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catena-Poly[[bis(1-ethyl-1*H*-imidazole-κN^3)copper(II)]-μ-benzene-1,4-dicarboxylato]

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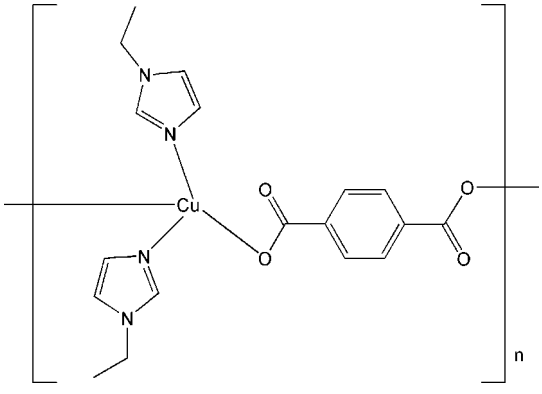
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.111; data-to-parameter ratio = 16.6.

In the title compound, $[Cu(C_8H_4O_4)(C_5H_8N_2)_2]_n$, each Cu^{II} atom is four-coordinated by two carboxylate O atoms from two different benzene-1,4-dicarboxylate (1,4-BDC) ligands and two N atoms from two 1-ethyl-1*H*-imidazole (EI) ligands in a slightly distorted square-planar coordination environment. There are two Cu atoms, both with site symmetry $\overline{1}$. Each 1,4-BDC acts as a bis-monodentate ligand that binds two Cu^{II} atoms, thus forming two unique chains. The EI ligands are attached on both sides of the chains.

Related literature

For related literature, see: Lehn (1990); Qi *et al.* (2003); De (2007).



Experimental

Crystal data

$[Cu(C_8H_4O_4)(C_5H_8N_2)_2]$
M_r = 419.92
Triclinic, $P\overline{1}$
a = 7.6864 (15) Å
b = 10.948 (2) Å
c = 11.372 (2) Å
α = 93.14 (3)°
β = 92.61 (3)°
γ = 105.54 (3)°
V = 918.8 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.22 mm^{-1}
T = 293 (2) K
0.33 × 0.27 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.661, T_{max} = 0.775
8970 measured reflections
4136 independent reflections
3397 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.111
S = 1.15
4136 reflections
249 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O1	1.9725 (14)	Cu2—O4	1.9505 (13)
Cu1—N1	1.9797 (18)	Cu2—N3	2.0088 (18)

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2556).

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supplementary materials

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catena-Poly[[bis(1-ethyl-1*H*-imidazole-κN^3)copper(II)]-μ-benzene-1,4-dicarboxylato]

G.-B. Che, Y. Liu, L. Lu, J. Sun and J. Wang

Comment

Chain structures have received much attention in coordination chemistry and materials chemistry (Lehn, 1990). An appropriate flexible bidentate organic acid bridge could be useful in the formation of chains in the presence of secondary ligands, such as 2,2'-bipyridine (bipy) and 1,10-phenanthroline (phen) (Qi *et al.*, 2003). The N atoms from the secondary ligand may occupy two coordination positions of metal ions; the rest of the coordination positions are available for other carboxylate ligands to allow the formation of chain. We selected 1,4-benzenedicarboxylic acid (1,4-H_2BDC) as a bridging ligand and 1-ethyl-1*H*-imidazole (EI) as a secondary ligand, generating the title compound, a new chain coordination polymer, [Cu(1,4-BDC)(EI)$_2$], (I), which is reported here.

In compound (I), there exist two unique Cu^{II} atoms, both with site symmetry $\bar{1}$. Each Cu^{II} atom is four-coordinated by two carboxylate O atoms from two different 1,4-BDC ligands, and two N atoms from two EI ligands in a square-planar coordination environment (Fig. 1). The Cu—O and Cu—N distances are within their normal ranges (Table 1). As shown in Fig. 2, each 1,4-BDC acts as a bis-modentate ligand that binds two Cu^{II} atoms, forming two unique chains, both propagating in [010]. The EI ligands are attached to both sides of the chains.

Experimental

A mixture of $CuCl_2{\cdot}2H_2O$ (0.5 mmol), 1,4-H_2BDC (0.5 mmol), EI (0.5 mmol), and H_2O (500 mmol) was adjusted to pH = 5.5 by addition of aqueous NaOH solution, and heated in a sealed vessel at 463 K for 2 days. After the mixture was slowly cooled to room temperature, blue blocks of (I) were yielded (21% yield).

Refinement

The H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

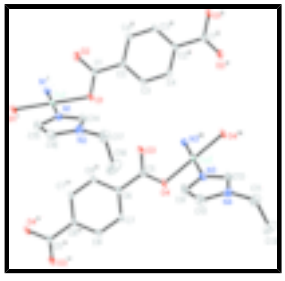

Fig. 1. The structure of (I), with displacement ellipsoids drawn at the 30% probability level. (H atoms have been omitted). Symmetry codes: (i) 2 − *x*, −*y*, 2 − *z*; (ii) 2 − *x*, 1 − *y*, 2 − *z*; (iii) 2 − *x*, 1 − *y*, 3 − *z*; (iv) 2 − *x*, −*y*, 3 − *z*.

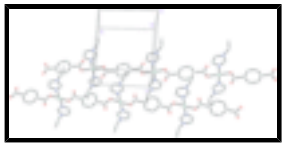

Fig. 2. View of the chain structure of (I).

catena-Poly[[bis(1-ethyl-1_H_-imidazole-κN^3)copper(II)]-μ- benzene-1,4-dicarboxylato]

Crystal data

$[Cu(C_8H_4O_4)(C_5H_8N_2)_2]$	$Z = 2$
$M_r = 419.92$	$F_{000} = 434$
Triclinic, $P\overline{1}$	$D_x = 1.518$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.6864$ (15) Å	Cell parameters from 7742 reflections
$b = 10.948$ (2) Å	$\theta = 3.0$–$27.5°$
$c = 11.372$ (2) Å	$\mu = 1.22$ mm^{-1}
$\alpha = 93.14$ (3)°	$T = 293$ (2) K
$\beta = 92.61$ (3)°	Block, blue
$\gamma = 105.54$ (3)°	0.33 × 0.27 × 0.21 mm
$V = 918.8$ (3) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	4136 independent reflections
Radiation source: rotating anode	3397 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.018$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 27.5°$
$T = 293$(2) K	$\theta_{min} = 3.2°$
ω scans	$h = -9 \rightarrow 9$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -13 \rightarrow 14$
$T_{min} = 0.661$, $T_{max} = 0.775$	$l = -14 \rightarrow 14$
8970 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H-atom parameters constrained
$wR(F^2) = 0.111$	$w = 1/[\sigma^2(F_o^2) + (0.0729P)^2 + 0.0254P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.15$	$(\Delta/\sigma)_{max} < 0.001$
4136 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}

249 parameters	$\Delta\rho_{min} = -0.49$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu2	1.0000	0.5000	1.5000	0.02771 (12)
Cu1	1.0000	0.0000	1.0000	0.02926 (12)
O3	0.9107 (2)	0.27569 (14)	1.36307 (14)	0.0467 (4)
O2	0.93649 (19)	0.17782 (13)	0.86458 (14)	0.0439 (4)
O1	1.04795 (19)	0.18231 (12)	1.04847 (13)	0.0374 (3)
C9	0.6494 (3)	0.3343 (2)	1.5848 (3)	0.0571 (7)
H9	0.6743	0.2585	1.5609	0.069*
O4	1.03966 (18)	0.33904 (12)	1.54287 (13)	0.0360 (3)
N2	0.5345 (3)	−0.0014 (2)	1.16622 (18)	0.0484 (5)
N1	0.7624 (2)	−0.03149 (17)	1.07038 (15)	0.0361 (4)
N4	0.5146 (2)	0.4683 (2)	1.65828 (17)	0.0414 (4)
N3	0.7593 (2)	0.45316 (18)	1.57218 (16)	0.0369 (4)
C8	1.0313 (3)	−0.03193 (18)	1.61379 (18)	0.0352 (4)
H8	1.0523	−0.0534	1.6901	0.042*
C13	0.4459 (4)	0.5512 (4)	1.8516 (3)	0.0774 (11)
H13A	0.4327	0.4717	1.8867	0.116*
H13B	0.3707	0.5970	1.8890	0.116*
H13C	0.5700	0.6006	1.8617	0.116*
C18	0.4524 (5)	0.0567 (5)	1.3606 (3)	0.0932 (14)
H18A	0.4053	−0.0296	1.3802	0.140*
H18B	0.3925	0.1101	1.4031	0.140*
H18C	0.5800	0.0844	1.3817	0.140*
C2	0.9975 (2)	0.37248 (17)	0.98204 (17)	0.0290 (4)
C14	0.6978 (3)	0.0531 (2)	1.1280 (2)	0.0426 (5)
H14	0.7576	0.1391	1.1405	0.051*
C4	1.0389 (3)	0.56046 (18)	1.11242 (18)	0.0333 (4)
H4	1.0650	0.6009	1.1877	0.040*
C3	1.0364 (2)	0.43359 (18)	1.09464 (18)	0.0337 (4)
H3	1.0607	0.3892	1.1580	0.040*
C15	0.6332 (3)	−0.1453 (2)	1.0739 (2)	0.0469 (5)

H15	0.6414	−0.2229	1.0406	0.056*
C1	0.9929 (2)	0.23451 (17)	0.96117 (18)	0.0315 (4)
C6	0.9910 (2)	0.12260 (17)	1.48043 (18)	0.0297 (4)
C5	0.9782 (2)	0.25449 (17)	1.45794 (19)	0.0327 (4)
C7	1.0223 (3)	0.09013 (18)	1.59434 (18)	0.0332 (4)
H7	1.0371	0.1503	1.6576	0.040*
C11	0.3898 (3)	0.5266 (3)	1.7217 (2)	0.0558 (7)
H11A	0.2681	0.4705	1.7114	0.067*
H11B	0.3889	0.6061	1.6883	0.067*
C16	0.4928 (3)	−0.1277 (3)	1.1329 (2)	0.0507 (6)
H16	0.3884	−0.1895	1.1479	0.061*
C12	0.6734 (3)	0.5318 (2)	1.6179 (2)	0.0410 (5)
H12	0.7168	0.6199	1.6218	0.049*
C10	0.4989 (3)	0.3439 (3)	1.6375 (3)	0.0605 (7)
H10	0.4029	0.2771	1.6559	0.073*
C17	0.4214 (4)	0.0649 (3)	1.2339 (3)	0.0689 (8)
H17A	0.4508	0.1534	1.2159	0.083*
H17B	0.2946	0.0265	1.2106	0.083*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu2	0.03678 (19)	0.01434 (17)	0.03383 (19)	0.00974 (12)	0.00320 (13)	0.00240 (12)
Cu1	0.04075 (19)	0.01696 (18)	0.0337 (2)	0.01396 (13)	0.00339 (13)	0.00183 (12)
O3	0.0661 (9)	0.0273 (8)	0.0518 (10)	0.0207 (7)	−0.0015 (7)	0.0100 (7)
O2	0.0558 (8)	0.0276 (7)	0.0504 (9)	0.0172 (6)	−0.0004 (7)	−0.0067 (7)
O1	0.0536 (8)	0.0189 (7)	0.0444 (8)	0.0174 (6)	0.0061 (7)	0.0024 (6)
C9	0.0574 (14)	0.0260 (11)	0.089 (2)	0.0094 (10)	0.0257 (13)	0.0077 (12)
O4	0.0467 (7)	0.0146 (6)	0.0489 (9)	0.0117 (5)	0.0022 (6)	0.0033 (6)
N2	0.0481 (10)	0.0546 (13)	0.0476 (11)	0.0225 (9)	0.0078 (9)	0.0009 (9)
N1	0.0440 (9)	0.0300 (9)	0.0383 (9)	0.0169 (7)	0.0027 (7)	0.0027 (7)
N4	0.0402 (9)	0.0469 (12)	0.0382 (9)	0.0138 (8)	0.0032 (7)	0.0009 (8)
N3	0.0418 (9)	0.0288 (9)	0.0419 (10)	0.0119 (7)	0.0060 (7)	0.0048 (7)
C8	0.0490 (10)	0.0235 (10)	0.0356 (10)	0.0136 (8)	0.0025 (8)	0.0045 (8)
C13	0.0614 (17)	0.121 (3)	0.0501 (16)	0.0303 (18)	0.0069 (13)	−0.0189 (18)
C18	0.0693 (19)	0.144 (4)	0.065 (2)	0.032 (2)	0.0096 (16)	−0.024 (2)
C2	0.0308 (8)	0.0195 (9)	0.0394 (10)	0.0107 (6)	0.0058 (7)	0.0022 (7)
C14	0.0492 (12)	0.0372 (12)	0.0456 (12)	0.0186 (9)	0.0076 (10)	0.0005 (9)
C4	0.0433 (10)	0.0224 (9)	0.0356 (10)	0.0122 (7)	0.0021 (8)	−0.0008 (7)
C3	0.0416 (10)	0.0236 (10)	0.0387 (11)	0.0131 (7)	0.0018 (8)	0.0041 (8)
C15	0.0462 (12)	0.0357 (12)	0.0586 (14)	0.0107 (9)	0.0049 (10)	0.0016 (10)
C1	0.0332 (9)	0.0202 (9)	0.0433 (11)	0.0101 (6)	0.0089 (8)	0.0002 (8)
C6	0.0324 (8)	0.0185 (9)	0.0402 (11)	0.0098 (6)	0.0048 (7)	0.0025 (7)
C5	0.0358 (9)	0.0202 (9)	0.0461 (11)	0.0121 (7)	0.0093 (8)	0.0082 (8)
C7	0.0442 (10)	0.0201 (9)	0.0369 (10)	0.0122 (7)	0.0036 (8)	−0.0018 (7)
C11	0.0443 (12)	0.0768 (19)	0.0492 (14)	0.0231 (12)	0.0070 (10)	−0.0056 (13)
C16	0.0445 (12)	0.0464 (15)	0.0614 (15)	0.0116 (10)	0.0042 (11)	0.0084 (12)
C12	0.0422 (11)	0.0358 (12)	0.0470 (12)	0.0129 (8)	0.0094 (9)	0.0016 (9)

C10	0.0479 (13)	0.0483 (15)	0.084 (2)	0.0063 (11)	0.0212 (13)	0.0156 (13)
C17	0.0745 (18)	0.072 (2)	0.0684 (18)	0.0332 (15)	0.0221 (15)	−0.0047 (15)

Geometric parameters (Å, °)

Cu1—O1	1.9725 (14)	C13—H13A	0.9600
Cu1—O1^{i}	1.9725 (14)	C13—H13B	0.9600
Cu1—N1^{i}	1.9797 (17)	C13—H13C	0.9600
Cu1—N1	1.9797 (18)	C18—C17	1.461 (5)
Cu2—O4^{ii}	1.9505 (13)	C18—H18A	0.9600
Cu2—O4	1.9505 (13)	C18—H18B	0.9600
Cu2—N3^{ii}	2.0088 (18)	C18—H18C	0.9600
Cu2—N3	2.0088 (18)	C2—C4^{iv}	1.393 (3)
C1—O1	1.283 (3)	C2—C3	1.393 (3)
C1—O2	1.232 (3)	C2—C1	1.507 (2)
C5—O3	1.236 (3)	C14—H14	0.9300
C5—O4	1.280 (3)	C4—C3	1.388 (3)
C9—C10	1.353 (4)	C4—C2^{iv}	1.393 (3)
C9—N3	1.368 (3)	C4—H4	0.9300
C9—H9	0.9300	C3—H3	0.9300
N2—C14	1.341 (3)	C15—C16	1.347 (3)
N2—C16	1.361 (3)	C15—H15	0.9300
N2—C17	1.487 (3)	C6—C7	1.389 (3)
N1—C14	1.321 (3)	C6—C8^{iii}	1.392 (3)
N1—C15	1.373 (3)	C6—C5	1.508 (2)
N4—C10	1.342 (3)	C7—H7	0.9300
N4—C12	1.347 (3)	C11—H11A	0.9700
N4—C11	1.479 (3)	C11—H11B	0.9700
N3—C12	1.318 (3)	C16—H16	0.9300
C8—C7	1.386 (3)	C12—H12	0.9300
C8—C6^{iii}	1.392 (3)	C10—H10	0.9300
C8—H8	0.9300	C17—H17A	0.9700
C13—C11	1.509 (4)	C17—H17B	0.9700
O1—Cu1—O1^{i}	180.0	C3—C2—C1	120.90 (18)
O1—Cu1—N1^{i}	90.68 (7)	N1—C14—N2	111.0 (2)
O1^{i}—Cu1—N1^{i}	89.32 (7)	N1—C14—H14	124.5
O1—Cu1—N1	89.32 (7)	N2—C14—H14	124.5
O1^{i}—Cu1—N1	90.68 (7)	C3—C4—C2^{iv}	120.28 (19)
N1^{i}—Cu1—N1	180.0	C3—C4—H4	119.9
O4^{ii}—Cu2—O4	180.0	C2^{iv}—C4—H4	119.9
O4^{ii}—Cu2—N3^{ii}	89.55 (7)	C4—C3—C2	120.14 (19)
O4—Cu2—N3^{ii}	90.45 (7)	C4—C3—H3	119.9
O4^{ii}—Cu2—N3	90.45 (7)	C2—C3—H3	119.9
O4—Cu2—N3	89.55 (7)	C16—C15—N1	109.8 (2)
N3^{ii}—Cu2—N3	180.0	C16—C15—H15	125.1

C1—O1—Cu1	106.68 (13)	N1—C15—H15	125.1
C10—C9—N3	109.6 (2)	O2—C1—O1	123.63 (18)
C10—C9—H9	125.2	O2—C1—C2	119.96 (19)
N3—C9—H9	125.2	O1—C1—C2	116.40 (18)
C5—O4—Cu2	109.27 (13)	C7—C6—C8^{iii}	119.66 (18)
C14—N2—C16	107.6 (2)	C7—C6—C5	120.69 (18)
C14—N2—C17	125.8 (2)	C8^{iii}—C6—C5	119.64 (18)
C16—N2—C17	126.6 (2)	O3—C5—O4	123.98 (18)
C14—N1—C15	105.37 (18)	O3—C5—C6	120.52 (19)
C14—N1—Cu1	126.74 (16)	O4—C5—C6	115.50 (18)
C15—N1—Cu1	127.86 (15)	C8—C7—C6	120.03 (19)
C10—N4—C12	107.14 (19)	C8—C7—H7	120.0
C10—N4—C11	127.1 (2)	C6—C7—H7	120.0
C12—N4—C11	125.6 (2)	N4—C11—C13	111.2 (2)
C12—N3—C9	105.09 (18)	N4—C11—H11A	109.4
C12—N3—Cu2	126.86 (15)	C13—C11—H11A	109.4
C9—N3—Cu2	128.05 (16)	N4—C11—H11B	109.4
C7—C8—C6^{iii}	120.31 (19)	C13—C11—H11B	109.4
C7—C8—H8	119.8	H11A—C11—H11B	108.0
C6^{iii}—C8—H8	119.8	C15—C16—N2	106.2 (2)
C11—C13—H13A	109.5	C15—C16—H16	126.9
C11—C13—H13B	109.5	N2—C16—H16	126.9
H13A—C13—H13B	109.5	N3—C12—N4	111.3 (2)
C11—C13—H13C	109.5	N3—C12—H12	124.3
H13A—C13—H13C	109.5	N4—C12—H12	124.3
H13B—C13—H13C	109.5	N4—C10—C9	106.9 (2)
C17—C18—H18A	109.5	N4—C10—H10	126.6
C17—C18—H18B	109.5	C9—C10—H10	126.6
H18A—C18—H18B	109.5	C18—C17—N2	110.6 (3)
C17—C18—H18C	109.5	C18—C17—H17A	109.5
H18A—C18—H18C	109.5	N2—C17—H17A	109.5
H18B—C18—H18C	109.5	C18—C17—H17B	109.5
C4^{iv}—C2—C3	119.57 (17)	N2—C17—H17B	109.5
C4^{iv}—C2—C1	119.52 (18)	H17A—C17—H17B	108.1

Symmetry codes: (i) −*x*+2, −*y*, −*z*+2; (ii) −*x*+2, −*y*+1, −*z*+3; (iii) −*x*+2, −*y*, −*z*+3; (iv) −*x*+2, −*y*+1, −*z*+2.

Fig. 1

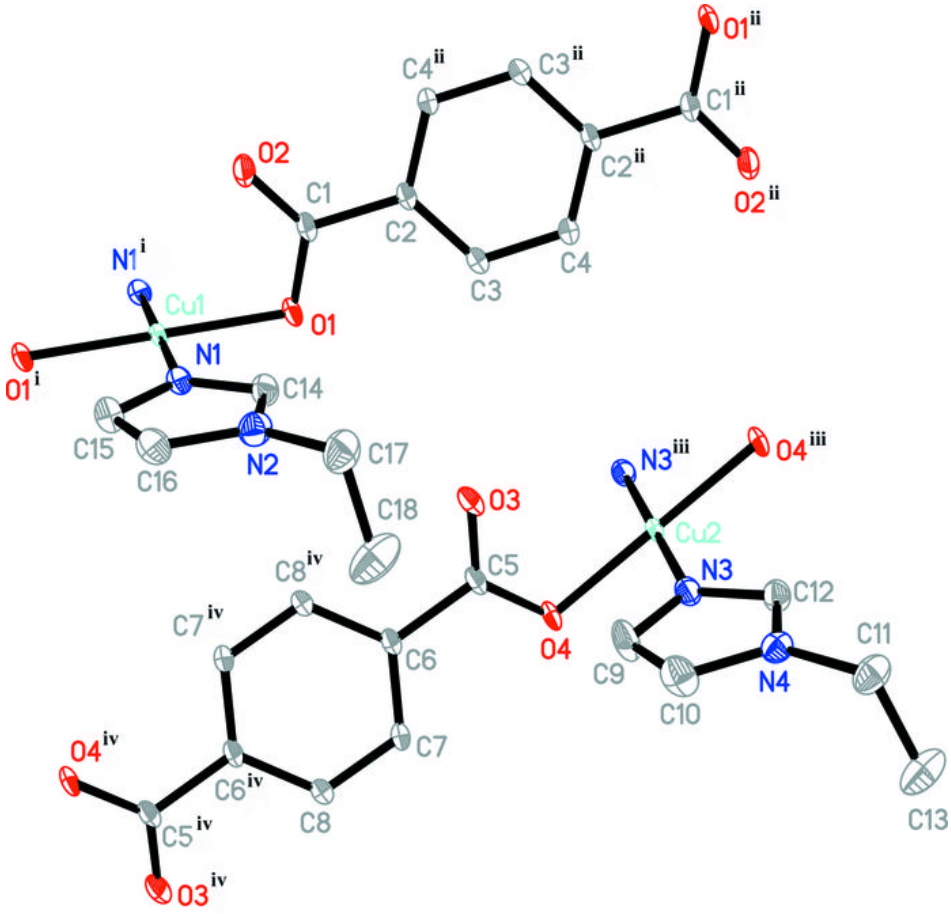
O1ii
C4ii
C3ii
C1ii
O2
C1
C2ii
O2ii
C2
C4
N1i
C3
Cu1
O1
O1i
N1
C14
C15
C16
N2
C17
C18
O3
N3iii
O4iii
Cu2
C8iv
C5
N3
C12
C7iv
O4
C6
C9
C10
N4
C11
O4iv
C7
C6iv
C8
C5iv
C13
O3iv

Fig. 2