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1,4-Bis{[2-(pyridin-2-yl)-1*H*-imidazol-1-yl]methyl}benzene dihydrate

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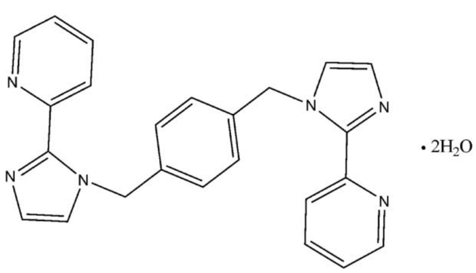
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.098; data-to-parameter ratio = 16.6.

In the title compound, $C_{24}H_{20}N_6 \cdot 2H_2O$, the 1,4-bis{[2-(pyridin-2-yl)-1*H*-imidazol-1-yl]methyl}benzene neutral molecule lies on a centre of symmetry; the molecule is linked to the solvent water molecule *via* O—H···N hydrogen bonds, generating a two-dimensional supramolecular layer parallel to (100).

Related literature

For related literature, see: Ayyappan *et al.* (2002); Eddaoudi *et al.* (2001); Kitaura *et al.* (2002); Russell *et al.* (1997); Tao *et al.* (2000).



Experimental

Crystal data

$C_{24}H_{20}N_6 \cdot 2H_2O$
M_r = 428.49
Monoclinic, $P2_1/c$
a = 7.503 (2) Å
b = 28.450 (2) Å
c = 5.030 (4) Å
β = 93.572 (2)°
V = 1071.6 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.40 × 0.38 × 0.36 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) T_{min} = 0.96, T_{max} = 0.97
6504 measured reflections
2513 independent reflections
1417 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.098
S = 0.98
2513 reflections
151 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1B···N2^{i}	0.860 (9)	2.115 (9)	2.9636 (16)	168.7 (17)
O1W—H1A···O1W^{ii}	0.873 (9)	1.955 (9)	2.8258 (19)	176.4 (18)

Symmetry codes: (i) $x-1, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; 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: BG2122).

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supplementary materials

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1,4-Bis{[2-(pyridin-2-yl)-1*H*-imidazol-1-yl]methyl}benzene dihydrate

R.-H. Cui and **Y.-Q. Lan**

Comment

Metal-organic extended structures have attracted considerable interest in coordination chemistry and material science because of their intriguing structural diversities and potential applications in functional materials, nanotechnology and biological recognition (Ayyappan *et al.*, 2002; Eddaoudi *et al.*, 2001; Kitaura *et al.*, 2002; Russell *et al.*, 1997; Tao *et al.*, 2000). Therefore, rational design and construction of coordination polymers with this potential diversity of architectures has become a particularly important subject. The key factor is the selection of the organic ligand, because it plays an important role in the formation of different metal-organic compounds. In this paper, we present a new organic N-donor ligand, $(C_{24}H_{20}N_6)(H_2O)_2$, (I).

Compound (I) is composed of *L* and solvent water molecules, in a 1:2 ratio: the main molecule lies onto a symmetry centre, thus rendering only half of it independent (Fig. 1). Interatomic bond distances and angles are normal. The *L* ligands are hydrogen bonded to the water molecules *via* O—H···N interactions, forming a two-dimensional supramolecular structure parallel to (100). (Table 1 andFig. 2).

Experimental

A mixture of 2-(2-pyridyl)imidazole (7.25 g, 50 mmol) and NaOH (2.00 g, 50 mmol) in DMSO (20 ml) was stirred at 60°C for 1 h, then 1,4-bis(chloromethyl)benzene (4.35 g, 25 mmol) was added. The mixture was cooled to room temperature after stirring at 60°C for 24 h, and then poured into 200 ml of water. A yellow solid of *L* formed immediately, which was isolated by filtration in 80% yield after drying in air. Crystals suitable for X-ray diffraction were recrystallized in 95% ethanol.

Refinement

All H atoms on C atoms were poisitioned geometrically and refined as riding atoms, with C—H = 0.93 − 0.97 Å, and U_{iso}=1.2U_{eq} (C). The H atoms of water molecule were located in a difference Fourier map and then refined isotropically.

Figures

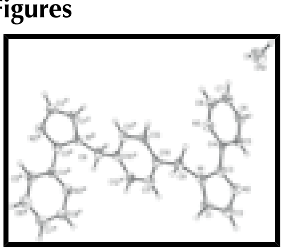

Fig. 1. A view of the molecule of (I). Displacement ellipsoids are drawn at the 30% probability level. Symmetry code: (iii) $1 - x, -y, -z$.

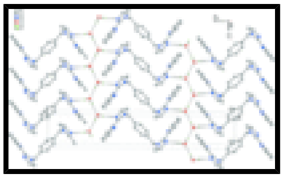

Fig. 2. Ball-stick representation of the two-dimensional supramolecular layer of (I).

1,4-Bis{[2-(pyridin-2-yl)-1*H*-imidazol-1-yl]methyl}benzene dihydrate

Crystal data

$C_{24}H_{20}N_6 \cdot 2H_2O$	$Z = 2$
$M_r = 428.49$	$F_{000} = 452$
Monoclinic, $P2_1/c$	$D_x = 1.328$ Mg m^{-3}
Hall symbol: -P2ybc	Mo $K\alpha$ radiation $\lambda = 0.71069$ Å
$a = 7.503$ (2) Å	$\theta = 1.4$–28.3°
$b = 28.450$ (2) Å	$\mu = 0.09$ mm^{-1}
$c = 5.030$ (4) Å	$T = 293$ (2) K
$\beta = 93.572$ (2)°	Block, colorless
$V = 1071.6$ (9) Å^3	0.40 × 0.38 × 0.36 mm

Data collection

Bruker APEX CCD area-detector diffractometer	2513 independent reflections
Radiation source: fine-focus sealed tube	1417 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.033$
$T = 293(2)$ K	$\theta_{max} = 28.3$°
ω scans	$\theta_{min} = 1.4$°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 7$
$T_{min} = 0.96$, $T_{max} = 0.97$	$k = -21 \rightarrow 37$
6504 measured reflections	$l = -5 \rightarrow 6$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.040$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.098$	$w = 1/[\sigma^2(F_o^2) + (0.045P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{max} < 0.001$
2513 reflections	$\Delta\rho_{max} = 0.15$ e Å^{-3}
151 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
3 restraints	Extinction correction: none

Primary atom site location: structure-invariant direct methods

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.9173 (2)	0.07266 (5)	0.5679 (3)	0.0547 (4)
H1	0.9156	0.0497	0.6992	0.066*
C2	1.0601 (2)	0.09773 (5)	0.4992 (3)	0.0576 (4)
H2	1.1749	0.0946	0.5781	0.069*
C3	0.83834 (18)	0.12158 (4)	0.2435 (2)	0.0419 (3)
C4	0.73301 (18)	0.14836 (4)	0.0402 (3)	0.0421 (3)
C5	0.81846 (19)	0.17646 (5)	−0.1371 (3)	0.0491 (4)
H5	0.9425	0.1781	−0.1297	0.059*
C6	0.7186 (2)	0.20188 (5)	−0.3232 (3)	0.0605 (4)
H6	0.7740	0.2207	−0.4447	0.073*
C7	0.5358 (2)	0.19924 (6)	−0.3287 (3)	0.0656 (5)
H7	0.4648	0.2164	−0.4518	0.079*
C8	0.4610 (2)	0.17053 (6)	−0.1468 (3)	0.0659 (5)
H8	0.3371	0.1687	−0.1511	0.079*
C9	0.59462 (18)	0.06872 (5)	0.4145 (3)	0.0500 (4)
H9A	0.5098	0.0945	0.4002	0.060*
H9B	0.5829	0.0536	0.5854	0.060*
C10	0.54828 (18)	0.03374 (4)	0.1959 (2)	0.0421 (3)
C11	0.66866 (18)	0.00005 (5)	0.1222 (3)	0.0486 (4)
H11	0.7837	−0.0002	0.2025	0.058*
C12	0.37921 (18)	0.03328 (5)	0.0689 (3)	0.0487 (4)
H12	0.2963	0.0558	0.1130	0.058*
N1	0.77573 (15)	0.08776 (4)	0.4063 (2)	0.0446 (3)
N2	1.01221 (15)	0.12840 (4)	0.2967 (2)	0.0514 (3)
N3	0.55510 (16)	0.14497 (4)	0.0368 (2)	0.0560 (3)
O1W	0.13387 (17)	0.27264 (4)	0.8409 (2)	0.0716 (3)
H1A	0.129 (2)	0.2590 (5)	0.685 (2)	0.107*
H1B	0.109 (2)	0.3018 (3)	0.811 (3)	0.107*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0708 (10)	0.0442 (8)	0.0481 (8)	0.0043 (8)	−0.0036 (8)	0.0046 (7)
C2	0.0562 (10)	0.0551 (9)	0.0599 (10)	0.0098 (8)	−0.0072 (8)	−0.0016 (8)
C3	0.0491 (9)	0.0356 (7)	0.0415 (7)	−0.0039 (6)	0.0051 (6)	−0.0037 (6)
C4	0.0503 (9)	0.0353 (7)	0.0406 (8)	−0.0004 (6)	0.0006 (6)	−0.0072 (6)
C5	0.0584 (9)	0.0443 (8)	0.0443 (8)	−0.0026 (7)	0.0017 (7)	−0.0010 (7)
C6	0.0864 (12)	0.0450 (9)	0.0495 (9)	0.0002 (8)	0.0002 (8)	0.0018 (7)
C7	0.0869 (13)	0.0510 (10)	0.0566 (10)	0.0121 (9)	−0.0148 (9)	−0.0015 (8)
C8	0.0549 (10)	0.0651 (11)	0.0757 (12)	0.0070 (8)	−0.0120 (8)	−0.0078 (10)
C9	0.0602 (9)	0.0452 (8)	0.0458 (8)	−0.0100 (7)	0.0121 (7)	−0.0021 (7)
C10	0.0519 (9)	0.0339 (7)	0.0413 (7)	−0.0065 (6)	0.0091 (6)	0.0023 (6)
C11	0.0487 (8)	0.0443 (8)	0.0526 (8)	−0.0032 (7)	0.0015 (7)	−0.0016 (7)
C12	0.0526 (9)	0.0404 (8)	0.0541 (9)	0.0018 (6)	0.0105 (7)	−0.0053 (7)
N1	0.0530 (7)	0.0379 (6)	0.0428 (6)	−0.0040 (5)	0.0019 (5)	−0.0016 (5)
N2	0.0487 (7)	0.0502 (7)	0.0549 (7)	−0.0010 (6)	0.0002 (6)	−0.0011 (6)
N3	0.0518 (8)	0.0544 (8)	0.0610 (8)	−0.0001 (6)	−0.0028 (6)	−0.0010 (6)
O1W	0.0977 (9)	0.0590 (7)	0.0571 (7)	0.0094 (7)	−0.0037 (6)	0.0049 (6)

Geometric parameters (Å, °)

C1—C2	1.3499 (19)	C7—H7	0.9300
C1—N1	1.3661 (17)	C8—N3	1.3411 (19)
C1—H1	0.9300	C8—H8	0.9300
C2—N2	1.3720 (18)	C9—N1	1.4658 (15)
C2—H2	0.9300	C9—C10	1.5074 (18)
C3—N2	1.3295 (16)	C9—H9A	0.9700
C3—N1	1.3657 (16)	C9—H9B	0.9700
C3—C4	1.4664 (19)	C10—C11	1.3834 (17)
C4—N3	1.3373 (16)	C10—C12	1.3844 (19)
C4—C5	1.3844 (18)	C11—C12^{i}	1.3815 (18)
C5—C6	1.3690 (19)	C11—H11	0.9300
C5—H5	0.9300	C12—C11^{i}	1.3815 (18)
C6—C7	1.372 (2)	C12—H12	0.9300
C6—H6	0.9300	O1W—H1A	0.873 (9)
C7—C8	1.372 (2)	O1W—H1B	0.860 (9)
C2—C1—N1	106.35 (13)	C7—C8—H8	117.9
C2—C1—H1	126.8	N1—C9—C10	113.30 (10)
N1—C1—H1	126.8	N1—C9—H9A	108.9
C1—C2—N2	110.54 (13)	C10—C9—H9A	108.9
C1—C2—H2	124.7	N1—C9—H9B	108.9
N2—C2—H2	124.7	C10—C9—H9B	108.9
N2—C3—N1	110.61 (12)	H9A—C9—H9B	107.7
N2—C3—C4	122.95 (12)	C11—C10—C12	117.67 (12)
N1—C3—C4	126.42 (12)	C11—C10—C9	121.88 (12)
N3—C4—C5	122.37 (13)	C12—C10—C9	120.40 (12)

N3—C4—C3	117.75 (12)	C12^{i}—C11—C10	121.08 (13)
C5—C4—C3	119.88 (12)	C12^{i}—C11—H11	119.5
C6—C5—C4	119.33 (14)	C10—C11—H11	119.5
C6—C5—H5	120.3	C11^{i}—C12—C10	121.24 (13)
C4—C5—H5	120.3	C11^{i}—C12—H12	119.4
C5—C6—C7	119.26 (15)	C10—C12—H12	119.4
C5—C6—H6	120.4	C3—N1—C1	107.13 (12)
C7—C6—H6	120.4	C3—N1—C9	129.14 (11)
C6—C7—C8	117.97 (14)	C1—N1—C9	123.72 (12)
C6—C7—H7	121.0	C3—N2—C2	105.36 (12)
C8—C7—H7	121.0	C4—N3—C8	116.85 (13)
N3—C8—C7	124.23 (15)	H1A—O1W—H1B	105.9 (12)
N3—C8—H8	117.9		

N1—C1—C2—N2	−0.12 (16)	C9—C10—C12—C11^{i}	−176.60 (12)
N2—C3—C4—N3	−167.83 (12)	N2—C3—N1—C1	−0.22 (14)
N1—C3—C4—N3	10.66 (19)	C4—C3—N1—C1	−178.86 (12)
N2—C3—C4—C5	11.21 (19)	N2—C3—N1—C9	−179.02 (11)
N1—C3—C4—C5	−170.30 (12)	C4—C3—N1—C9	2.3 (2)
N3—C4—C5—C6	0.0 (2)	C2—C1—N1—C3	0.20 (15)
C3—C4—C5—C6	−178.95 (12)	C2—C1—N1—C9	179.08 (11)
C4—C5—C6—C7	0.5 (2)	C10—C9—N1—C3	77.88 (17)
C5—C6—C7—C8	−0.7 (2)	C10—C9—N1—C1	−100.74 (15)
C6—C7—C8—N3	0.3 (2)	N1—C3—N2—C2	0.14 (14)
N1—C9—C10—C11	41.69 (17)	C4—C3—N2—C2	178.84 (12)
N1—C9—C10—C12	−140.92 (12)	C1—C2—N2—C3	−0.01 (16)
C12—C10—C11—C12^{i}	−0.9 (2)	C5—C4—N3—C8	−0.45 (19)
C9—C10—C11—C12^{i}	176.56 (12)	C3—C4—N3—C8	178.56 (12)
C11—C10—C12—C11^{i}	0.9 (2)	C7—C8—N3—C4	0.3 (2)

Symmetry codes: (i) −*x*+1, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1B···N2^{ii}	0.860 (9)	2.115 (9)	2.9636 (16)	168.7 (17)
O1W—H1A···O1W^{iii}	0.873 (9)	1.955 (9)	2.8258 (19)	176.4 (18)

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

Fig. 1

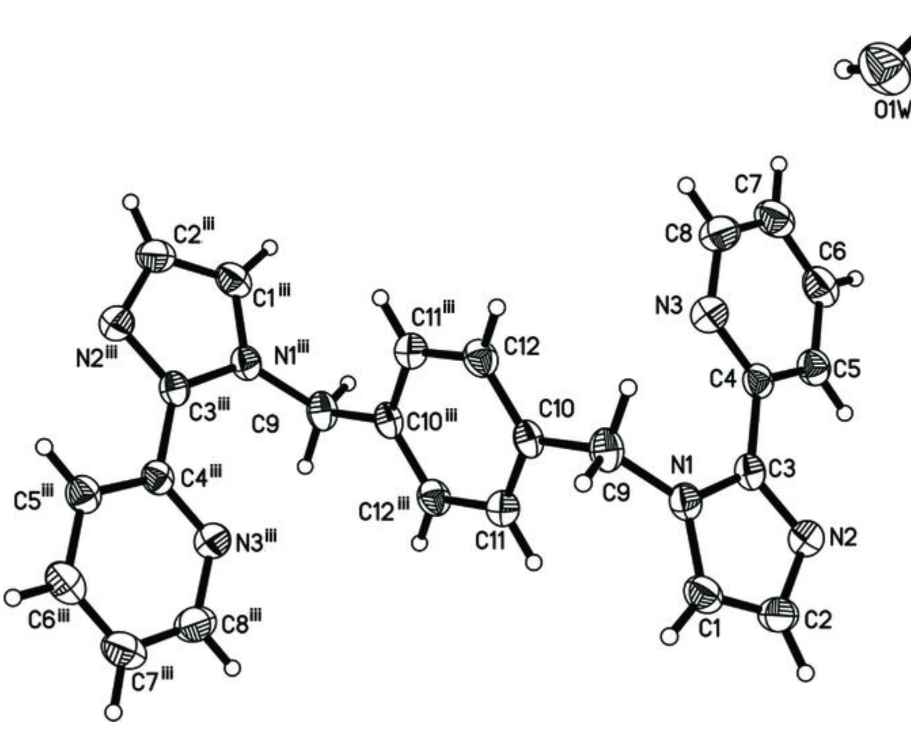
O1W
C7
C8
C6
N3
C2iii
C1iii
C11iii
C12
N2iii
N1iii
C4
C5
C10
C3iii
C9
C10iii
C4iii
C9
N1
C3
C5iii
C12iii
C11
N3iii
N2
C6iii
C8iii
C1
C2
C7iii

Fig. 2