C(7)	61	81	128	-24	-46	17
C(8)	43	75	146	-36	-24	23
C(11)	85	167	86	-67	10	43
C(80)	39	84	129	-16	2	-6
C(84)	101	163	84	-64	-36	-13
C(81)	56	77	142	-31	-29	-6
C(57)	32	136	284	-79	150	-135
C(54)	144	16	173	-31	-049	40
C(63)	100	300	185	62	-107	-72

Table F5Hydrogen coordinates [x  $10^4$ ] and isotropic displacement parameters[Ų x  $10^3$ ] for [Cu<sub>6</sub>(phen)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>( $\mu$ -O<sub>2</sub>CC<sub>2</sub>H<sub>5</sub>)<sub>12</sub>]<sub>n</sub>[Cu<sub>2</sub>( $\mu$ -O<sub>2</sub>CC<sub>2</sub>H<sub>5</sub>)<sub>4</sub>(H<sub>2</sub>O)<sub>2</sub>]<sub>2n</sub>(H<sub>2</sub>O)<sub>0.5n</sub> VI

	X	У	Z	U(eq)
H(10)	7050(3)	2681(15)	8351(15)	55(1)
H(20)	6990(3)	2194(14)	8451(15)	47(1)
H(30)	5300(3)	2304(14)	11612(13)	37(1)
H(40)	5540(3)	2805(15)	11542(16)	55(1)
H(50)	3270(4)	5200(19)	3721(18)	96(1)
H(60)	3350(3)	5678(12)	3781(13)	21(1)
H(80)	2920(3)	10651(12)	3758(14)	32(1)
H(90)	0670(4)	10803(18)	3183(16)	73(1)
H(100)	1380(5)	10700(2)	2790(2)	123(1)
H(110)	6180(5)	5710(2)	3270(2)	160(1)
H(120)	5690(4)	568.(2)	2800(2)	111(1)