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Supporting Information for

Preparation and Characterization of Chiral Copper 12-Metallacrown-4 Complexes, Inorganic Analogs of Tetraphenylporphyrinatocopper(II)

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Received:

Contains: Synthetic details and characterization data for new compounds (2 pages). Full details of the X-ray crystallographic analysis of *S,S,S,S*-**2**/*S,S,S,S*-**2'** including thermal ellipsoid representations of the structure of the *S,S,S,S*-**2**/*S,S,S,S*-**2'** pair and *S,S,S,S*-**2'** alone, tables of bond lengths and angles, atomic positional and anisotropic displacement parameters, and atomic displacements from the mean plane of the 4 hydroximate oxygen atoms for both *S,S,S,S*-**2** and *S,S,S,S*-**2'**. (17 pages).

General Procedures: All reagents and solvents were obtained from commercial sources and were used as received. The synthetic intermediates *rac*-3-amino-3-phenylpropanoic acid,[1] methyl *rac*-3-amino-3-phenylpropanoate,[2] methyl *S*-3-amino-3-phenylpropanoate,[1] and methyl *R*-3-amino-3-phenylpropanoate[4] were prepared as described in the literature.

***S*-3-amino-3-phenylproprionohydroxamic acid (*S*-β-phenylalaninehydroxamic acid; *S*-β-pheha).**[4] A solution of KOH (5.99 g, 107 mmol) in CH_3OH (15 ml) was added to a warm solution of $NH_2OH{\cdot}HCl$ (4.12 g, 59.3 mmol) in CH_3OH (20 ml) resulting in the deposition of KCl. After standing for 10 minutes at 0 °C under N_2 the mixture was filtered, and to the filtrate was added a solution of methyl *S*-3-amino-3-phenylpropanoate (5.30 g, 29.6 mmol) in CH_3OH (5 ml). The resultant solution stirred under nitrogen at room temperature overnight. To the then yellow solution was added 12 M HCl (2.5 ml, 30 mmol) causing the deposition of KCl. The mixture was filtered and the filtrate stored at -20 °C for several hours, yielding the product as colorless crystals, 3.23 g (61%), Mp 148-150 °C, $[\alpha]_D^{26}$ = + 13.6 ± 0.2 (*c* 0.51 M, 0.15 M NaOH) ^{1}H NMR (200 MHz, D_2O) δ 7.46-7.34 (m, 5H), 4.37 (t, *J* = 8 Hz, 1H), 2.57 (m, *J* = 0.8 Hz, 8 Hz, 2H) ppm; FTIR (KBr) 3339, 3282, 3029, 2959, 2917, 1657, 1585, 1525, 1490, 1454, 1370, 1264, 1243, 1152, 1068, 1019, 927, 842, 759, 737, 702, 604, 526 cm^{-1}; LRCIMS (CH_4) *m/z* 163 ($[M\text{-}OH]^+$, 100%); Anal. Calcd for $C_9H_{12}N_2O_2{\cdot}0.33$ HCl: C, 56.20; H, 6.46; N, 14.56. Found: C, 56.21; H, 6.37; N, 14.59. The structure of *S*-β-pheha was further confirmed by X-ray crystallography. X-ray data for *S*-β-pheha: $C_9H_{12}N_2O_2$, MW = 180.21, colorless plate crystal, monoclinic space group $P2_1$ (#4) with *a* = 4.7884(6) Å, *b* = 6.5067(9) Å, *c* = 14.625(2) Å, β = 95.954(2)°, *V* = 453.6(1) $Å^3$ at 173(2) K, *Z* = 2, ρ_{calcd} = 1.319 g cm^{-3}, $2\theta_{max}$ = 50.00° (Mo Kα). Data were collected on a Siemens SMART system, and the structure was solved by direct methods. Full-matrix least squares refinement on F^2 converged to current residuals *R*1 = 0.0455, w*R*2 = 0.0888, and *S* = 1.148 for 1330 independent reflections with $I > 2(\sigma)$ *I* and 122 parameters. Full details will be reported separately.

***R*-3-amino-3-phenylproprionohydroxamic acid (*R*-β-pheha).** A procedure identical to that used for the preparation of the *S*-isomer was followed, substituting methyl *R*-3-amino-3-phenylpropanoate. The yield of crystalline product was 60%, Mp 151-152.5 °C, $[\alpha]_D^{26}$ = - 8.48 ± 0.1 (*c* 0.25 M, 0.15 M NaOH); Anal. Calcd for $C_9H_{12}N_2O_2{\cdot}0.50$ HCl: C, 54.48; H, 6.35; N, 14.12. Found: C, 54.78; H, 6.23; N, 14.18.

Cu(II)SO_4[12-$MC_{Cu(II)N(S\text{-}\beta\text{-}pheha)}$-4], *S,S,S,S*-1: To a stirred suspension of *S*-β-phenylalaninehydroxamic acid (0.201 g, 1.12 mmol) in H_2O (10 mL) was added a solution of $CuSO_4{\cdot}5H_2O$ (0.348 g, 1.28 mmol)

and NaOAc (0.183 g, 2.07 mmol) in H_2O (10 mL). The ligand dissolved within minutes, and the product began to precipitate soon thereafter. The suspension was stirred for 0.5 h, and the solid product was then collected, washed with Et_2O and dried *in vacuo*, 0.275 g (87%), Mp > 220 °C. ^1H NMR (200 MHz, CD_3OD) δ 34.82, 8.53, 5.31, -2.69, -8.32 ppm; FAB-MS (MNBA) *m/z* 1124 ($[M+H]^+$, 100%); Anal. Calc'd for $C_{36}H_{40}N_8O_{12}SCu_5 \cdot 2H_2O$ ($C_{36}H_{44}N_8O_{14}SCu_5$): C, 37.19; H, 3.81; N, 9.64. Found: C, 37.24; H, 3.90; N, 9.52.

Cu(II)(OAc)$_2$[12-MC$_{Cu(II)N(S\text{-}\beta\text{-}pheha)}$-4], *S,S,S,S*-2, and Cu(II)Cl[12-MC$_{Cu(II)N(S\text{-}\beta\text{-}pheha)4}$]·Cu(II)(OAc)$_3$, *S,S,S,S*-2'. *S*-β-phenylalaninehydroxamic acid (0.180 g, 1.00 mmol) was dissolved in 15ml of methanol. $Cu(OAc)_2 \cdot H_2O$ (0.250 g, 1.25 mmol) and NaOAc (0.083 g, 1.01mmol) were added and the reaction was stirred for 2 hours before being gravity filtered. The product crystallized as dark green prisms, 0.245 g, (79%). ^1H NMR (200 MHz, CD_3OD) 43.6, -10.0, -17.0 ppm; FAB-MS (MNBA) *m/z* 1088 ($[M-OAc]^+$, 45%), 1029 (100%, $[M]^+$); Anal. Calcd for $C_{84}H_{127}O_{40}N_{16}Cu_{11}Cl_1$: C, 36.75; H, 5.03; N, 8.16, Cu, 25.46; Found: C, 36.40; H, 4.40; N, 7.96; Cu, 25.2.

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Table 1. Crystal data and structure refinement for *S,S,S,S*-**2**/*S,S,S,S*-**2'**.

Identification code		*S,S,S,S*-**2**/*S,S,S,S*-**2'**
Empirical formula		$Cu_{11}C_{85}H_{100}N_{16}O_{42}Cl$
Formula weight		2752.20
Temperature		158(2) K
Wavelength		0.71073 Å
Crystal system		Triclinic
Space group		P1
Unit cell dimensions	a =12.5406(3) Å	alpha =88.7370(10)°
	b =13.8416(3) Å	beta =76.0010(10)°
	c =16.6932(4) Å	gamma =71.1350(10)°
Volume		2655.57(11) $Å^3$
Z		1
Density (calculated)		1.721 Mg/m^3
Absorption coefficient		2.274 mm^{-1}
F(000)		1394
Crystal size		0.08 x 0.12 x 0.18 mm
q range for data collection		2.42 to 29.38°
Limiting indices		-17<h<16,-17<k<18,-22<l<22
Reflections collected		30681
Independent reflections		23856 (R_{int} = 0.0198)
Absorption correction		None
Refinement method		Full-matrix least-squares on F2
Data / restraints / parameters		23856 / 9 / 1397
Goodness-of-fit on F2		1.041
Final R indices [I>2s(I)]		R1 = 0.0376, wR2 = 0.0849
R indices (all data)		R1 = 0.0458, wR2 = 0.0905
Absolute structure parameter		0.011(7)
Largest diff. peak and hole		1.449 and -0.851 $eÅ^{-3}$

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Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [A^2 x 10^3] for *S,S,S,S*-**2**/*S,S,S,S*-**2'**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cu(1)	2278(1)	-7815(1)	-9486(1)	14(1)
Cu(2)	2235(1)	-6639(1)	-6943(1)	14(1)
Cu(3)	3881(1)	-4236(1)	-8072(1)	15(1)
Cu(4)	4538(1)	-5817(1)	-10603(1)	16(1)
Cu(5)	2919(1)	-5903(1)	-8781(1)	12(1)
N(1)	1775(3)	-7199(3)	-7817(2)	15(1)
N(2)	1620(3)	-7493(3)	-6116(2)	15(1)
N(3)	2956(3)	-4929(3)	-7300(2)	14(1)
N(4)	4204(3)	-3518(3)	-7188(2)	15(1)
N(5)	4209(3)	-4712(3)	-9759(2)	16(1)
N(6)	5693(4)	-5315(3)	-11377(2)	24(1)
N(7)	3132(3)	-7065(3)	-10266(2)	15(1)
N(8)	2501(3)	-8860(3)	-10348(2)	18(1)
O(1)	2195(3)	-6908(2)	-8625(2)	18(1)
O(2)	1477(3)	-8399(2)	-8556(2)	19(1)
O(3)	2429(2)	-5534(2)	-7626(2)	13(1)
O(4)	2821(3)	-5977(2)	-6216(2)	18(1)
O(5)	3562(3)	-4841(2)	-8967(2)	17(1)
O(6)	4746(3)	-3675(3)	-9006(2)	19(1)
O(7)	3231(3)	-6162(2)	-9955(2)	14(1)
O(8)	4547(3)	-6893(3)	-11353(2)	20(1)
C(1)	1432(4)	-7984(3)	-7857(3)	14(1)
C(2)	974(4)	-8425(3)	-7077(3)	15(1)
C(3)	613(4)	-7778(3)	-6260(3)	14(1)
C(4)	146(4)	-8344(3)	-5540(3)	16(1)
C(5)	-1022(4)	-7972(4)	-5124(3)	22(1)
C(6)	-1467(4)	-8485(4)	-4465(3)	27(1)
C(7)	-735(5)	-9371(4)	-4213(3)	25(1)
C(8)	434(4)	-9744(4)	-4648(3)	24(1)
C(9)	860(4)	-9236(4)	-5298(3)	20(1)
C(10)	3105(4)	-5222(3)	-6563(3)	16(1)
C(11)	3657(4)	-4672(3)	-6114(3)	18(1)
C(12)	3521(4)	-3562(3)	-6324(3)	14(1)
C(13)	3862(4)	-2998(3)	-5714(3)	15(1)
C(14)	3245(4)	-1974(3)	-5489(3)	18(1)
C(15)	3564(4)	-1441(4)	-4948(3)	21(1)
C(16)	4484(4)	-1921(4)	-4611(3)	24(1)
C(17)	5100(4)	-2946(4)	-4821(3)	23(1)
C(18)	4798(4)	-3482(4)	-5374(3)	21(1)
C(19)	4783(4)	-4088(4)	-9699(3)	18(1)
C(20)	5546(5)	-3842(4)	-10472(3)	28(1)
C(21)	5447(4)	-4189(4)	-11303(3)	22(1)
C(22)	6263(4)	-3855(4)	-12011(3)	21(1)
C(23)	5802(5)	-3112(5)	-12502(4)	37(1)
C(24)	6553(6)	-2821(5)	-13172(4)	45(2)
C(25)	7707(6)	-3262(5)	-13315(3)	43(2)
C(26)	8188(5)	-3991(5)	-12822(4)	41(1)
C(27)	7467(5)	-4290(4)	-12157(4)	35(1)
C(28)	3833(4)	-7359(3)	-10998(3)	16(1)
C(29)	3747(4)	-8248(4)	-11474(3)	21(1)
C(30)	2596(4)	-8458(4)	-11185(3)	17(1)
C(31)	2406(4)	-9151(4)	-11795(3)	20(1)
C(32)	1527(4)	-8741(4)	-12205(3)	24(1)
C(33)	1287(4)	-9359(4)	-12720(3)	29(1)

C(34)	1918(5)	-10396(4)	-12848(3)	29(1)
C(35)	2804(5)	-10794(4)	-12462(3)	32(1)
C(36)	3047(5)	-10182(4)	-11931(3)	27(1)
O(9)	5971(3)	-6893(2)	-10034(2)	22(1)
O(10)	4782(3)	-7321(3)	-8618(2)	30(1)
O(11)	4224(3)	-8061(3)	-7470(2)	23(1)
C(37)	4576(4)	-8071(4)	-8245(3)	19(1)
C(38)	4767(5)	-9034(4)	-8743(3)	29(1)
Cu(11)	-2184(1)	-8398(1)	-7821(1)	14(1)
Cu(12)	-912(1)	-7478(1)	-10412(1)	14(1)
Cu(13)	482(1)	-5155(1)	-9530(1)	14(1)
Cu(14)	-1643(1)	-5441(1)	-6958(1)	14(1)
Cu(15)	-744(1)	-6865(1)	-8689(1)	12(1)
Cu(16)	-1570(1)	-11044(1)	-8545(1)	19(1)
N(11)	-1292(3)	-8328(3)	-9521(2)	14(1)
N(12)	-1696(3)	-8023(3)	-11108(2)	17(1)
N(13)	334(3)	-6198(3)	-10228(2)	14(1)
N(14)	1166(3)	-4477(3)	-10471(2)	16(1)
N(15)	-446(3)	-5193(3)	-7849(2)	14(1)
N(16)	-1641(3)	-4291(3)	-6246(2)	23(1)
N(17)	-2126(3)	-7255(3)	-7151(2)	15(1)
N(18)	-3472(3)	-8626(3)	-6959(2)	16(1)
O(12)	-1105(3)	-8089(2)	-8756(2)	15(1)
O(13)	-2349(3)	-9225(2)	-8710(2)	16(1)
O(14)	92(3)	-7069(2)	-9862(2)	15(1)
O(15)	-502(3)	-6547(3)	-11218(2)	21(1)
O(16)	-278(3)	-5714(2)	-8608(2)	19(1)
O(17)	672(3)	-4350(2)	-8662(2)	18(1)
O(18)	-1319(3)	-6754(2)	-7516(2)	15(1)
O(19)	-2792(3)	-5912(2)	-6184(2)	19(1)
C(41)	-1931(4)	-8931(3)	-9428(3)	15(1)
C(42)	-2222(4)	-9279(3)	-10173(3)	16(1)
C(43)	-1533(4)	-9127(3)	-11026(3)	14(1)
C(44)	-1909(4)	-9597(4)	-11679(3)	18(1)
C(45)	-2803(4)	-9031(4)	-12028(3)	20(1)
C(46)	-3168(4)	-9514(4)	-12591(3)	26(1)
C(47)	-2649(4)	-10544(4)	-12799(3)	24(1)
C(48)	-1761(5)	-11110(4)	-12441(3)	30(1)
C(49)	-1399(4)	-10636(4)	-11898(3)	23(1)
C(50)	12(4)	-6025(3)	-10927(3)	18(1)
C(51)	313(4)	-5179(4)	-11424(3)	23(1)
C(52)	1388(4)	-4971(3)	-11316(3)	16(1)
C(53)	1838(4)	-4334(4)	-11988(3)	19(1)
C(54)	1071(4)	-3476(4)	-12232(3)	23(1)
C(55)	1476(5)	-2901(4)	-12845(3)	25(1)
C(56)	2652(5)	-3182(4)	-13229(3)	30(1)
C(57)	3424(5)	-4023(4)	-12987(3)	32(1)
C(58)	3018(5)	-4608(4)	-12363(3)	27(1)
C(59)	82(4)	-4512(3)	-7944(3)	14(1)
C(60)	-22(4)	-3859(3)	-7204(3)	15(1)
C(61)	-448(4)	-4220(3)	-6350(3)	16(1)
C(62)	-384(4)	-3510(4)	-5700(3)	18(1)
C(63)	-1084(5)	-2483(4)	-5578(3)	28(1)
C(64)	-924(5)	-1829(4)	-5031(3)	32(1)
C(65)	-114(5)	-2194(4)	-4578(3)	29(1)
C(66)	577(5)	-3211(4)	-4691(3)	32(1)
C(67)	436(4)	-3867(4)	-5235(3)	27(1)
C(68)	-2831(4)	-6762(3)	-6471(3)	16(1)
C(69)	-3741(4)	-7192(3)	-5987(3)	17(1)
C(70)	-3473(4)	-8345(3)	-6103(2)	14(1)
C(71)	-4344(4)	-8675(3)	-5446(3)	15(1)

C(72)	-5538(4)	-8289(4)	-5387(3)	22(1)
C(73)	-6315(4)	-8565(4)	-4762(3)	22(1)
C(74)	-5924(4)	-9214(4)	-4166(3)	26(1)
C(75)	-4744(5)	-9609(4)	-4230(3)	29(1)
C(76)	-3958(4)	-9348(4)	-4854(3)	22(1)
O(20)	-2378(3)	-11472(3)	-9293(2)	24(1)
O(21)	-949(3)	-9685(2)	-7300(2)	25(1)
O(22)	-440(3)	-11267(3)	-7875(2)	23(1)
C(82)	-350(4)	-10609(3)	-7392(3)	19(1)
C(83)	572(5)	-10999(4)	-6923(3)	29(1)
O(23)	-278(3)	-11078(3)	-9502(2)	24(1)
O(24)	-314(3)	-12342(3)	-10300(2)	32(1)
C(84)	177(4)	-11752(4)	-10118(3)	22(1)
C(85)	1359(5)	-11788(5)	-10630(3)	38(1)
O(25)	-2854(3)	-10863(3)	-7579(2)	23(1)
O(26)	-2407(3)	-12559(3)	-7581(3)	41(1)
C(86)	-2998(4)	-11684(4)	-7284(3)	30(1)
C(87)	-3946(5)	-11530(5)	-6497(4)	45(2)
O(43)	1804(16)	-6742(7)	-13318(6)	306(13)
O(44)	3562(22)	-6911(7)	-13014(6)	585(28)
C(88)	2810(24)	-6574(8)	-13443(6)	681(48)
C(89)	2789(15)	-5892(7)	-14133(6)	154(7)
O(30)	-3140(3)	-4299(3)	-7572(2)	24(1)
O(31)	-567(13)	-5838(6)	-14744(5)	173(6)
C(90)	508(17)	-6333(8)	-14418(5)	141(7)
O(32)	4473(4)	-10784(4)	-10345(3)	50(1)
C(91)	5705(7)	-11007(6)	-10628(6)	68(2)
O(33)	5482(3)	-5942(4)	-7819(3)	47(1)
O(34)	-1520(4)	-3921(4)	-9555(3)	60(1)
O(35)	1081(3)	-9967(3)	-9292(2)	25(1)
O(36)	3616(3)	-9554(3)	-6678(2)	27(1)
O(37)	3820(3)	-11313(3)	-7612(2)	33(1)
O(38)	1783(3)	-12770(3)	-8604(3)	40(1)
O(39)	2998(3)	-11354(3)	-8983(2)	36(1)
O(40)	-4122(4)	-12275(4)	-8780(3)	56(1)
O(41)	6080(8)	-6110(7)	-13091(4)	140(4)
O(42)	-3047(9)	-5285(5)	-14542(4)	170(5)
O(45)	-1324(16)	-7061(10)	-12730(7)	232(8)
C(93)	-367(42)	-6524(15)	-13732(22)	553(29)
Cl(1)	-2607(1)	-5731(1)	-9356(1)	36(1)

Table 3. Bond lengths [Å] for *S,S,S,S*-**2**/*S,S,S,S*-**2'**.

Cu(1)-O(1)	1.891(3)	C(22)-C(27)	1.394(7)
Cu(1)-O(2)	1.946(3)	C(23)-C(24)	1.419(8)
Cu(1)-N(8)	1.969(4)	C(24)-C(25)	1.339(9)
Cu(1)-N(7)	1.975(4)	C(25)-C(26)	1.366(9)
Cu(2)-O(3)	1.931(3)	C(26)-C(27)	1.399(8)
Cu(2)-O(4)	1.942(3)	C(28)-C(29)	1.526(6)
Cu(2)-N(1)	1.951(4)	C(29)-C(30)	1.526(6)
Cu(2)-N(2)	1.976(4)	C(30)-C(31)	1.524(6)
Cu(3)-O(5)	1.912(3)	C(31)-C(36)	1.385(7)
Cu(3)-N(3)	1.967(4)	C(31)-C(32)	1.396(7)
Cu(3)-O(6)	1.971(3)	C(32)-C(33)	1.374(7)
Cu(3)-N(4)	1.986(4)	C(33)-C(34)	1.389(8)
Cu(4)-O(7)	1.927(3)	C(34)-C(35)	1.374(8)
Cu(4)-O(8)	1.962(3)	C(35)-C(36)	1.388(7)
Cu(4)-N(5)	1.975(4)	O(10)-C(37)	1.264(6)
Cu(4)-N(6)	1.988(4)	O(11)-C(37)	1.261(5)
Cu(4)-O(9)	2.320(3)	C(37)-C(38)	1.507(7)
Cu(5)-O(1)	1.876(3)	Cu(11)-O(12)	1.943(3)
Cu(5)-O(5)	1.879(3)	Cu(11)-O(13)	1.983(3)
Cu(5)-O(3)	1.904(3)	Cu(11)-N(17)	1.988(4)
Cu(5)-O(7)	1.921(3)	Cu(11)-N(18)	1.991(4)
N(1)-C(1)	1.300(6)	Cu(11)-O(21)	2.264(3)
N(1)-O(1)	1.423(4)	Cu(12)-O(15)	1.939(3)
N(2)-C(3)	1.511(5)	Cu(12)-N(11)	1.941(4)
N(3)-C(10)	1.325(6)	Cu(12)-O(14)	1.946(3)
N(3)-O(3)	1.408(4)	Cu(12)-N(12)	1.991(4)
N(4)-C(12)	1.499(5)	Cu(13)-O(16)	1.894(3)
N(5)-C(19)	1.309(6)	Cu(13)-O(17)	1.951(3)
N(5)-O(5)	1.415(4)	Cu(13)-N(13)	1.956(4)
N(6)-C(21)	1.489(6)	Cu(13)-N(14)	1.972(4)
N(7)-C(28)	1.306(5)	Cu(14)-O(18)	1.937(3)
N(7)-O(7)	1.416(4)	Cu(14)-N(15)	1.953(4)
N(8)-C(30)	1.484(6)	Cu(14)-O(19)	1.959(3)
O(2)-C(1)	1.293(5)	Cu(14)-N(16)	2.009(4)
O(4)-C(10)	1.292(5)	Cu(15)-O(16)	1.884(3)
O(6)-C(19)	1.286(5)	Cu(15)-O(12)	1.902(3)
O(8)-C(28)	1.291(5)	Cu(15)-O(18)	1.906(3)
C(1)-C(2)	1.492(6)	Cu(15)-O(14)	1.964(3)
C(2)-C(3)	1.537(6)	Cu(16)-O(25)	1.937(3)
C(3)-C(4)	1.522(6)	Cu(16)-O(22)	1.955(3)
C(4)-C(5)	1.389(6)	Cu(16)-O(23)	1.970(3)
C(4)-C(9)	1.388(6)	Cu(16)-O(20)	1.993(3)
C(5)-C(6)	1.396(7)	Cu(16)-O(13)	2.425(3)
C(6)-C(7)	1.401(7)	N(11)-C(41)	1.315(6)
C(7)-C(8)	1.399(7)	N(11)-O(12)	1.417(4)
C(8)-C(9)	1.372(6)	N(12)-C(43)	1.482(6)
C(10)-C(11)	1.495(6)	N(13)-C(50)	1.318(6)
C(11)-C(12)	1.533(6)	N(13)-O(14)	1.425(4)
C(12)-C(13)	1.514(6)	N(14)-C(52)	1.504(5)
C(13)-C(14)	1.387(6)	N(15)-C(59)	1.303(6)
C(13)-C(18)	1.395(6)	N(15)-O(16)	1.408(4)
C(14)-C(15)	1.383(6)	N(16)-C(61)	1.498(6)
C(15)-C(16)	1.375(7)	N(17)-C(68)	1.302(5)
C(16)-C(17)	1.384(7)	N(17)-O(18)	1.418(4)
C(17)-C(18)	1.387(6)	N(18)-C(70)	1.489(5)
C(19)-C(20)	1.513(6)	O(13)-C(41)	1.300(5)
C(20)-C(21)	1.524(7)	O(15)-C(50)	1.281(5)
C(21)-C(22)	1.535(6)	O(17)-C(59)	1.304(5)
C(22)-C(23)	1.367(7)	O(19)-C(68)	1.300(5)

C(41)-C(42)	1.508(6)	C(66)-C(67)	1.379(7)
C(42)-C(43)	1.525(6)	C(68)-C(69)	1.511(6)
C(43)-C(44)	1.521(6)	C(69)-C(70)	1.527(6)
C(44)-C(49)	1.389(7)	C(70)-C(71)	1.525(6)
C(44)-C(45)	1.392(7)	C(71)-C(72)	1.396(6)
C(45)-C(46)	1.404(6)	C(71)-C(76)	1.406(6)
C(46)-C(47)	1.374(7)	C(72)-C(73)	1.384(6)
C(47)-C(48)	1.396(7)	C(73)-C(74)	1.396(7)
C(48)-C(49)	1.368(7)	C(74)-C(75)	1.379(8)
C(50)-C(51)	1.515(6)	C(75)-C(76)	1.380(7)
C(51)-C(52)	1.518(6)	O(21)-C(82)	1.247(5)
C(52)-C(53)	1.525(6)	O(22)-C(82)	1.278(5)
C(53)-C(54)	1.389(7)	C(82)-C(83)	1.503(7)
C(53)-C(58)	1.388(7)	O(23)-C(84)	1.292(5)
C(54)-C(55)	1.384(6)	O(24)-C(84)	1.250(6)
C(55)-C(56)	1.386(7)	C(84)-C(85)	1.507(7)
C(56)-C(57)	1.376(8)	O(25)-C(86)	1.278(6)
C(57)-C(58)	1.405(7)	O(26)-C(86)	1.237(7)
C(59)-C(60)	1.501(5)	C(86)-C(87)	1.509(7)
C(60)-C(61)	1.529(6)	O(43)-C(88)	1.32(2)
C(61)-C(62)	1.514(6)	O(44)-C(88)	1.28(2)
C(62)-C(63)	1.397(7)	C(88)-C(89)	1.473(11)
C(62)-C(67)	1.394(7)	O(31)-C(90)	1.52(2)
C(63)-C(64)	1.390(7)	O(32)-C(91)	1.431(9)
C(64)-C(65)	1.372(8)	O(45)-C(93)	2.08(5)
C(65)-C(66)	1.382(8)		

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Table 4. Bond angles [°] for *S,S,S,S*-**2**/*S,S,S,S*-**2'**.

O(1)-Cu(1)-O(2)	81.07(13)	N(5)-O(5)-Cu(3)	114.3(2)
O(1)-Cu(1)-N(8)	174.1(2)	Cu(5)-O(5)-Cu(3)	120.1(2)
O(2)-Cu(1)-N(8)	97.76(14)	C(19)-O(6)-Cu(3)	110.8(3)
O(1)-Cu(1)-N(7)	88.15(13)	N(7)-O(7)-Cu(5)	119.5(2)
O(2)-Cu(1)-N(7)	169.06(13)	N(7)-O(7)-Cu(4)	113.1(2)
N(8)-Cu(1)-N(7)	92.8(2)	Cu(5)-O(7)-Cu(4)	115.10(14)
O(3)-Cu(2)-O(4)	82.04(12)	C(28)-O(8)-Cu(4)	111.0(3)
O(3)-Cu(2)-N(1)	89.51(13)	O(2)-C(1)-N(1)	121.9(4)
O(4)-Cu(2)-N(1)	170.74(14)	O(2)-C(1)-C(2)	118.7(4)
O(3)-Cu(2)-N(2)	164.47(14)	N(1)-C(1)-C(2)	119.4(4)
O(4)-Cu(2)-N(2)	96.98(13)	C(1)-C(2)-C(3)	118.3(4)
N(1)-Cu(2)-N(2)	92.17(14)	N(2)-C(3)-C(4)	110.8(3)
O(5)-Cu(3)-N(3)	88.75(13)	N(2)-C(3)-C(2)	110.8(3)
O(5)-Cu(3)-O(6)	80.64(12)	C(4)-C(3)-C(2)	110.6(3)
N(3)-Cu(3)-O(6)	169.37(13)	C(5)-C(4)-C(9)	119.1(4)
O(5)-Cu(3)-N(4)	175.87(14)	C(5)-C(4)-C(3)	119.5(4)
N(3)-Cu(3)-N(4)	94.58(14)	C(9)-C(4)-C(3)	121.4(4)
O(6)-Cu(3)-N(4)	96.05(14)	C(4)-C(5)-C(6)	120.3(5)
O(7)-Cu(4)-O(8)	80.81(12)	C(7)-C(6)-C(5)	120.2(5)
O(7)-Cu(4)-N(5)	88.82(13)	C(8)-C(7)-C(6)	118.7(4)
O(8)-Cu(4)-N(5)	168.83(14)	C(9)-C(8)-C(7)	120.6(5)
O(7)-Cu(4)-N(6)	170.1(2)	C(8)-C(9)-C(4)	121.1(4)
O(8)-Cu(4)-N(6)	97.64(14)	O(4)-C(10)-N(3)	123.3(4)
N(5)-Cu(4)-N(6)	91.9(2)	O(4)-C(10)-C(11)	117.9(4)
O(7)-Cu(4)-O(9)	98.31(12)	N(3)-C(10)-C(11)	118.8(4)
O(8)-Cu(4)-O(9)	94.45(13)	C(10)-C(11)-C(12)	116.4(4)
N(5)-Cu(4)-O(9)	91.13(14)	N(4)-C(12)-C(13)	110.5(3)
N(6)-Cu(4)-O(9)	91.5(2)	N(4)-C(12)-C(11)	110.8(4)
O(1)-Cu(5)-O(5)	176.16(14)	C(13)-C(12)-C(11)	112.5(3)
O(1)-Cu(5)-O(3)	90.67(13)	C(14)-C(13)-C(18)	118.6(4)
O(5)-Cu(5)-O(3)	90.35(12)	C(14)-C(13)-C(12)	119.9(4)
O(1)-Cu(5)-O(7)	88.81(12)	C(18)-C(13)-C(12)	121.5(4)
O(5)-Cu(5)-O(7)	89.73(12)	C(13)-C(14)-C(15)	120.6(4)
O(3)-Cu(5)-O(7)	173.03(13)	C(16)-C(15)-C(14)	120.6(4)
C(1)-N(1)-O(1)	110.6(3)	C(15)-C(16)-C(17)	119.5(4)
C(1)-N(1)-Cu(2)	132.0(3)	C(16)-C(17)-C(18)	120.2(4)
O(1)-N(1)-Cu(2)	114.6(2)	C(17)-C(18)-C(13)	120.4(4)
C(3)-N(2)-Cu(2)	115.9(3)	O(6)-C(19)-N(5)	123.2(4)
C(10)-N(3)-O(3)	110.6(3)	O(6)-C(19)-C(20)	117.3(4)
C(10)-N(3)-Cu(3)	125.9(3)	N(5)-C(19)-C(20)	119.5(4)
O(3)-N(3)-Cu(3)	118.5(2)	C(19)-C(20)-C(21)	117.5(4)
C(12)-N(4)-Cu(3)	115.9(3)	N(6)-C(21)-C(20)	111.8(4)
C(19)-N(5)-O(5)	110.2(3)	N(6)-C(21)-C(22)	110.7(4)
C(19)-N(5)-Cu(4)	130.3(3)	C(20)-C(21)-C(22)	110.1(4)
O(5)-N(5)-Cu(4)	114.9(3)	C(23)-C(22)-C(27)	119.5(5)
C(21)-N(6)-Cu(4)	114.7(3)	C(23)-C(22)-C(21)	119.5(5)
C(28)-N(7)-O(7)	110.9(3)	C(27)-C(22)-C(21)	121.0(5)
C(28)-N(7)-Cu(1)	129.9(3)	C(22)-C(23)-C(24)	119.6(6)
O(7)-N(7)-Cu(1)	117.7(2)	C(25)-C(24)-C(23)	120.2(6)
C(30)-N(8)-Cu(1)	112.6(3)	C(24)-C(25)-C(26)	121.2(5)
N(1)-O(1)-Cu(5)	120.9(2)	C(25)-C(26)-C(27)	119.8(6)
N(1)-O(1)-Cu(1)	114.1(2)	C(22)-C(27)-C(26)	119.7(5)
Cu(5)-O(1)-Cu(1)	123.5(2)	O(8)-C(28)-N(7)	122.7(4)
C(1)-O(2)-Cu(1)	111.6(3)	O(8)-C(28)-C(29)	118.9(4)
N(3)-O(3)-Cu(5)	118.6(2)	N(7)-C(28)-C(29)	118.3(4)
N(3)-O(3)-Cu(2)	113.0(2)	C(30)-C(29)-C(28)	114.7(4)
Cu(5)-O(3)-Cu(2)	113.99(14)	N(8)-C(30)-C(31)	112.0(4)
C(10)-O(4)-Cu(2)	110.7(3)	N(8)-C(30)-C(29)	109.7(4)
N(5)-O(5)-Cu(5)	121.7(2)	C(31)-C(30)-C(29)	113.5(4)

C(36)-C(31)-C(32)	118.9(4)	O(14)-N(13)-Cu(13)	119.4(2)
C(36)-C(31)-C(30)	122.2(4)	C(52)-N(14)-Cu(13)	116.1(3)
C(32)-C(31)-C(30)	118.8(4)	C(59)-N(15)-O(16)	111.2(3)
C(33)-C(32)-C(31)	120.3(5)	C(59)-N(15)-Cu(14)	133.6(3)
C(32)-C(33)-C(34)	120.8(5)	O(16)-N(15)-Cu(14)	113.7(2)
C(35)-C(34)-C(33)	118.9(5)	C(61)-N(16)-Cu(14)	112.5(3)
C(34)-C(35)-C(36)	120.9(5)	C(68)-N(17)-O(18)	111.4(3)
C(31)-C(36)-C(35)	120.1(5)	C(68)-N(17)-Cu(11)	130.6(3)
O(11)-C(37)-O(10)	123.3(4)	O(18)-N(17)-Cu(11)	117.0(2)
O(11)-C(37)-C(38)	117.7(4)	C(70)-N(18)-Cu(11)	113.4(3)
O(10)-C(37)-C(38)	119.0(4)	N(11)-O(12)-Cu(15)	116.0(2)
O(12)-Cu(11)-O(13)	80.49(12)	N(11)-O(12)-Cu(11)	111.9(2)
O(12)-Cu(11)-N(17)	89.58(13)	Cu(15)-O(12)-Cu(11)	118.69(14)
O(13)-Cu(11)-N(17)	163.53(14)	C(41)-O(13)-Cu(11)	109.8(3)
O(12)-Cu(11)-N(18)	171.25(14)	C(41)-O(13)-Cu(16)	114.8(3)
O(13)-Cu(11)-N(18)	94.94(14)	Cu(11)-O(13)-Cu(16)	111.82(13)
N(17)-Cu(11)-N(18)	93.1(2)	N(13)-O(14)-Cu(12)	110.0(2)
O(12)-Cu(11)-O(21)	100.71(13)	N(13)-O(14)-Cu(15)	115.5(2)
O(13)-Cu(11)-O(21)	97.56(12)	Cu(12)-O(14)-Cu(15)	104.44(14)
N(17)-Cu(11)-O(21)	97.18(13)	C(50)-O(15)-Cu(12)	109.7(3)
N(18)-Cu(11)-O(21)	87.24(14)	N(15)-O(16)-Cu(15)	123.0(2)
O(15)-Cu(12)-N(11)	174.12(14)	N(15)-O(16)-Cu(13)	113.3(2)
O(15)-Cu(12)-O(14)	82.76(13)	Cu(15)-O(16)-Cu(13)	123.7(2)
N(11)-Cu(12)-O(14)	91.96(13)	C(59)-O(17)-Cu(13)	109.8(3)
O(15)-Cu(12)-N(12)	94.21(14)	N(17)-O(18)-Cu(15)	119.1(2)
N(11)-Cu(12)-N(12)	91.4(2)	N(17)-O(18)-Cu(14)	112.7(2)
O(14)-Cu(12)-N(12)	170.53(14)	Cu(15)-O(18)-Cu(14)	117.0(2)
O(16)-Cu(13)-O(17)	82.13(13)	C(68)-O(19)-Cu(14)	110.7(3)
O(16)-Cu(13)-N(13)	87.49(14)	O(13)-C(41)-N(11)	122.4(4)
O(17)-Cu(13)-N(13)	167.40(14)	O(13)-C(41)-C(42)	118.1(4)
O(16)-Cu(13)-N(14)	175.6(2)	N(11)-C(41)-C(42)	119.4(4)
O(17)-Cu(13)-N(14)	96.61(14)	C(41)-C(42)-C(43)	117.7(4)
N(13)-Cu(13)-N(14)	94.3(2)	N(12)-C(43)-C(44)	113.6(4)
O(18)-Cu(14)-N(15)	88.43(14)	N(12)-C(43)-C(42)	109.3(3)
O(18)-Cu(14)-O(19)	81.35(12)	C(44)-C(43)-C(42)	108.7(3)
N(15)-Cu(14)-O(19)	169.74(14)	C(49)-C(44)-C(45)	118.6(4)
O(18)-Cu(14)-N(16)	164.9(2)	C(49)-C(44)-C(43)	119.2(4)
N(15)-Cu(14)-N(16)	90.8(2)	C(45)-C(44)-C(43)	122.1(4)
O(19)-Cu(14)-N(16)	99.27(14)	C(44)-C(45)-C(46)	119.9(4)
O(16)-Cu(15)-O(12)	175.68(14)	C(47)-C(46)-C(45)	120.4(5)
O(16)-Cu(15)-O(18)	88.95(13)	C(46)-C(47)-C(48)	119.5(4)
O(12)-Cu(15)-O(18)	90.78(12)	C(49)-C(48)-C(47)	120.1(5)
O(16)-Cu(15)-O(14)	88.84(12)	C(48)-C(49)-C(44)	121.6(5)
O(12)-Cu(15)-O(14)	90.77(12)	O(15)-C(50)-N(13)	124.1(4)
O(18)-Cu(15)-O(14)	171.01(13)	O(15)-C(50)-C(51)	118.7(4)
O(25)-Cu(16)-O(22)	92.57(14)	N(13)-C(50)-C(51)	117.2(4)
O(25)-Cu(16)-O(23)	173.97(14)	C(50)-C(51)-C(52)	115.4(4)
O(22)-Cu(16)-O(23)	86.42(14)	N(14)-C(52)-C(51)	110.7(4)
O(25)-Cu(16)-O(20)	93.57(14)	N(14)-C(52)-C(53)	110.7(3)
O(22)-Cu(16)-O(20)	154.88(14)	C(51)-C(52)-C(53)	113.0(4)
O(23)-Cu(16)-O(20)	89.83(14)	C(54)-C(53)-C(58)	119.4(4)
O(25)-Cu(16)-O(13)	87.76(12)	C(54)-C(53)-C(52)	120.4(4)
O(22)-Cu(16)-O(13)	108.64(12)	C(58)-C(53)-C(52)	120.3(4)
O(23)-Cu(16)-O(13)	86.94(12)	C(55)-C(54)-C(53)	120.5(5)
O(20)-Cu(16)-O(13)	95.94(12)	C(54)-C(55)-C(56)	120.2(5)
C(41)-N(11)-O(12)	111.3(3)	C(57)-C(56)-C(55)	120.0(4)
C(41)-N(11)-Cu(12)	131.5(3)	C(56)-C(57)-C(58)	120.1(5)
O(12)-N(11)-Cu(12)	115.2(2)	C(53)-C(58)-C(57)	119.9(5)
C(43)-N(12)-Cu(12)	113.4(3)	O(17)-C(59)-N(15)	122.7(4)
C(50)-N(13)-O(14)	111.3(3)	O(17)-C(59)-C(60)	118.3(4)
C(50)-N(13)-Cu(13)	124.5(3)	N(15)-C(59)-C(60)	119.0(4)

C(59)-C(60)-C(61)	117.4(4)
N(16)-C(61)-C(62)	113.2(3)
N(16)-C(61)-C(60)	110.7(4)
C(62)-C(61)-C(60)	108.6(4)
C(63)-C(62)-C(67)	118.4(4)
C(63)-C(62)-C(61)	121.9(4)
C(67)-C(62)-C(61)	119.6(4)
C(64)-C(63)-C(62)	120.3(5)
C(65)-C(64)-C(63)	120.5(5)
C(64)-C(65)-C(66)	119.6(5)
C(67)-C(66)-C(65)	120.6(5)
C(66)-C(67)-C(62)	120.5(5)
O(19)-C(68)-N(17)	123.1(4)
O(19)-C(68)-C(69)	118.0(4)
N(17)-C(68)-C(69)	118.9(4)
C(68)-C(69)-C(70)	116.4(4)
N(18)-C(70)-C(71)	112.5(3)
N(18)-C(70)-C(69)	110.3(4)
C(71)-C(70)-C(69)	109.2(3)
C(72)-C(71)-C(76)	118.3(4)
C(72)-C(71)-C(70)	121.8(4)
C(76)-C(71)-C(70)	119.9(4)
C(73)-C(72)-C(71)	120.6(4)
C(72)-C(73)-C(74)	120.7(5)
C(75)-C(74)-C(73)	118.8(4)
C(74)-C(75)-C(76)	121.2(5)
C(75)-C(76)-C(71)	120.5(5)
C(82)-O(21)-Cu(11)	145.1(3)
C(82)-O(22)-Cu(16)	127.1(3)
O(21)-C(82)-O(22)	125.0(4)
O(21)-C(82)-C(83)	119.0(4)
O(22)-C(82)-C(83)	116.0(4)
C(84)-O(23)-Cu(16)	126.8(3)
O(24)-C(84)-O(23)	123.6(4)
O(24)-C(84)-C(85)	120.6(4)
O(23)-C(84)-C(85)	115.7(4)
C(86)-O(25)-Cu(16)	115.8(3)
O(26)-C(86)-O(25)	124.9(5)
O(26)-C(86)-C(87)	120.0(5)
O(25)-C(86)-C(87)	115.0(5)
O(44)-C(88)-O(43)	125.7(12)
O(44)-C(88)-C(89)	131(2)
O(43)-C(88)-C(89)	103(2)

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Table 5. Anisotropic displacement parameters [$Å^2$ x 10^3] for *S,S,S,S*-**2**/*S,S,S,S*-**2'**.The anisotropic displacement factor exponent takes the form: $-2p^2$ [(ha*)2U11 + ... + 2hka*b*U12]

	U11	U22	U33	U23	U13	U12
Cu(1)	18(1)	16(1)	10(1)	-1(1)	-1(1)	-11(1)
Cu(2)	20(1)	14(1)	11(1)	1(1)	-4(1)	-10(1)
Cu(3)	19(1)	16(1)	11(1)	-2(1)	-1(1)	-11(1)
Cu(4)	20(1)	16(1)	12(1)	-1(1)	0(1)	-11(1)
Cu(5)	16(1)	13(1)	11(1)	0(1)	-3(1)	-9(1)
N(1)	20(2)	19(2)	10(2)	4(1)	-3(1)	-12(2)
N(2)	21(2)	16(2)	12(2)	1(1)	-5(1)	-11(2)
N(3)	20(2)	11(2)	16(2)	-1(1)	-7(1)	-9(2)
N(4)	18(2)	15(2)	15(2)	1(1)	-1(1)	-11(2)
N(5)	21(2)	18(2)	10(2)	1(1)	2(1)	-12(2)
N(6)	30(2)	22(2)	19(2)	0(2)	3(2)	-16(2)
N(7)	22(2)	15(2)	13(2)	-1(1)	-4(1)	-13(2)
N(8)	21(2)	22(2)	15(2)	1(2)	-1(2)	-15(2)
O(1)	28(2)	25(2)	8(1)	1(1)	0(1)	-19(1)
O(2)	28(2)	24(2)	10(1)	-2(1)	-2(1)	-19(1)
O(3)	18(1)	11(1)	13(1)	0(1)	-5(1)	-8(1)
O(4)	28(2)	16(2)	17(2)	3(1)	-9(1)	-14(1)
O(5)	26(2)	22(2)	8(1)	1(1)	2(1)	-19(1)
O(6)	24(2)	23(2)	13(2)	-2(1)	-1(1)	-15(1)
O(7)	22(2)	13(2)	11(1)	-2(1)	-2(1)	-12(1)
O(8)	25(2)	23(2)	14(2)	-1(1)	4(1)	-17(1)
C(1)	16(2)	15(2)	14(2)	-1(2)	-7(2)	-5(2)
C(2)	21(2)	15(2)	12(2)	3(2)	-7(2)	-9(2)
C(3)	17(2)	14(2)	15(2)	3(2)	-5(2)	-9(2)
C(4)	22(2)	18(2)	11(2)	1(2)	-4(2)	-12(2)
C(5)	23(2)	21(2)	22(2)	0(2)	-1(2)	-11(2)
C(6)	25(2)	35(3)	22(2)	1(2)	0(2)	-15(2)
C(7)	35(3)	30(3)	16(2)	2(2)	2(2)	-23(2)
C(8)	33(3)	23(3)	20(2)	7(2)	-6(2)	-13(2)
C(9)	23(2)	22(2)	17(2)	4(2)	-3(2)	-10(2)
C(10)	16(2)	12(2)	20(2)	1(2)	-7(2)	-4(2)
C(11)	29(2)	16(2)	15(2)	4(2)	-11(2)	-12(2)
C(12)	15(2)	15(2)	13(2)	1(2)	-2(2)	-7(2)
C(13)	20(2)	11(2)	16(2)	-3(2)	-3(2)	-9(2)
C(14)	22(2)	15(2)	17(2)	-1(2)	-5(2)	-4(2)
C(15)	35(3)	12(2)	19(2)	-3(2)	-6(2)	-10(2)
C(16)	37(3)	26(3)	16(2)	-1(2)	-6(2)	-21(2)
C(17)	27(2)	26(3)	22(2)	1(2)	-11(2)	-13(2)
C(18)	24(2)	19(2)	22(2)	-3(2)	-5(2)	-9(2)
C(19)	19(2)	17(2)	19(2)	-1(2)	0(2)	-10(2)
C(20)	39(3)	37(3)	16(2)	-1(2)	1(2)	-27(3)
C(21)	26(2)	22(2)	18(2)	3(2)	3(2)	-15(2)
C(22)	28(2)	24(2)	15(2)	2(2)	-2(2)	-18(2)
C(23)	43(3)	41(3)	40(3)	18(3)	-19(3)	-29(3)
C(24)	69(4)	58(4)	40(3)	31(3)	-33(3)	-50(4)
C(25)	68(4)	62(4)	19(3)	9(3)	-5(3)	-53(4)
C(26)	39(3)	44(4)	42(3)	3(3)	1(3)	-22(3)
C(27)	36(3)	27(3)	38(3)	8(2)	1(2)	-13(2)
C(28)	20(2)	18(2)	12(2)	3(2)	-4(2)	-10(2)
C(29)	25(2)	22(2)	17(2)	-5(2)	2(2)	-13(2)
C(30)	22(2)	19(2)	13(2)	-2(2)	-3(2)	-12(2)
C(31)	24(2)	24(2)	13(2)	-3(2)	1(2)	-16(2)
C(32)	25(2)	25(3)	21(2)	-8(2)	0(2)	-9(2)
C(33)	26(3)	40(3)	22(2)	-4(2)	-6(2)	-13(2)
C(34)	42(3)	35(3)	16(2)	-4(2)	-1(2)	-28(3)

C(35)	51(3)	24(3)	24(3)	-1(2)	-12(2)	-16(2)
C(36)	46(3)	22(3)	22(2)	0(2)	-15(2)	-16(2)
O(9)	20(2)	19(2)	25(2)	-5(1)	-4(1)	-5(1)
O(10)	33(2)	24(2)	31(2)	3(2)	-3(2)	-11(2)
O(11)	21(2)	26(2)	23(2)	3(1)	-6(1)	-9(1)
C(37)	13(2)	23(2)	20(2)	3(2)	-4(2)	-7(2)
C(38)	31(3)	26(3)	29(3)	-3(2)	-3(2)	-11(2)
Cu(11)	17(1)	15(1)	11(1)	-1(1)	-1(1)	-10(1)
Cu(12)	19(1)	15(1)	11(1)	1(1)	-3(1)	-10(1)
Cu(13)	22(1)	16(1)	9(1)	1(1)	-3(1)	-12(1)
Cu(14)	16(1)	14(1)	12(1)	-1(1)	-1(1)	-9(1)
Cu(15)	15(1)	13(1)	10(1)	0(1)	-2(1)	-9(1)
Cu(16)	18(1)	17(1)	23(1)	-1(1)	-3(1)	-9(1)
N(11)	18(2)	14(2)	14(2)	-1(1)	-4(1)	-9(2)
N(12)	23(2)	18(2)	12(2)	1(1)	-3(1)	-11(2)
N(13)	18(2)	10(2)	16(2)	3(1)	0(1)	-7(2)
N(14)	20(2)	18(2)	12(2)	0(1)	-4(1)	-11(2)
N(15)	18(2)	18(2)	7(2)	-2(1)	-3(1)	-9(2)
N(16)	22(2)	27(2)	19(2)	-9(2)	4(2)	-15(2)
N(17)	17(2)	13(2)	17(2)	3(1)	-2(1)	-10(2)
N(18)	19(2)	18(2)	13(2)	2(1)	-6(1)	-8(2)
O(12)	23(2)	21(2)	7(1)	-2(1)	-2(1)	-14(1)
O(13)	21(2)	20(2)	11(1)	0(1)	-2(1)	-13(1)
O(14)	21(2)	14(2)	12(1)	2(1)	-3(1)	-11(1)
O(15)	35(2)	22(2)	14(2)	4(1)	-10(1)	-17(2)
O(16)	32(2)	22(2)	8(1)	-4(1)	0(1)	-20(2)
O(17)	26(2)	19(2)	13(2)	2(1)	-4(1)	-15(1)
O(18)	19(2)	16(2)	12(1)	-2(1)	1(1)	-12(1)
O(19)	24(2)	15(2)	17(2)	-1(1)	1(1)	-10(1)
C(41)	19(2)	10(2)	16(2)	1(2)	-4(2)	-7(2)
C(42)	22(2)	16(2)	14(2)	1(2)	-4(2)	-10(2)
C(43)	18(2)	14(2)	14(2)	-4(2)	-4(2)	-8(2)
C(44)	23(2)	24(2)	10(2)	-2(2)	-3(2)	-14(2)
C(45)	19(2)	23(2)	19(2)	-7(2)	-3(2)	-9(2)
C(46)	23(2)	45(3)	15(2)	1(2)	-6(2)	-17(2)
C(47)	29(3)	32(3)	17(2)	-7(2)	-6(2)	-17(2)
C(48)	38(3)	26(3)	28(3)	-8(2)	-6(2)	-15(2)
C(49)	29(3)	20(2)	21(2)	-1(2)	-8(2)	-9(2)
C(50)	26(2)	17(2)	15(2)	2(2)	-8(2)	-9(2)
C(51)	32(3)	26(3)	19(2)	6(2)	-10(2)	-20(2)
C(52)	24(2)	15(2)	10(2)	1(2)	-2(2)	-10(2)
C(53)	30(2)	18(2)	12(2)	0(2)	-2(2)	-16(2)
C(54)	28(2)	23(3)	20(2)	4(2)	-4(2)	-14(2)
C(55)	43(3)	20(2)	19(2)	9(2)	-10(2)	-19(2)
C(56)	50(3)	32(3)	15(2)	6(2)	0(2)	-29(3)
C(57)	30(3)	33(3)	29(3)	3(2)	8(2)	-18(2)
C(58)	31(3)	27(3)	24(3)	3(2)	-5(2)	-12(2)
C(59)	14(2)	19(2)	10(2)	-1(2)	-3(2)	-8(2)
C(60)	22(2)	15(2)	15(2)	-3(2)	-6(2)	-12(2)
C(61)	22(2)	16(2)	11(2)	-4(2)	-1(2)	-9(2)
C(62)	21(2)	22(2)	13(2)	-2(2)	0(2)	-14(2)
C(63)	43(3)	17(2)	24(3)	-3(2)	-13(2)	-6(2)
C(64)	50(3)	18(3)	26(3)	-7(2)	-9(2)	-10(2)
C(65)	38(3)	37(3)	21(2)	-1(2)	-7(2)	-25(2)
C(66)	32(3)	44(3)	23(3)	-11(2)	-14(2)	-11(2)
C(67)	23(2)	33(3)	24(2)	-9(2)	-8(2)	-5(2)
C(68)	21(2)	15(2)	13(2)	2(2)	-2(2)	-8(2)
C(69)	18(2)	15(2)	16(2)	-1(2)	4(2)	-7(2)
C(70)	14(2)	17(2)	12(2)	-1(2)	-1(2)	-6(2)
C(71)	20(2)	14(2)	11(2)	0(2)	-2(2)	-8(2)
C(72)	23(2)	25(3)	20(2)	4(2)	-3(2)	-12(2)

C(73)	21(2)	30(3)	19(2)	3(2)	0(2)	-16(2)
C(74)	34(3)	34(3)	17(2)	1(2)	1(2)	-25(2)
C(75)	49(3)	31(3)	21(2)	14(2)	-18(2)	-25(3)
C(76)	26(2)	21(2)	27(2)	9(2)	-12(2)	-13(2)
O(20)	25(2)	22(2)	29(2)	-2(1)	-6(1)	-14(1)
O(21)	28(2)	15(2)	31(2)	0(1)	-11(2)	-4(1)
O(22)	25(2)	21(2)	26(2)	-1(1)	-9(1)	-7(1)
C(82)	18(2)	15(2)	21(2)	2(2)	0(2)	-7(2)
C(83)	34(3)	25(3)	32(3)	1(2)	-15(2)	-10(2)
O(23)	25(2)	25(2)	23(2)	-6(1)	1(1)	-13(2)
O(24)	30(2)	32(2)	34(2)	-14(2)	-2(2)	-16(2)
C(84)	26(2)	18(2)	22(2)	-3(2)	-7(2)	-6(2)
C(85)	35(3)	48(4)	29(3)	-15(3)	5(2)	-22(3)
O(25)	20(2)	22(2)	28(2)	9(1)	-3(1)	-10(1)
O(26)	28(2)	25(2)	74(3)	17(2)	-16(2)	-13(2)
C(86)	17(2)	31(3)	44(3)	18(2)	-12(2)	-9(2)
C(87)	26(3)	51(4)	52(4)	35(3)	-1(3)	-15(3)
O(43)	661(32)	62(6)	82(7)	-20(5)	110(13)	-115(12)
O(44)	1655(85)	95(8)	127(10)	78(7)	-402(26)	-324(23)
C(88)	2000(142)	140(13)	41(6)	53(7)	-248(26)	-541(42)
C(89)	361(22)	51(6)	53(6)	22(5)	-44(9)	-78(9)
O(30)	18(2)	27(2)	26(2)	4(1)	-4(1)	-6(1)
O(31)	399(17)	85(6)	63(5)	-19(4)	10(7)	-164(9)
C(90)	378(21)	42(5)	24(4)	4(4)	-47(8)	-99(9)
O(32)	38(2)	56(3)	50(3)	9(2)	-6(2)	-10(2)
C(91)	60(5)	56(5)	90(6)	7(4)	-30(4)	-13(4)
O(33)	28(2)	72(3)	42(2)	-20(2)	-4(2)	-20(2)
O(34)	50(3)	39(3)	75(4)	21(2)	0(2)	-9(2)
O(35)	28(2)	21(2)	28(2)	-6(1)	-4(1)	-12(2)
O(36)	27(2)	22(2)	33(2)	4(2)	-9(2)	-8(2)
O(37)	43(2)	24(2)	36(2)	5(2)	-14(2)	-15(2)
O(38)	27(2)	22(2)	63(3)	-7(2)	3(2)	-6(2)
O(39)	42(2)	32(2)	40(2)	10(2)	-19(2)	-13(2)
O(40)	41(2)	74(3)	61(3)	-27(3)	11(2)	-43(3)
O(41)	172(8)	147(7)	48(4)	-39(4)	-30(5)	24(6)
O(42)	296(12)	73(5)	50(4)	-36(3)	-81(6)	91(6)
O(45)	428(23)	162(11)	150(10)	86(9)	-135(13)	-115(13)
C(93)	1254(84)	86(15)	549(42)	34(22)	-739(54)	-151(31)
Cl(1)	26(1)	31(1)	51(1)	1(1)	-9(1)	-10(1)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for *S,S,S,S*-**2**/*S,S,S,S*-**2'**.

	x	y	z	U(eq)
H(2C)	2217(3)	-8086(3)	-6099(2)	18
H(2D)	1389(3)	-7151(3)	-5604(2)	18
H(4C)	4983(3)	-3792(3)	-7205(2)	18
H(4D)	4059(3)	-2842(3)	-7306(2)	18
H(6C)	6415(4)	-5638(3)	-11285(2)	28
H(6D)	5721(4)	-5499(3)	-11910(2)	28
H(8C)	3166(3)	-9398(3)	-10351(2)	22
H(8D)	1884(3)	-9106(3)	-10223(2)	22
H(2A)	1577(4)	-9077(3)	-7024(3)	18
H(2B)	290(4)	-8596(3)	-7141(3)	18
H(3A)	-24(4)	-7133(3)	-6299(3)	17
H(5A)	-1520(4)	-7367(4)	-5289(3)	27
H(6A)	-2269(4)	-8232(4)	-4187(3)	33
H(7A)	-1027(5)	-9713(4)	-3755(3)	31
H(8A)	938(4)	-10353(4)	-4494(3)	29
H(9A)	1656(4)	-9500(4)	-5587(3)	24
H(11A)	4498(4)	-5063(3)	-6227(3)	22
H(11B)	3325(4)	-4678(3)	-5513(3)	22
H(12A)	2681(4)	-3202(3)	-6299(3)	17
H(14A)	2598(4)	-1635(3)	-5708(3)	22
H(15A)	3142(4)	-736(4)	-4807(3)	26
H(16A)	4696(4)	-1552(4)	-4238(3)	28
H(17A)	5731(4)	-3284(4)	-4586(3)	27
H(18A)	5231(4)	-4183(4)	-5521(3)	25
H(20A)	6366(5)	-4151(4)	-10444(3)	34
H(20B)	5371(5)	-3091(4)	-10461(3)	34
H(21A)	4630(4)	-3845(4)	-11347(3)	26
H(23A)	4983(5)	-2792(5)	-12395(4)	44
H(24A)	6236(6)	-2313(5)	-13519(4)	54
H(25A)	8201(6)	-3063(5)	-13767(3)	52
H(26A)	9009(5)	-4294(5)	-12931(4)	49
H(27A)	7797(5)	-4787(4)	-11807(4)	42
H(29A)	3864(4)	-8105(4)	-12067(3)	25
H(29B)	4386(4)	-8874(4)	-11424(3)	25
H(30A)	1960(4)	-7785(4)	-11132(3)	20
H(32A)	1093(4)	-8032(4)	-12127(3)	29
H(33A)	682(4)	-9074(4)	-12992(3)	34
H(34A)	1741(5)	-10824(4)	-13198(3)	34
H(35A)	3256(5)	-11498(4)	-12559(3)	38
H(36A)	3654(5)	-10470(4)	-11662(3)	33
H(9B)	5900(19)	-6610(14)	-9483(9)	33
H(9C)	6739(3)	-6952(21)	-10390(11)	33
H(38A)	5039(5)	-8941(4)	-9332(3)	43
H(38B)	4034(5)	-9181(4)	-8648(3)	43
H(38C)	5353(5)	-9606(4)	-8574(3)	43
H(12C)	-2480(3)	-7662(3)	-10964(2)	20
H(12D)	-1412(3)	-7919(3)	-11653(2)	20
H(14C)	678(3)	-3815(3)	-10455(2)	19
H(14D)	1860(3)	-4448(3)	-10400(2)	19
H(16C)	-2121(3)	-3684(3)	-6378(2)	27
H(16D)	-1935(3)	-4386(3)	-5701(2)	27
H(18C)	-4170(3)	-8246(3)	-7064(2)	19
H(18D)	-3413(3)	-9304(3)	-6994(2)	19
H(42A)	-3056(4)	-8917(3)	-10135(3)	20
H(42B)	-2120(4)	-10017(3)	-10139(3)	20
H(43A)	-689(4)	-9498(3)	-11073(3)	17

H(45A)	-3167(4)	-8319(4)	-11886(3)	24
H(46A)	-3776(4)	-9127(4)	-12830(3)	32
H(47A)	-2893(4)	-10869(4)	-13182(3)	29
H(48A)	-1407(5)	-11824(4)	-12574(3)	36
H(49A)	-785(4)	-11028(4)	-11666(3)	28
H(51A)	-359(4)	-4541(4)	-11268(3)	27
H(51B)	426(4)	-5354(4)	-12017(3)	27
H(52A)	2015(4)	-5647(3)	-11355(3)	19
H(54A)	263(4)	-3284(4)	-11976(3)	27
H(55A)	946(5)	-2310(4)	-13003(3)	30
H(56A)	2926(5)	-2796(4)	-13659(3)	36
H(57A)	4232(5)	-4207(4)	-13243(3)	38
H(58A)	3550(5)	-5191(4)	-12199(3)	32
H(60A)	-559(4)	-3166(3)	-7245(3)	18
H(60B)	751(4)	-3795(3)	-7237(3)	18
H(61A)	94(4)	-4919(3)	-6307(3)	19
H(63A)	-1671(5)	-2229(4)	-5870(3)	34
H(64A)	-1379(5)	-1125(4)	-4971(3)	38
H(65A)	-29(5)	-1751(4)	-4189(3)	34
H(66A)	1155(5)	-3460(4)	-4390(3)	38
H(67A)	902(4)	-4568(4)	-5295(3)	33
H(69A)	-4481(4)	-6844(3)	-6140(3)	21
H(69B)	-3867(4)	-7017(3)	-5392(3)	21
H(70A)	-2678(4)	-8696(3)	-6020(2)	17
H(72A)	-5819(4)	-7833(4)	-5780(3)	26
H(73A)	-7123(4)	-8310(4)	-4738(3)	27
H(74A)	-6461(4)	-9380(4)	-3724(3)	31
H(75A)	-4468(5)	-10068(4)	-3838(3)	35
H(76A)	-3149(4)	-9625(4)	-4884(3)	27
H(20C)	-3103(3)	-10922(3)	-9295(2)	36
H(20D)	-2555(3)	-12089(3)	-9097(2)	36
H(83A)	965(5)	-11733(4)	-7059(3)	44
H(83B)	211(5)	-10880(4)	-6328(3)	44
H(83C)	1140(5)	-10637(4)	-7076(3)	44
H(85A)	1608(5)	-11277(5)	-10399(3)	56
H(85B)	1317(5)	-11639(5)	-11201(3)	56
H(85C)	1919(5)	-12470(5)	-10624(3)	56
H(87A)	-4325(5)	-10796(5)	-6348(4)	67
H(87B)	-3607(5)	-11863(5)	-6050(4)	67
H(87C)	-4522(5)	-11830(5)	-6581(4)	67
H(89A)	2068(15)	-5774(7)	-14308(6)	231
H(89B)	3458(15)	-6210(7)	-14598(6)	231
H(89C)	2827(15)	-5238(7)	-13952(6)	231

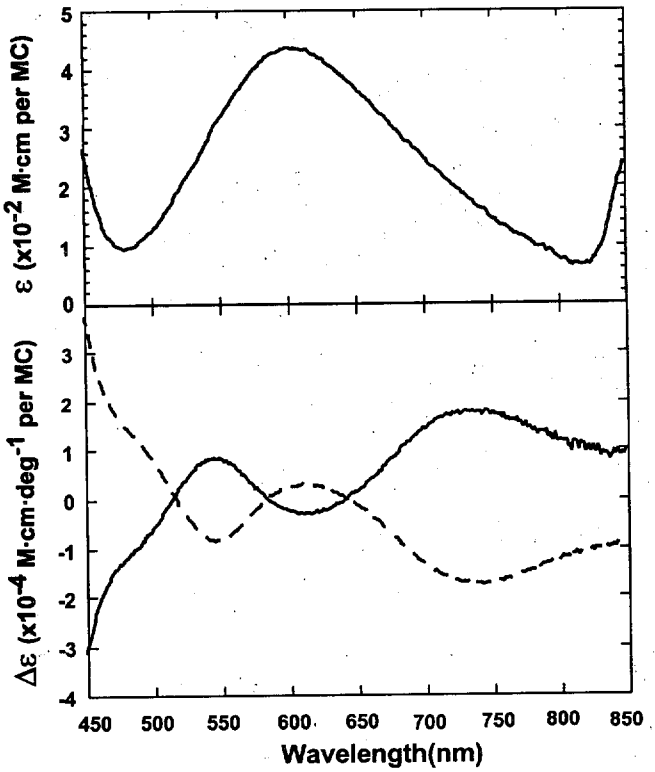


Figure S1: Visible spectrum (top) of S,S,S,S-2/S,S,S,S-2' and circular dichroism (CD) spectra (bottom) of S,S,S,S-2/S,S,S,S-2' (solid line) and R,R,R,R-2/R,R,R,R-2' (broken line) in methanol.

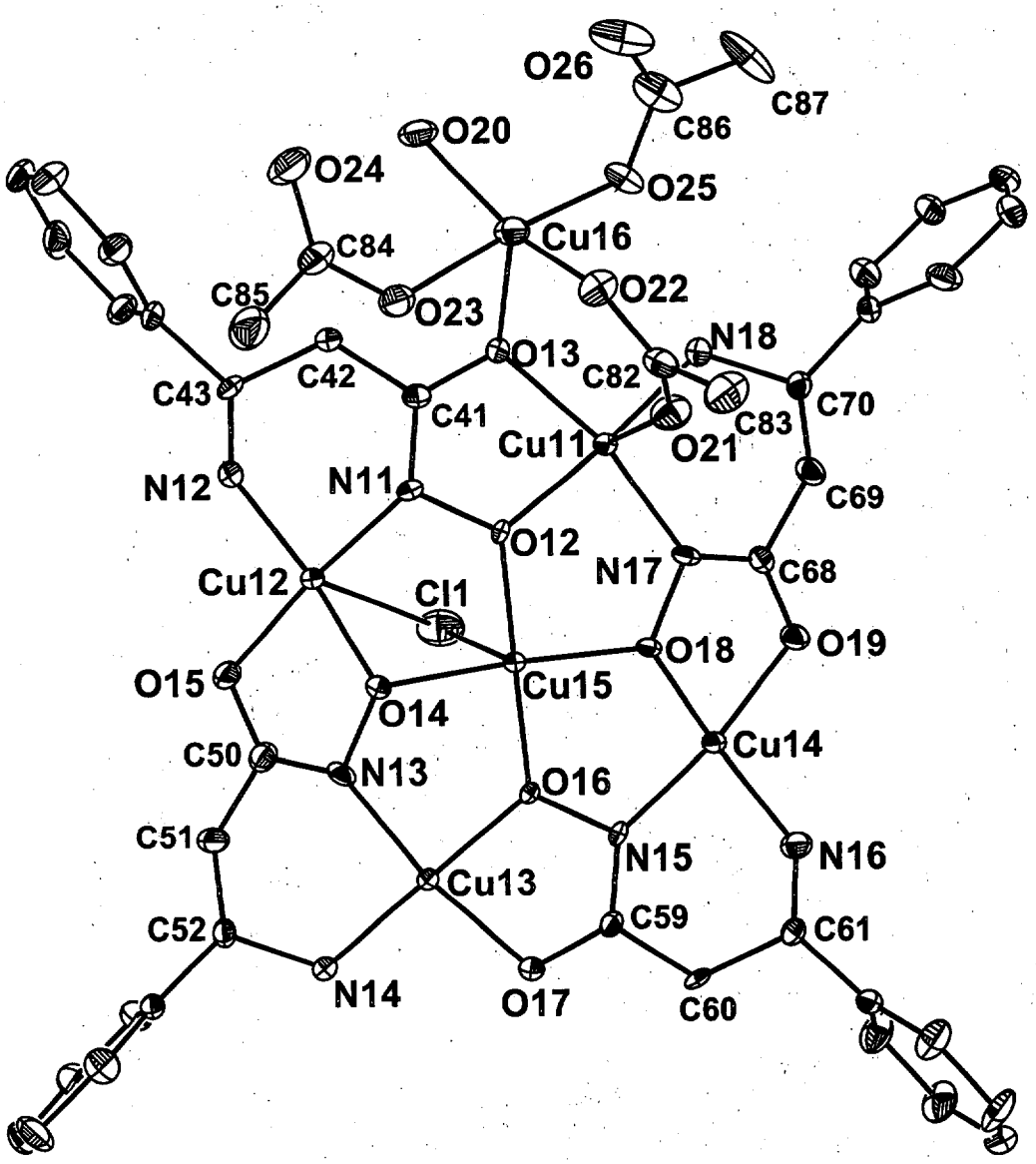


Figure S2: Thermal ellipsoid representation and numbering scheme for *S,S,S,S*-**2'**

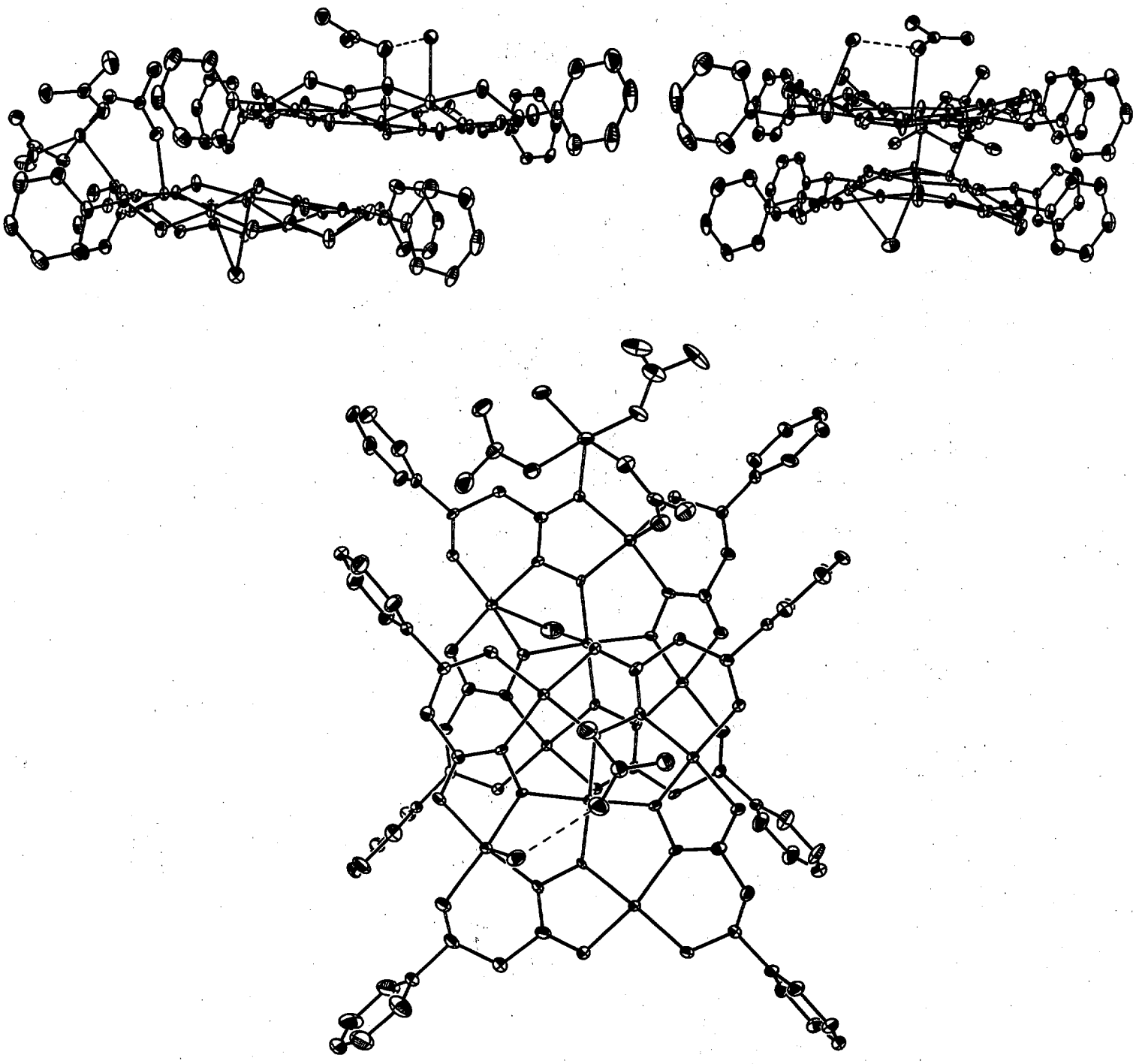


Figure S3: Thermal ellipsoid representation of *S,S,S,S*-**2**/*S,S,S,S*-**2'** as found in the crystal structure. The top 2 views are orthogonal side-on view of the pair of metalla-crowns and the bottom is a top view of the pair.

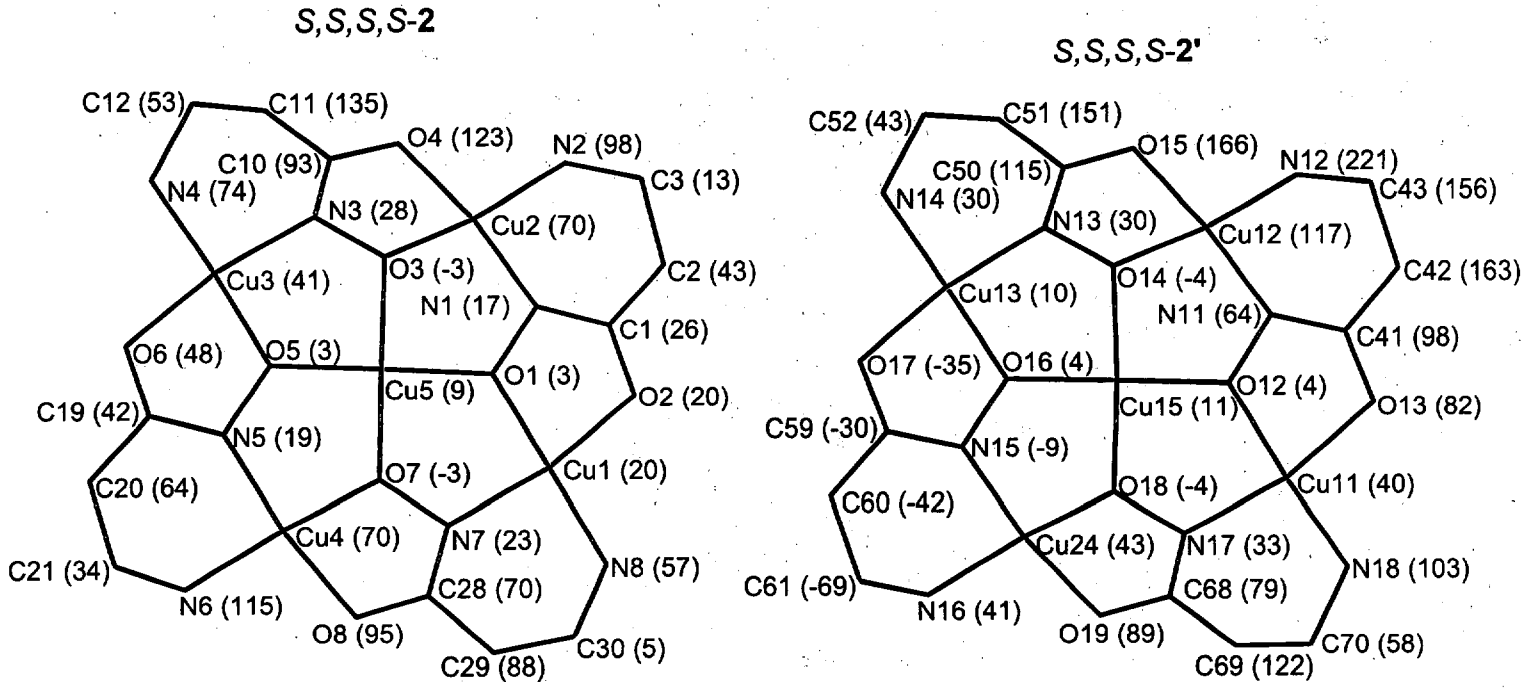


Figure S4: Displacement of metallacrown core atoms from the mean plane of the 4 metallacrown ring oxygens (O1, O3, O5, O7 for *S,S,S,S*-**2**; O12, O14, O16, O18 for *S,S,S,S*-**2'**). Displacements are given in units of 0.01Å.

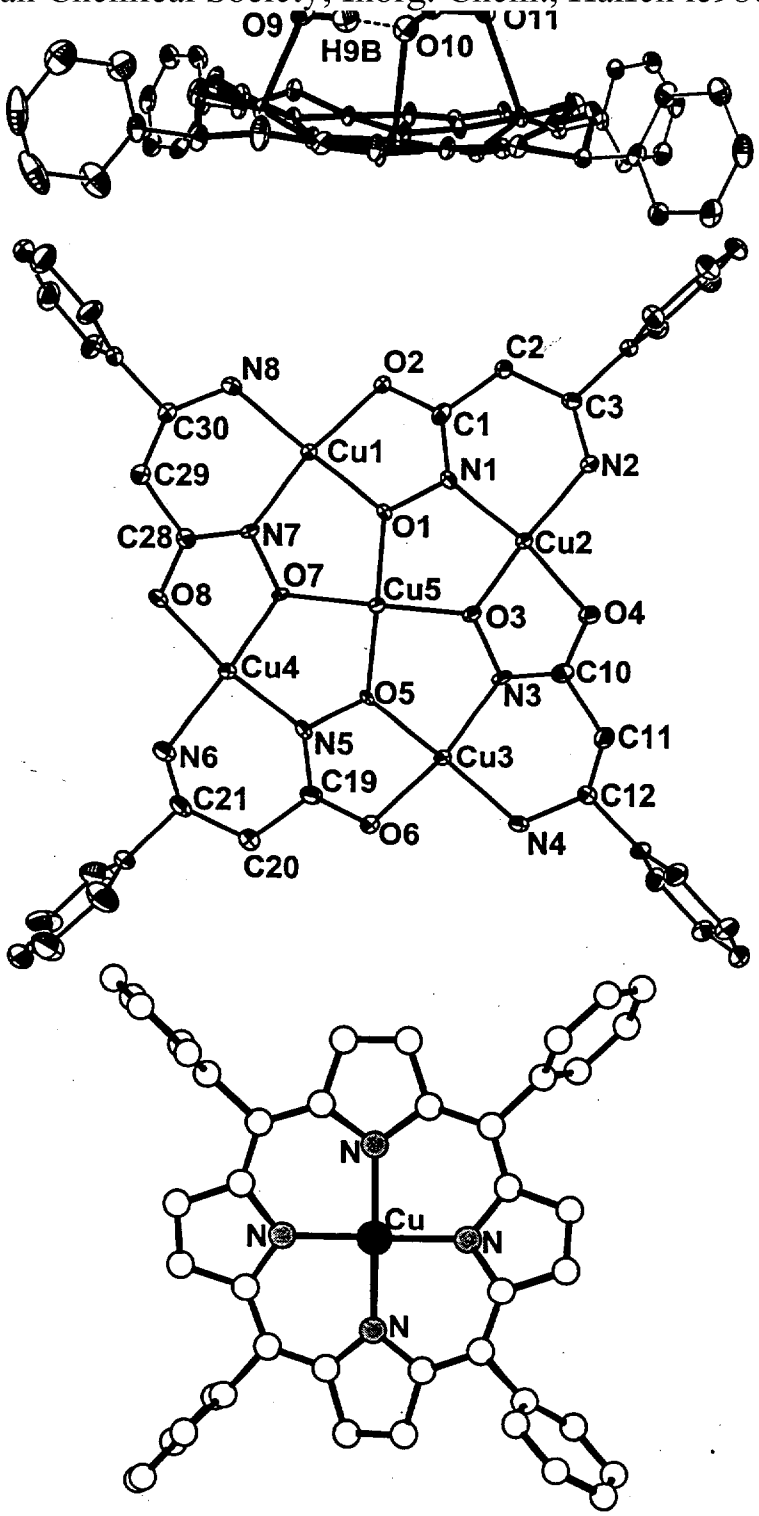
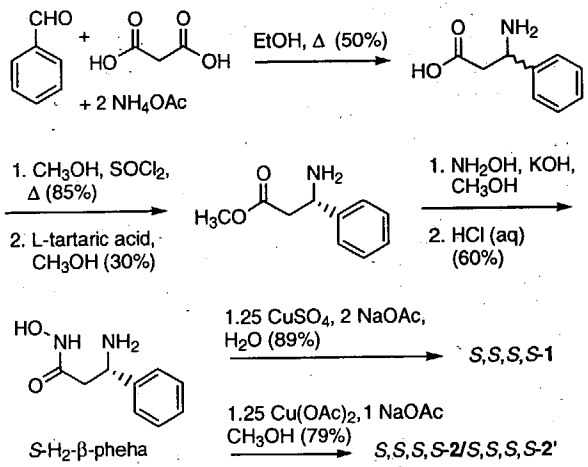


Figure 5. (Top) Side view thermal ellipsoid representation (50% probability) of the X-ray crystal structure of S,S,S,S-**2** including bound acetate and water; all nonwater hydrogen atoms are omitted for clarity. (Middle) Top view thermal ellipsoid representation of *S,S,S,S*-**2** with bound acetate, bound water and hydrogen atoms omitted for clarity. Selected interatomic distances (Å) and angles (deg): Cu5−O1, 1.877-(3); Cu5−O5, 1.881(3); Cu5−O3, 1.906(3); Cu5−O7, 1.921(3); Cu1−Cu5, 3.3176(7); Cu2−Cu5, 3.2155(7); Cu3−Cu5, 3.2850(7); Cu4−Cu5, 3.2469(7); Cu1−Cu2, 4.5620(7); Cu1−Cu4, 4.6308(7); Cu2−Cu3, 4.5989(7); Cu3−Cu4, 4.5694(7); O1−Cu5−O5, 176.2(2); O1−Cu5−O3, 90.71(14); O5−Cu5−O3, 90.33(13); O1−Cu5−O7, 88.74(13); O5−Cu5−O7, 89.78(13); O3−Cu5−O7, 173.11(14). (Bottom) Representation of **3** drawn from crystallographic positional parameters reported in ref 12. All three structures are on the same scale.



Scheme S1 (Manuscript # IC9807386)