Supporting Information

A Novel 3D Poly*pseudo*-rotaxane Metal-organic Framework Based on a Flexible Bis-pyridyl-bis-amide Ligand

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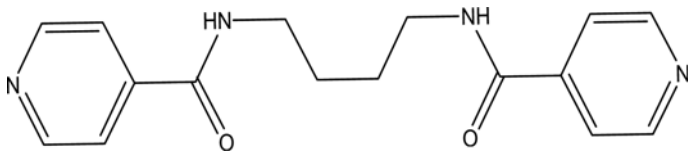

Scheme S1. The flexible ligand N,N-bis(4-pyridinecarboxamide)-1,4-butane (L)

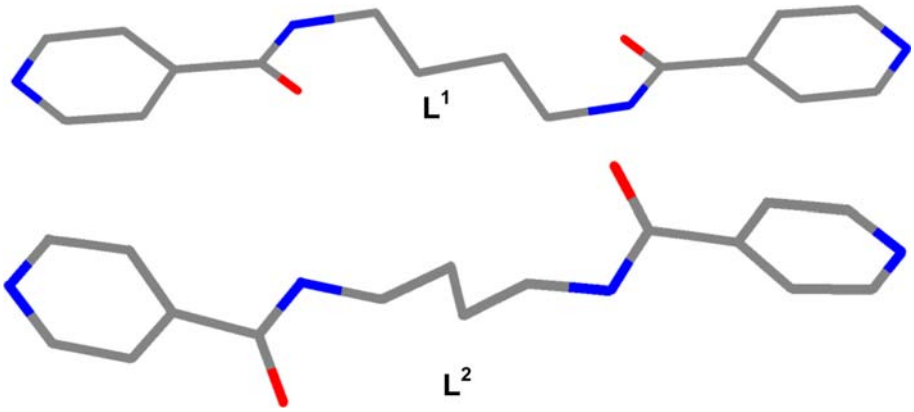

Fig S1. Two different conformations of L ligand.

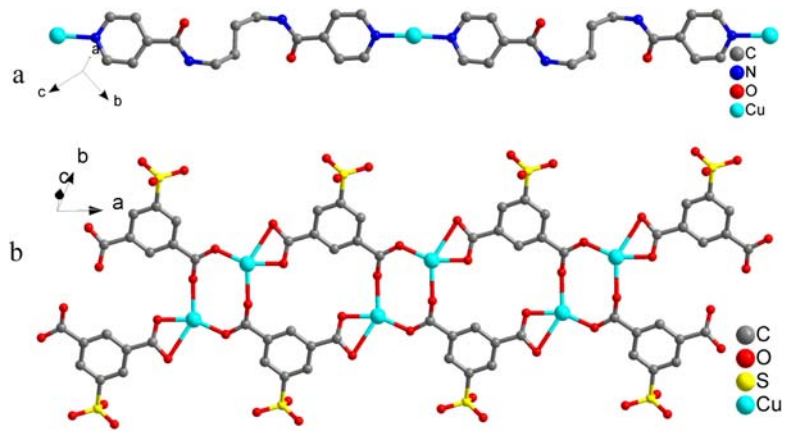

Fig S2. a) 1D $[CuL]_n$ chain bridged by L^2; b) $[Cu_2(SIP)_2]_{2n}^{2n-}$ 1D double-chain in **1**.

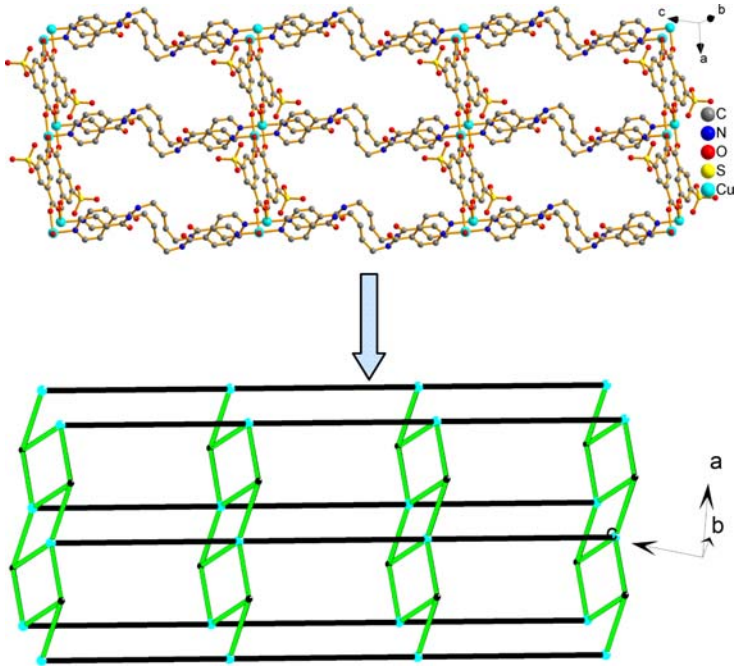

Fig S3. The ball-and-stick model of 2D double-layer in compound **1** (top). The schematic view of this 2D double-layer (bottom).

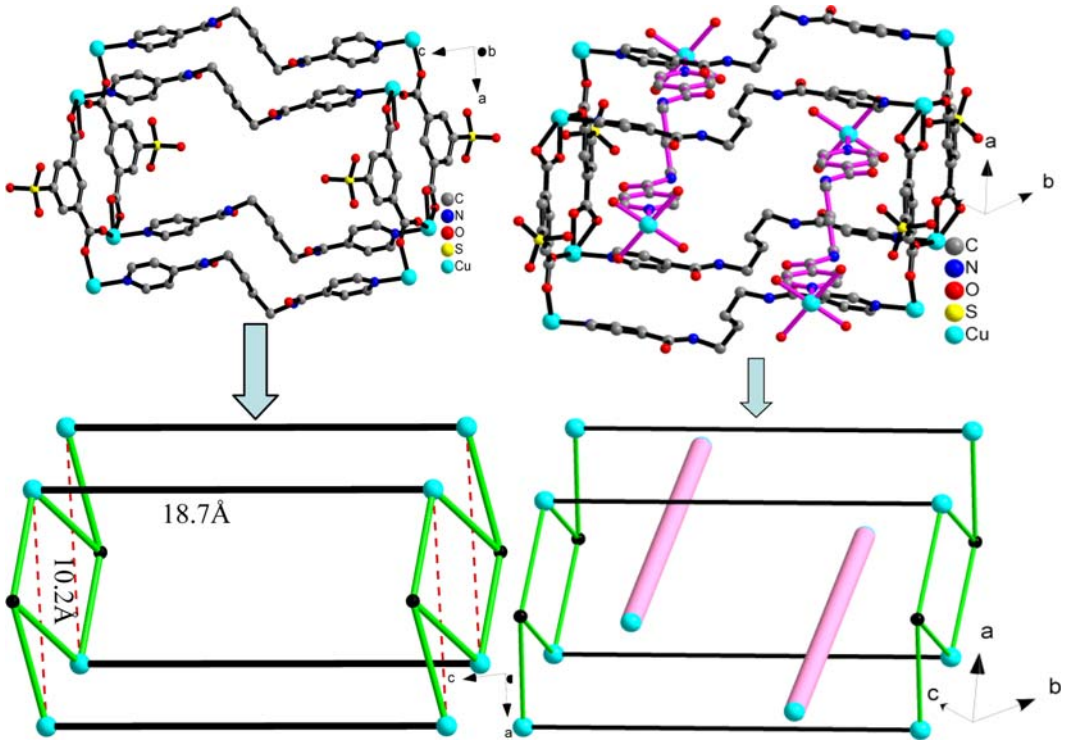

Fig S4. The building unit of compound **1**

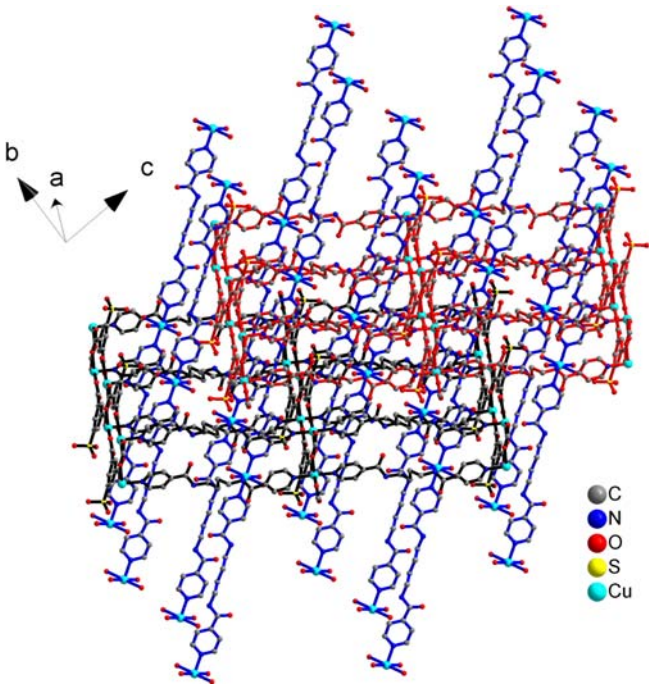

Fig S5. The 3D poly*pseudo*-rotaxane MOF of compound **1**.

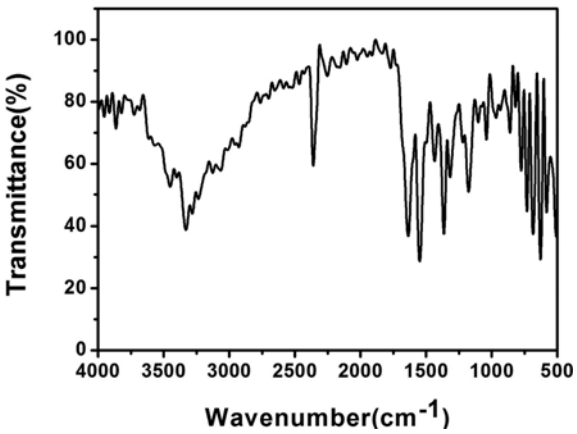

Fig S6. IR spectrum of compound **1**

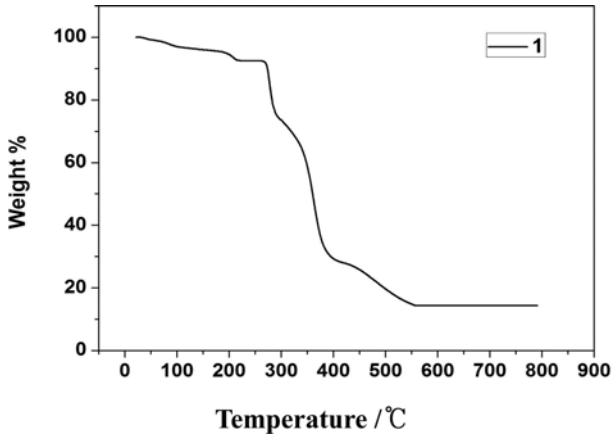

Fig S7. The TGA curve of compound **1**

Table S1. Crystal Data and Structure Refinements for Compound **1**

formula	$C_{64}H_{72}Cu_3N_{12}O_{26}S_2$
*F*w	1680.13
space group	P -1
a (Å)	10.2137(8)
b (Å)	11.6628(13)
c (Å)	15.7133(13)
α (°)	85.055(8)
β (°)	82.932(7)
γ (°)	90.000
V (Å^3)	1732.9(13)
Z	1
D_c (g·cm^{-3})	1.610
μ (mm^{-1})	1.066
F(000)	867
final$R_1{}^a$, $wR_2{}^b$ [$I > 2\sigma(I)$]	0.0415, 0.0987
final$R_1{}^a$, $wR_2{}^b$ (all data)	0.0561, 0.1054
GOF on F^2	1.034
largest diff. peak and holes (eÅ^3)	0.586 and -0.633

$^aR_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. $^bwR_2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$

Table S2. Selected Bond Lengths (Å) and Bond Angles (°) for Compound **1**

Cu(1)-N(1)	2.021(2)	Cu(1)-N(4)	2.031(2)
Cu(1)-O(1)	2.003(2)	Cu(1)-O(2)	2.578(2)
Cu(1)-O(7)#5	1.958(2)	Cu(1)-O(6)#3	2.222(2)
Cu(2)-N(5)	2.055(2)	Cu(2)-N(5)#7	2.055(2)
Cu(2)-O(1W)	2.341(3)	Cu(2)-O(1W)#7	2.341(3)
Cu(2)-O(2W)	2.027(2)	Cu(2)-O(2W)#7	2.027(2)
O(1)-Cu(1)-O(2)	56.14(7)	N(1)-Cu(1)-O(2)	84.88(9)
O(7)#5-Cu(1)-O(1)	154.29(8)	O(7)#5-Cu(1)-N(1)	91.32(9)
O(1)-Cu(1)-N(1)	91.58(9)	O(7)#5-Cu(1)-N(4)	86.62(9)
O(1)-Cu(1)-N(4)	89.27(9)	N(1)-Cu(1)-N(4)	176.87(10)
O(7)#5-Cu(1)-O(6)#3	115.52(8)	O(1)-Cu(1)-O(6)#3	89.78(8)
N(1)-Cu(1)-O(6)#3	93.60(9)	N(4)-Cu(1)-O(6)#3	89.41(9)
O(7)#5-Cu(1)-O(2)	98.74(8)	O(6)#3-Cu(1)-O(2)	145.75(7)
N(4)-Cu(1)-O(2)	93.10(9)	N(5)-Cu(2)-O(1W)	93.14(10)
O(1W)-Cu(2)-O(2W)#7	89.66(10)	N(5)-Cu(2)-O(1W)#7	86.86(9)
O(2W)#7-Cu(2)-N(5)	91.09(9)	O(2W)#7-Cu(2)-O(2W)	179.998(2)
N(5)#7-Cu(2)-N(5)	180.0	O(1W)#7-Cu(2)-O(1W)	180.0
O(1W)-Cu(2)-O(2W)	90.34(10)	O(2W)-Cu(2)-N(5)	88.91(9)

Symmetry codes: #3 -x,-y+2,-z #5 x+1,y,z #7 -x,-y+2,-z+1

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F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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C2 0.0163(13) 0.0192(15) 0.0191(14) 0.0029(11) -0.0026(11) -0.0087(12)
C3 0.0167(13) 0.0214(15) 0.0209(15) -0.0024(11) 0.0033(11) -0.0076(12)
C4 0.0221(14) 0.0178(15) 0.0167(14) -0.0007(11) -0.0020(11) -0.0084(12)
C5 0.0159(13) 0.0236(16) 0.0197(14) -0.0003(11) -0.0049(11) -0.0083(12)
C6 0.0170(13) 0.0178(15) 0.0186(14) 0.0017(11) -0.0030(11) -0.0070(11)
C7 0.0190(13) 0.0183(15) 0.0158(14) 0.0016(11) -0.0035(11) -0.0058(12)
C8 0.0204(14) 0.0153(14) 0.0180(14) -0.0011(11) -0.0025(11) -0.0074(11)
C9 0.0329(17) 0.0271(18) 0.0302(18) 0.0011(14) 0.0034(14) -0.0003(14)
C10 0.0370(18) 0.0327(19) 0.0243(17) -0.0001(14) 0.0046(14) -0.0052(15)
C11 0.0251(15) 0.0259(17) 0.0251(16) 0.0045(13) -0.0029(12) -0.0088(13)
C12 0.0286(16) 0.0294(18) 0.0234(16) 0.0020(13) 0.0008(13) -0.0062(14)
C13 0.0316(17) 0.0290(18) 0.0295(17) 0.0095(14) -0.0011(14) -0.0041(14)
C14 0.0393(18) 0.0275(18) 0.0270(17) 0.0033(13) 0.0014(14) -0.0090(15)
C15 0.0396(18) 0.0272(18) 0.0240(16) 0.0033(13) -0.0025(14) -0.0078(15)
C16 0.0301(16) 0.0285(18) 0.0226(16) 0.0036(13) -0.0006(13) -0.0025(14)
C17 0.0248(15) 0.0312(18) 0.0240(16) -0.0007(13) 0.0012(12) -0.0124(14)
C18 0.0245(15) 0.0268(17) 0.0227(15) -0.0011(12) 0.0008(12) -0.0107(13)
C19 0.059(2) 0.0263(19) 0.0211(16) -0.0039(13) 0.0021(15) -0.0093(17)
C20 0.0380(18) 0.0194(16) 0.0257(16) 0.0018(13) -0.0033(14) -0.0045(14)
C21 0.048(2) 0.0263(19) 0.0305(19) 0.0021(14) 0.0028(16) 0.0013(16)
C22 0.0423(19) 0.036(2) 0.0240(17) 0.0010(14) 0.0050(15) -0.0036(16)
C23 0.061(2) 0.0243(18) 0.0259(18) -0.0035(14) 0.0031(16) -0.0081(17)
C24 0.0368(18) 0.0279(18) 0.0258(17) -0.0046(13) 0.0001(14) -0.0091(15)
N1 0.0203(12) 0.0260(14) 0.0220(13) 0.0027(10) -0.0036(10) -0.0078(11)
N2 0.0313(14) 0.0276(15) 0.0232(14) 0.0025(11) -0.0006(11) -0.0064(12)
N3 0.0365(14) 0.0271(15) 0.0166(13) -0.0012(10) -0.0020(11) -0.0097(12)
N4 0.0215(12) 0.0225(14) 0.0237(13) -0.0014(10) 0.0015(10) -0.0083(11)
O1 0.0182(10) 0.0235(11) 0.0279(11) -0.0030(9) -0.0029(8) -0.0104(9)

O2 0.0166(10) 0.0353(13) 0.0401(13) -0.0124(10) -0.0029(9) -0.0071(10)
O3 0.0425(14) 0.0356(15) 0.0434(15) -0.0187(11) -0.0090(11) 0.0050(12)
O4 0.0451(13) 0.0365(14) 0.0294(12) -0.0045(10) -0.0047(10) -0.0263(11)
O5 0.0605(15) 0.0345(14) 0.0223(12) 0.0009(10) 0.0008(10) -0.0264(12)
O6 0.0250(11) 0.0314(13) 0.0273(12) -0.0128(9) 0.0031(9) -0.0090(10)
O7 0.0160(10) 0.0406(14) 0.0296(12) -0.0107(10) 0.0000(8) -0.0128(10)
O8 0.0683(17) 0.0321(14) 0.0269(13) -0.0007(10) -0.0053(12) -0.0100(12)
O9 0.0526(15) 0.0337(14) 0.0277(12) -0.0053(10) -0.0077(11) -0.0137(12)
S1 0.0298(4) 0.0193(4) 0.0185(4) -0.0034(3) -0.0014(3) -0.0097(3)
Cu1 0.01525(17) 0.0231(2) 0.01803(19) 0.00018(14) -0.00194(13) -0.00927(14)
C25 0.0436(18) 0.0262(17) 0.0189(15) 0.0024(12) -0.0070(13) -0.0170(15)
C26 0.0445(19) 0.0220(17) 0.0242(16) 0.0025(13) -0.0080(14) -0.0168(15)
C27 0.0333(16) 0.0253(17) 0.0214(15) 0.0016(12) -0.0058(13) -0.0144(14)
C28 0.0432(18) 0.0292(18) 0.0224(16) -0.0016(13) -0.0051(14) -0.0179(15)
C29 0.075(3) 0.036(2) 0.0217(17) -0.0067(14) 0.0004(17) -0.0259(19)
C30 0.072(3) 0.036(2) 0.0211(17) -0.0032(15) -0.0025(17) -0.0262(19)
C31 0.0450(19) 0.0237(17) 0.0244(16) 0.0041(13) -0.0067(14) -0.0138(15)
C32 0.0447(19) 0.0211(17) 0.0275(17) 0.0000(13) -0.0051(14) -0.0132(15)
N5 0.0341(14) 0.0218(14) 0.0247(14) -0.0031(11) -0.0055(11) -0.0105(11)
N6 0.075(2) 0.0340(17) 0.0172(13) -0.0040(11) -0.0010(13) -0.0306(16)
O1W 0.0750(18) 0.0507(17) 0.0418(15) 0.0031(12) -0.0195(13) -0.0398(15)
O2W 0.0504(14) 0.0247(13) 0.0326(13) -0.0016(10) -0.0080(11) -0.0113(11)
O10 0.129(3) 0.0401(16) 0.0222(13) 0.0050(11) -0.0108(15) -0.0370(17)
Cu2 0.0311(3) 0.0190(3) 0.0216(3) -0.0033(2) -0.0049(2) -0.0091(2)
O3W 0.0550(17) 0.0504(18) 0.0647(19) -0.0123(14) 0.0157(14) -0.0143(14)

_geom_special_details
;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
;

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C1 O1 1.258(3) . ?
C1 C2 1.514(3) . ?
C2 C3 1.382(4) . ?
C2 C8 1.399(4) . ?
C3 C4 1.381(4) . ?
C3 H3 0.9300 . ?
C4 C5 1.382(4) . ?
C4 S1 1.769(3) . ?
C5 C6 1.388(4) . ?
C5 H5 0.9300 . ?
C6 C8 1.399(4) . ?
C6 C7 1.515(4) . ?
C7 O6 1.226(3) . ?
C7 O7 1.272(3) . ?

C8 H8 0.9300 . ?
C9 N1 1.332(4) . ?
C9 C10 1.373(4) . ?
C9 H9 0.9300 . ?
C10 C11 1.375(4) . ?
C10 H10 0.9300 . ?
C11 C21 1.380(4) . ?
C11 C12 1.505(4) . ?
C12 O8 1.232(4) . ?
C12 N2 1.336(4) . ?
C13 N2 1.455(4) . ?
C13 C14 1.520(4) . ?
C13 H13A 0.9700 . ?
C13 H13B 0.9700 . ?
C14 C15 1.512(4) . ?
C14 H14A 0.9700 . ?
C14 H14B 0.9700 . ?
C15 C16 1.529(4) . ?
C15 H15A 0.9700 . ?
C15 H15B 0.9700 . ?
C16 N3 1.460(4) . ?
C16 H16A 0.9700 . ?
C16 H16B 0.9700 . ?
C17 O9 1.238(4) . ?
C17 N3 1.321(4) . ?
C17 C18 1.501(4) . ?
C18 C20 1.386(4) . ?
C18 C19 1.386(4) . ?
C19 C23 1.364(4) 1_546 ?
C19 H19 0.9300 . ?
C20 C24 1.374(4) 1_546 ?
C20 H20 0.9300 . ?
C21 C22 1.381(5) . ?
C21 H21 0.9300 . ?
C22 N1 1.335(4) . ?
C22 H22 0.9300 . ?
C23 N4 1.336(4) . ?
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C23 H23 0.9300 . ?
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C24 C20 1.374(4) 1_564 ?
C24 H24 0.9300 . ?
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N2 H2 0.8600 . ?
N3 H3A 0.8600 . ?
N4 Cu1 2.031(2) . ?
O1 Cu1 2.0034(18) . ?
O3 S1 1.441(2) . ?
O4 S1 1.447(2) . ?
O5 S1 1.463(2) . ?
O6 Cu1 2.222(2) 2_575 ?
O7 Cu1 1.9580(18) 1_455 ?
Cu1 O7 1.9580(19) 1_655 ?
Cu1 O6 2.222(2) 2_575 ?
C25 N5 1.335(4) . ?
C25 C26 1.379(4) . ?
C25 H25 0.9300 . ?

C26 C27 1.391(4) . ?
C26 H26 0.9300 . ?
C27 C31 1.383(4) . ?
C27 C28 1.514(4) . ?
C28 O10 1.214(4) . ?
C28 N6 1.335(4) . ?
C29 N6 1.467(4) . ?
C29 C30 1.513(5) . ?
C29 H29A 0.9700 . ?
C29 H29B 0.9700 . ?
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C30 H30A 0.9700 . ?
C30 H30B 0.9700 . ?
C31 C32 1.378(4) . ?
C31 H31 0.9300 . ?
C32 N5 1.345(4) . ?
C32 H32 0.9300 . ?
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N6 H6 0.8600 . ?
O1W Cu2 2.341(3) . ?
O1W H1WA 0.8501 . ?
O1W H1WB 0.8500 . ?
O2W Cu2 2.027(2) . ?
O2W H2WA 0.8500 . ?
O2W H2WB 0.8499 . ?
Cu2 O2W 2.027(2) 2_576 ?
Cu2 N5 2.055(2) 2_576 ?
Cu2 O1W 2.341(3) 2_576 ?
Cu2 H2WA 1.8921 . ?
O3W H3WA 0.8499 . ?
O3W H3WB 0.8501 . ?

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O1 C1 C2 118.4(2) . . ?
C3 C2 C8 119.2(2) . . ?
C3 C2 C1 116.7(2) . . ?
C8 C2 C1 124.0(2) . . ?
C4 C3 C2 121.1(2) . . ?
C4 C3 H3 119.5 . . ?
C2 C3 H3 119.5 . . ?
C3 C4 C5 120.3(2) . . ?
C3 C4 S1 118.3(2) . . ?
C5 C4 S1 121.4(2) . . ?
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C4 C5 H5 120.3 . . ?
C6 C5 H5 120.3 . . ?
C5 C6 C8 120.4(2) . . ?
C5 C6 C7 118.7(2) . . ?

C8 C6 C7 120.8(2) . . ?
O6 C7 O7 125.6(3) . . ?
O6 C7 C6 120.0(2) . . ?
O7 C7 C6 114.4(2) . . ?
C2 C8 C6 119.4(2) . . ?
C2 C8 H8 120.3 . . ?
C6 C8 H8 120.3 . . ?
N1 C9 C10 123.2(3) . . ?
N1 C9 H9 118.4 . . ?
C10 C9 H9 118.4 . . ?
C9 C10 C11 119.9(3) . . ?
C9 C10 H10 120.1 . . ?
C11 C10 H10 120.1 . . ?
C10 C11 C21 117.6(3) . . ?
C10 C11 C12 118.2(3) . . ?
C21 C11 C12 124.2(3) . . ?
O8 C12 N2 122.6(3) . . ?
O8 C12 C11 119.7(3) . . ?
N2 C12 C11 117.7(3) . . ?
N2 C13 C14 114.5(3) . . ?
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C14 C13 H13A 108.6 . . ?
N2 C13 H13B 108.6 . . ?
C14 C13 H13B 108.6 . . ?
H13A C13 H13B 107.6 . . ?
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C15 C14 H14A 108.5 . . ?
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C15 C14 H14B 108.5 . . ?
C13 C14 H14B 108.5 . . ?
H14A C14 H14B 107.5 . . ?
C14 C15 C16 112.3(3) . . ?
C14 C15 H15A 109.1 . . ?
C16 C15 H15A 109.1 . . ?
C14 C15 H15B 109.1 . . ?
C16 C15 H15B 109.1 . . ?
H15A C15 H15B 107.9 . . ?
N3 C16 C15 112.6(3) . . ?
N3 C16 H16A 109.1 . . ?
C15 C16 H16A 109.1 . . ?
N3 C16 H16B 109.1 . . ?
C15 C16 H16B 109.1 . . ?
H16A C16 H16B 107.8 . . ?
O9 C17 N3 123.8(3) . . ?
O9 C17 C18 118.7(3) . . ?
N3 C17 C18 117.5(3) . . ?
C20 C18 C19 117.0(3) . . ?
C20 C18 C17 124.3(3) . . ?
C19 C18 C17 118.6(3) . . ?
C23 C19 C18 119.9(3) 1_546 . ?
C23 C19 H19 120.1 1_546 . ?
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C24 C20 C18 119.6(3) 1_546 . ?
C24 C20 H20 120.2 1_546 . ?
C18 C20 H20 120.2 . . ?
C11 C21 C22 118.8(3) . . ?
C11 C21 H21 120.6 . . ?

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C19 C23 H23 118.2 1_564 . ?
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C20 C24 H24 118.4 1_564 . ?
C9 N1 C22 116.7(3) . . ?
C9 N1 Cu1 122.0(2) . . ?
C22 N1 Cu1 121.3(2) . . ?
C12 N2 C13 122.3(3) . . ?
C12 N2 H2 118.8 . . ?
C13 N2 H2 118.8 . . ?
C17 N3 C16 124.0(3) . . ?
C17 N3 H3A 118.0 . . ?
C16 N3 H3A 118.0 . . ?
C23 N4 C24 116.8(3) . . ?
C23 N4 Cu1 118.9(2) . . ?
C24 N4 Cu1 124.2(2) . . ?
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C7 O6 Cu1 156.6(2) . 2_575 ?
C7 O7 Cu1 126.71(18) . 1_455 ?
O3 S1 O4 114.17(15) . . ?
O3 S1 O5 112.59(15) . . ?
O4 S1 O5 111.80(14) . . ?
O3 S1 C4 105.69(13) . . ?
O4 S1 C4 106.12(13) . . ?
O5 S1 C4 105.68(13) . . ?
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O1 Cu1 N1 91.58(9) . . ?
O7 Cu1 N4 86.62(9) 1_655 . ?
O1 Cu1 N4 89.27(9) . . ?
N1 Cu1 N4 176.87(10) . . ?
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O1 Cu1 O6 89.78(8) . 2_575 ?
N1 Cu1 O6 93.60(9) . 2_575 ?
N4 Cu1 O6 89.41(9) . 2_575 ?
N5 C25 C26 124.1(3) . . ?
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C26 C25 H25 118.0 . . ?
C25 C26 C27 119.3(3) . . ?
C25 C26 H26 120.4 . . ?
C27 C26 H26 120.4 . . ?
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C31 C27 C28 117.6(3) . . ?
C26 C27 C28 125.6(3) . . ?
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O10 C28 C27 118.8(3) . . ?
N6 C28 C27 118.6(3) . . ?
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C30 C29 H29A 108.7 . . ?
N6 C29 H29B 108.7 . . ?

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H29A C29 H29B 107.6 . . ?
C29 C30 C30 112.3(4) . 2_565 ?
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C30 C30 H30B 109.1 2_565 . ?
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C32 C31 C27 120.4(3) . . ?
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C27 C31 H31 119.8 . . ?
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C31 C32 H32 118.5 . . ?
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C32 N5 Cu2 120.4(2) . . ?
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C28 N6 H6 119.2 . . ?
C29 N6 H6 119.2 . . ?
Cu2 O1W H1WA 140.3 . . ?
Cu2 O1W H1WB 105.5 . . ?
H1WA O1W H1WB 107.7 . . ?
Cu2 O2W H2WA 68.7 . . ?
Cu2 O2W H2WB 122.9 . . ?
H2WA O2W H2WB 107.7 . . ?
O2W Cu2 O2W 179.998(2) 2_576 . ?
O2W Cu2 N5 88.91(9) 2_576 2_576 ?
O2W Cu2 N5 91.09(9) . 2_576 ?
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O2W Cu2 O1W 89.66(9) . 2_576 ?
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O1 C1 C2 C8 -21.7(4) . . . . ?
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C1 C2 C3 C4 -175.6(2) . . . . ?
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C3 C4 C5 C6 0.0(4) . . . . ?
S1 C4 C5 C6 179.7(2) . . . . ?
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C8 C6 C7 O6 1.8(4) . . . . ?
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N1 C9 C10 C11 -2.8(5) . . . . ?
C9 C10 C11 C21 -0.6(5) . . . . ?
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C10 C11 C12 N2 150.3(3) . . . . ?
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O9 C17 C18 C20 -161.0(3) . . . . ?
N3 C17 C18 C20 16.7(4) . . . . ?
O9 C17 C18 C19 14.3(4) . . . . ?
N3 C17 C18 C19 -168.0(3) . . . . ?
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C17 C18 C19 C23 -174.5(3) . . . 1_546 ?
C19 C18 C20 C24 -2.1(5) . . . 1_546 ?
C17 C18 C20 C24 173.2(3) . . . 1_546 ?
C10 C11 C21 C22 3.4(5) . . . . ?
C12 C11 C21 C22 -175.5(3) . . . . ?
C11 C21 C22 N1 -3.2(6) . . . . ?
C10 C9 N1 C22 3.1(5) . . . . ?
C10 C9 N1 Cu1 -176.2(3) . . . . ?
C21 C22 N1 C9 -0.1(5) . . . . ?
C21 C22 N1 Cu1 179.3(3) . . . . ?
O8 C12 N2 C13 -5.8(5) . . . . ?
C11 C12 N2 C13 174.5(3) . . . . ?
C14 C13 N2 C12 95.4(4) . . . . ?
O9 C17 N3 C16 5.3(5) . . . . ?
C18 C17 N3 C16 -172.3(3) . . . . ?
C15 C16 N3 C17 -99.0(4) . . . . ?
C19 C23 N4 C24 -2.3(5) 1_564 . . . ?
C19 C23 N4 Cu1 174.3(3) 1_564 . . . ?
C20 C24 N4 C23 1.2(5) 1_564 . . . ?
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C20 C24 N4 Cu1 -175.2(2) 1_564 . . . ?
O2 C1 O1 Cu1 4.2(3) . . . . ?
C2 C1 O1 Cu1 -172.66(19) . . . . ?
O7 C7 O6 Cu1 -72.6(6) . . . 2_575 ?
C6 C7 O6 Cu1 108.3(5) . . . 2_575 ?
O6 C7 O7 Cu1 8.6(4) . . . 1_455 ?
C6 C7 O7 Cu1 -172.30(18) . . . 1_455 ?
C3 C4 S1 O3 37.9(3) . . . . ?
C5 C4 S1 O3 -141.8(2) . . . . ?
C3 C4 S1 O4 159.5(2) . . . . ?
C5 C4 S1 O4 -20.2(3) . . . . ?
C3 C4 S1 O5 -81.6(2) . . . . ?
C5 C4 S1 O5 98.6(3) . . . . ?
C1 O1 Cu1 O7 11.5(3) . . . 1_655 ?
C1 O1 Cu1 N1 -84.81(18) . . . . ?
C1 O1 Cu1 N4 92.18(18) . . . . ?
C1 O1 Cu1 O6 -178.41(18) . . . 2_575 ?
C9 N1 Cu1 O7 137.3(2) . . . 1_655 ?
C22 N1 Cu1 O7 -41.9(3) . . . 1_655 ?
C9 N1 Cu1 O1 -68.2(2) . . . . ?
C22 N1 Cu1 O1 112.5(3) . . . . ?
C9 N1 Cu1 N4 -173.9(16) . . . . ?
C22 N1 Cu1 N4 6.9(18) . . . . ?
C9 N1 Cu1 O6 21.7(3) . . . 2_575 ?
C22 N1 Cu1 O6 -157.6(2) . . . 2_575 ?
C23 N4 Cu1 O7 58.6(2) . . . 1_655 ?
C24 N4 Cu1 O7 -125.1(2) . . . 1_655 ?
C23 N4 Cu1 O1 -96.0(2) . . . . ?
C24 N4 Cu1 O1 80.3(2) . . . . ?
C23 N4 Cu1 N1 9.7(18) . . . . ?
C24 N4 Cu1 N1 -174.0(16) . . . . ?
C23 N4 Cu1 O6 174.2(2) . . . 2_575 ?
C24 N4 Cu1 O6 -9.5(2) . . . 2_575 ?
N5 C25 C26 C27 0.6(5) . . . . ?
C25 C26 C27 C31 -2.3(5) . . . . ?
C25 C26 C27 C28 176.2(3) . . . . ?
C31 C27 C28 O10 8.5(5) . . . . ?
C26 C27 C28 O10 -170.0(3) . . . . ?
C31 C27 C28 N6 -173.3(3) . . . . ?
C26 C27 C28 N6 8.2(5) . . . . ?
N6 C29 C30 C30 -178.7(4) . . . 2_565 ?
C26 C27 C31 C32 2.1(5) . . . . ?
C28 C27 C31 C32 -176.6(3) . . . . ?
C27 C31 C32 N5 0.0(5) . . . . ?
C26 C25 N5 C32 1.4(5) . . . . ?
C26 C25 N5 Cu2 -174.7(2) . . . . ?
C31 C32 N5 C25 -1.7(5) . . . . ?
C31 C32 N5 Cu2 174.5(2) . . . . ?
O10 C28 N6 C29 1.9(5) . . . . ?
C27 C28 N6 C29 -176.3(3) . . . . ?
C30 C29 N6 C28 -93.0(4) . . . . ?
C25 N5 Cu2 O2W 35.9(2) . . . 2_576 ?
C32 N5 Cu2 O2W -140.1(2) . . . 2_576 ?
C25 N5 Cu2 O2W -144.1(2) . . . . ?
C32 N5 Cu2 O2W 39.9(2) . . . . ?
C25 N5 Cu2 N5 -80(15) . . . 2_576 ?
C32 N5 Cu2 N5 104(15) . . . 2_576 ?

C25 N5 Cu2 O1W 126.2(2) . . . 2_576 ?
C32 N5 Cu2 O1W -49.8(2) . . . 2_576 ?
C25 N5 Cu2 O1W -53.8(2) . . . . ?
C32 N5 Cu2 O1W 130.2(2) . . . . ?

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_refine_diff_density_min -0.632
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