

# 1,1'-(Butane-1,4-diyl)di-1*H*-imidazole-benzene-1,3,5-triol-water (1/1/1)

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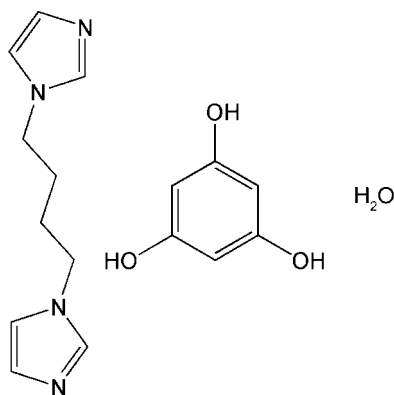
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Key indicators: single-crystal X-ray study;  $T = 291$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.057;  $wR$  factor = 0.195; data-to-parameter ratio = 17.8.

The asymmetric unit of the title compound,  $\text{C}_{10}\text{H}_{14}\text{N}_4 \cdot \text{C}_6\text{H}_6\text{O}_3 \cdot \text{H}_2\text{O}$ , contains one molecule of benzene-1,3,5-triol, two half-molecules of 1,1'-butane-1,4-diyl-di-1*H*-imidazole (each molecule is centrosymmetric) and one solvent water molecule. In the crystal structure, intermolecular  $\text{O}-\text{H} \cdots \text{O}$  and  $\text{O}-\text{H} \cdots \text{N}$  hydrogen bonds link all molecules into a three-dimensional supramolecular network.

## Related literature

For background and details of the synthesis of 1,1'-(1,4-butanediyl)diimidazole, see: Ma *et al.* (2003). For the related crystal structure of 1,1'-(1,4-butanediyl)diimidazole, see: Yu *et al.* (2008).



## Experimental

### Crystal data

$\text{C}_{10}\text{H}_{14}\text{N}_4 \cdot \text{C}_6\text{H}_6\text{O}_3 \cdot \text{H}_2\text{O}$   
 $M_r = 334.38$   
Triclinic,  $P\bar{1}$   
 $a = 7.964$  (5) Å  
 $b = 8.405$  (7) Å  
 $c = 14.800$  (9) Å  
 $\alpha = 98.40$  (3)°  
 $\beta = 92.93$  (2)°

$\gamma = 117.47$  (3)°  
 $V = 861.5$  (10) Å<sup>3</sup>  
 $Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 291$  (2) K  
 $0.31 \times 0.31 \times 0.19$  mm

### Data collection

Rigaku R-AXIS RAPID diffractometer  
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)  
 $T_{\min} = 0.971$ ,  $T_{\max} = 0.982$

8527 measured reflections  
3911 independent reflections  
2370 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.028$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$   
 $wR(F^2) = 0.195$   
 $S = 1.05$   
3911 reflections

220 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.20$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.27$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O4}-\text{H22} \cdots \text{O2}$	0.85	1.94	2.789 (3)	176
$\text{O4}-\text{H21} \cdots \text{O1}^{\text{i}}$	0.85	2.02	2.751 (3)	143
$\text{O3}-\text{H2} \cdots \text{O4}^{\text{ii}}$	0.82	1.84	2.658 (3)	173
$\text{O2}-\text{H6} \cdots \text{N2}^{\text{iii}}$	0.82	1.84	2.636 (3)	164
$\text{O1}-\text{H4} \cdots \text{N4}^{\text{iv}}$	0.82	1.79	2.596 (3)	170

Symmetry codes: (i)  $x, y + 1, z$ ; (ii)  $x - 1, y - 1, z$ ; (iii)  $-x + 2, -y + 1, -z + 1$ ; (iv)  $x, y - 1, z$ .

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: CV2422).

## References

- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.  
Ma, J.-F., Yang, J., Zheng, G.-L. & Liu, J.-F. (2003). *Inorg. Chem.* **42**, 7531–7534.  
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.  
Rigaku/MS (2002). *CrystalStructure*. Rigaku/MS Inc., The Woodlands, Texas, USA.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
Yu, Y.-H., Shi, A.-E., Su, Y., Hou, G.-F. & Gao, J.-S. (2008). *Acta Cryst.* **E64**, m628.

**supplementary materials**

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## 1,1'-(Butane-1,4-diyl)di-1*H*-imidazole-benzene-1,3,5-triol-water (1/1/1)

J.-S. Gao, Y.-H. Yu and G.-F. Hou

### Comment

The 1,1'-(1,4-butanediyl)diimidazole can be used as a flexible ligand to construct coordination polymer materials (Ma *et al.*, 2003; Yu *et al.*, 2008). In this paper, we report the new title compound, (I), synthesized by the reaction of 1,1'-(1,4-butanediyl)diimidazole and *m*-trihydroxybenzene in an methanol solution.

The asymmetric unit of the title compound, C<sub>10</sub>H<sub>14</sub>N<sub>4</sub>.C<sub>6</sub>H<sub>6</sub>O<sub>3</sub>.H<sub>2</sub>O, contains one molecule of benzene-1,3,5-triol, two halves of two independent centrosymmetric molecules of 1,1'-butane-1,4-diyl-di-1*H*-imidazole and one crystalline water molecule (Figure 1). The two 1,1'-(1,4-butanediyl)diimidazole molecules both lie on inversion center.

There are five symmetry independent 'active' H atoms in the crystal structure; all of them participate in hydrogen bonds, which link the 1,1'-(1,4-butanediyl)diimidazole molecules, *m*-trihydroxybenzene molecule and water solvent molecule into an infinite three-dimensional network (Table 1, Figure 2).

### Experimental

1,1'-(1,4-Butanediyl)diimidazole was prepared from imidazole and 1,4-dibromobutane in dimethylsulfoxide solution (Ma *et al.*, 2003). *m*-trihydroxybenzene (0.126 g, 1 mmol) and 1,1'-(1,4-butanediyl)diimidazole (0.380 g, 2 mmol) were dissolved in hot methanol solution (15 ml) then a clear solution was obtained. The resulting solution was allowed to stand in a desiccator at room temperature for several days. Red crystals of (I) were obtained.

### Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic); C—H = 0.97 Å (methylene) and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The hydroxy H atoms were placed in calculated positions and treated as riding on their parent atoms, with O—H = 0.82 Å and with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ . Water H atoms were initially located in a difference Fourier map, but they were treated as riding on their parent atoms with O—H = 0.85 Å and with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ .

## Figures

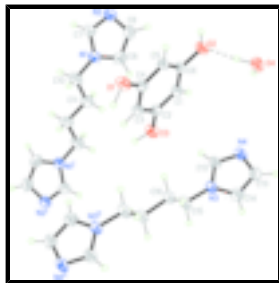


Fig. 1. A portion of the crystal structure of (I), showing the atomic numbering and 30% probability displacement ellipsoids [symmetry code: (I)  $-x, -y, -z + 1$ ; (II)  $-x, -y, -z$ ]. Dashed line indicates the hydrogen-bonding interaction.

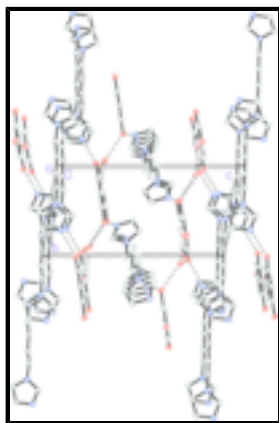


Fig. 2. A partial packing view, showing the three-dimensional hydrogen-bonding network. Dashed lines indicate the hydrogen-bonding interactions. H atoms have been omitted for clarity.

### 1,1'-(Butane-1,4-diyl)di-1*H*-imidazole-benzene-1,3,5-triol-water (1/1/1)

#### Crystal data

$C_{10}H_{14}N_4 \cdot C_6H_6O_3 \cdot H_2O$

$M_r = 334.38$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 7.964\ (5)\ \text{\AA}$

$b = 8.405\ (7)\ \text{\AA}$

$c = 14.800\ (9)\ \text{\AA}$

$\alpha = 98.40\ (3)^\circ$

$\beta = 92.93\ (2)^\circ$

$\gamma = 117.47\ (3)^\circ$

$V = 861.5\ (10)\ \text{\AA}^3$

$Z = 2$

$F_{000} = 356$

$D_x = 1.289\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 5362 reflections

$\theta = 3.1\text{--}27.6^\circ$

$\mu = 0.09\ \text{mm}^{-1}$

$T = 291\ (2)\ \text{K}$

Block, red

$0.31 \times 0.31 \times 0.19\ \text{mm}$

#### Data collection

Rigaku R-Axis RAPID  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 291\ (2)\ \text{K}$

3911 independent reflections

2370 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.028$

$\theta_{\text{max}} = 27.5^\circ$

$\omega$ scans	$\theta_{\min} = 3.1^\circ$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -10 \rightarrow 10$
$T_{\min} = 0.971$ , $T_{\max} = 0.982$	$k = -10 \rightarrow 10$
8527 measured reflections	$l = -18 \rightarrow 19$

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.057$	H-atom parameters constrained
$wR(F^2) = 0.195$	$w = 1/[\sigma^2(F_o^2) + (0.1078P)^2 + 0.0441P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
3911 reflections	$(\Delta/\sigma)_{\max} < 0.001$
220 parameters	$\Delta\rho_{\max} = 0.20 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.27 \text{ e } \text{\AA}^{-3}$
	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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6082 (3)	0.4322 (3)	0.27525 (15)	0.0495 (5)
H1	0.5935	0.5359	0.2907	0.059*
C2	0.4512 (3)	0.2634 (3)	0.24735 (14)	0.0463 (5)
C3	0.4707 (3)	0.1074 (3)	0.22121 (14)	0.0440 (5)
H3	0.3639	-0.0060	0.2009	0.053*
C4	0.6534 (3)	0.1248 (3)	0.22616 (14)	0.0431 (5)
C5	0.8124 (3)	0.2923 (3)	0.25642 (14)	0.0445 (5)
H5	0.9340	0.3024	0.2609	0.053*
C6	0.7880 (3)	0.4458 (3)	0.28012 (14)	0.0461 (5)
C7	0.5669 (4)	0.2164 (4)	0.62310 (17)	0.0599 (6)
H7	0.5388	0.1550	0.6722	0.072*
C8	0.7113 (4)	0.4008 (4)	0.5372 (2)	0.0807 (9)
H8	0.8061	0.4952	0.5144	0.097*

## supplementary materials

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C9	0.5333 (4)	0.2938 (5)	0.4948 (2)	0.0814 (9)
H9	0.4827	0.2997	0.4381	0.098*
C10	0.2441 (4)	0.0249 (4)	0.5326 (2)	0.0770 (8)
H10	0.2144	-0.0270	0.5878	0.092*
H11	0.2360	-0.0698	0.4837	0.092*
C11	0.0998 (3)	0.0796 (4)	0.50659 (19)	0.0655 (7)
H12	0.1248	0.1263	0.4498	0.079*
H13	0.1094	0.1768	0.5543	0.079*
C12	0.2720 (3)	0.5418 (3)	0.10952 (16)	0.0561 (6)
H16	0.2520	0.5172	0.1684	0.067*
C13	0.3851 (4)	0.6740 (4)	-0.00145 (17)	0.0606 (6)
H14	0.4595	0.7618	-0.0344	0.073*
C14	0.2445 (4)	0.5074 (4)	-0.03878 (17)	0.0613 (6)
H15	0.2052	0.4582	-0.1013	0.074*
C15	0.0159 (3)	0.2379 (3)	0.02391 (18)	0.0572 (6)
H17	-0.0806	0.2134	-0.0265	0.069*
H18	-0.0429	0.2277	0.0801	0.069*
C16	0.0830 (3)	0.0959 (3)	0.00706 (15)	0.0502 (6)
H19	0.1731	0.1147	0.0593	0.060*
H20	0.1485	0.1102	-0.0471	0.060*
N1	0.4412 (3)	0.1758 (3)	0.54990 (13)	0.0574 (5)
N2	0.7338 (3)	0.3514 (3)	0.61894 (15)	0.0661 (6)
N3	0.1703 (3)	0.4238 (2)	0.03210 (12)	0.0497 (5)
N4	0.4031 (3)	0.6959 (3)	0.09239 (14)	0.0573 (5)
O1	0.6793 (2)	-0.0244 (2)	0.20167 (12)	0.0587 (5)
H4	0.5847	-0.1054	0.1677	0.088*
O2	0.9405 (2)	0.6159 (2)	0.30773 (14)	0.0675 (5)
H6	1.0348	0.6068	0.3247	0.101*
O3	0.2755 (2)	0.2535 (2)	0.24808 (13)	0.0643 (5)
H2	0.1939	0.1464	0.2426	0.096*
O4	0.9883 (2)	0.9172 (3)	0.23236 (15)	0.0838 (6)
H21	0.8952	0.9328	0.2485	0.101*
H22	0.9716	0.8225	0.2530	0.101*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0515 (13)	0.0396 (12)	0.0590 (13)	0.0239 (11)	0.0033 (10)	0.0078 (10)
C2	0.0425 (11)	0.0467 (13)	0.0518 (12)	0.0225 (10)	0.0043 (9)	0.0113 (9)
C3	0.0374 (10)	0.0401 (12)	0.0503 (11)	0.0165 (9)	-0.0001 (9)	0.0055 (9)
C4	0.0432 (11)	0.0403 (12)	0.0464 (11)	0.0210 (10)	0.0037 (9)	0.0067 (9)
C5	0.0380 (11)	0.0443 (13)	0.0502 (11)	0.0192 (10)	0.0014 (9)	0.0090 (9)
C6	0.0416 (11)	0.0352 (12)	0.0532 (12)	0.0118 (10)	0.0007 (9)	0.0086 (9)
C7	0.0559 (14)	0.0609 (16)	0.0589 (14)	0.0246 (13)	0.0035 (11)	0.0120 (12)
C8	0.0605 (17)	0.069 (2)	0.117 (2)	0.0253 (16)	0.0187 (17)	0.0479 (18)
C9	0.074 (2)	0.096 (2)	0.0739 (17)	0.0352 (19)	0.0028 (15)	0.0350 (16)
C10	0.0540 (16)	0.0608 (18)	0.104 (2)	0.0216 (14)	-0.0041 (15)	0.0053 (15)
C11	0.0538 (14)	0.0644 (17)	0.0701 (15)	0.0261 (13)	-0.0046 (12)	0.0007 (13)

C12	0.0588 (14)	0.0445 (14)	0.0537 (13)	0.0177 (12)	0.0049 (11)	0.0011 (10)
C13	0.0570 (14)	0.0543 (16)	0.0706 (16)	0.0231 (13)	0.0136 (12)	0.0216 (12)
C14	0.0626 (15)	0.0632 (17)	0.0537 (13)	0.0266 (14)	0.0070 (12)	0.0095 (12)
C15	0.0451 (12)	0.0400 (13)	0.0717 (15)	0.0117 (10)	0.0073 (11)	-0.0024 (11)
C16	0.0418 (12)	0.0415 (13)	0.0559 (12)	0.0134 (10)	0.0030 (10)	0.0000 (10)
N1	0.0483 (11)	0.0548 (13)	0.0616 (12)	0.0200 (10)	-0.0006 (9)	0.0080 (10)
N2	0.0545 (13)	0.0524 (13)	0.0832 (15)	0.0220 (11)	-0.0070 (11)	0.0064 (11)
N3	0.0477 (10)	0.0376 (11)	0.0563 (11)	0.0159 (9)	0.0070 (9)	0.0026 (8)
N4	0.0512 (11)	0.0358 (11)	0.0724 (13)	0.0131 (9)	0.0036 (10)	0.0020 (9)
O1	0.0444 (9)	0.0438 (9)	0.0818 (12)	0.0222 (8)	-0.0023 (8)	-0.0069 (8)
O2	0.0494 (10)	0.0371 (9)	0.1014 (13)	0.0126 (8)	-0.0109 (9)	0.0056 (9)
O3	0.0432 (9)	0.0548 (11)	0.0984 (13)	0.0274 (8)	0.0079 (9)	0.0107 (10)
O4	0.0461 (10)	0.0723 (14)	0.1375 (18)	0.0247 (10)	0.0120 (11)	0.0456 (12)

*Geometric parameters (Å, °)*

C1—C2	1.373 (3)	C11—C11 <sup>i</sup>	1.512 (5)
C1—C6	1.380 (3)	C11—H12	0.9700
C1—H1	0.9300	C11—H13	0.9700
C2—O3	1.364 (3)	C12—N4	1.306 (3)
C2—C3	1.392 (3)	C12—N3	1.336 (3)
C3—C4	1.390 (3)	C12—H16	0.9300
C3—H3	0.9300	C13—C14	1.335 (4)
C4—O1	1.364 (3)	C13—N4	1.365 (3)
C4—C5	1.378 (3)	C13—H14	0.9300
C5—C6	1.390 (3)	C14—N3	1.356 (3)
C5—H5	0.9300	C14—H15	0.9300
C6—O2	1.365 (3)	C15—N3	1.458 (3)
C7—N2	1.302 (3)	C15—C16	1.512 (3)
C7—N1	1.326 (3)	C15—H17	0.9700
C7—H7	0.9300	C15—H18	0.9700
C8—C9	1.334 (4)	C16—C16 <sup>ii</sup>	1.516 (4)
C8—N2	1.364 (4)	C16—H19	0.9700
C8—H8	0.9300	C16—H20	0.9700
C9—N1	1.347 (4)	O1—H4	0.8200
C9—H9	0.9300	O2—H6	0.8200
C10—N1	1.471 (3)	O3—H2	0.8200
C10—C11	1.475 (4)	O4—H21	0.8501
C10—H10	0.9700	O4—H22	0.8500
C10—H11	0.9700		
C2—C1—C6	119.1 (2)	C10—C11—H13	109.4
C2—C1—H1	120.4	C11 <sup>i</sup> —C11—H13	109.4
C6—C1—H1	120.4	H12—C11—H13	108.0
O3—C2—C1	117.6 (2)	N4—C12—N3	111.8 (2)
O3—C2—C3	121.2 (2)	N4—C12—H16	124.1
C1—C2—C3	121.2 (2)	N3—C12—H16	124.1
C4—C3—C2	118.5 (2)	C14—C13—N4	109.7 (2)
C4—C3—H3	120.7	C14—C13—H14	125.1

## supplementary materials

C2—C3—H3	120.7	N4—C13—H14	125.1
O1—C4—C5	118.36 (19)	C13—C14—N3	106.8 (2)
O1—C4—C3	120.58 (19)	C13—C14—H15	126.6
C5—C4—C3	121.07 (19)	N3—C14—H15	126.6
C4—C5—C6	118.88 (19)	N3—C15—C16	112.84 (19)
C4—C5—H5	120.6	N3—C15—H17	109.0
C6—C5—H5	120.6	C16—C15—H17	109.0
O2—C6—C1	117.4 (2)	N3—C15—H18	109.0
O2—C6—C5	121.5 (2)	C16—C15—H18	109.0
C1—C6—C5	121.1 (2)	H17—C15—H18	107.8
N2—C7—N1	112.9 (2)	C15—C16—C16 <sup>ii</sup>	111.3 (2)
N2—C7—H7	123.6	C15—C16—H19	109.4
N1—C7—H7	123.6	C16 <sup>ii</sup> —C16—H19	109.4
C9—C8—N2	110.0 (3)	C15—C16—H20	109.4
C9—C8—H8	125.0	C16 <sup>ii</sup> —C16—H20	109.4
N2—C8—H8	125.0	H19—C16—H20	108.0
C8—C9—N1	106.8 (3)	C7—N1—C9	106.2 (2)
C8—C9—H9	126.6	C7—N1—C10	125.6 (2)
N1—C9—H9	126.6	C9—N1—C10	128.2 (2)
N1—C10—C11	113.9 (2)	C7—N2—C8	104.1 (2)
N1—C10—H10	108.8	C12—N3—C14	106.6 (2)
C11—C10—H10	108.8	C12—N3—C15	127.4 (2)
N1—C10—H11	108.8	C14—N3—C15	126.0 (2)
C11—C10—H11	108.8	C12—N4—C13	105.2 (2)
H10—C10—H11	107.7	C4—O1—H4	109.5
C10—C11—C11 <sup>i</sup>	111.3 (3)	C6—O2—H6	109.5
C10—C11—H12	109.4	C2—O3—H2	109.5
C11 <sup>i</sup> —C11—H12	109.4	H21—O4—H22	102.9

Symmetry codes: (i)  $-x, -y, -z+1$ ; (ii)  $-x, -y, -z$ .

### Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H22 $\cdots$ O2	0.85	1.94	2.789 (3)	176
O4—H21 $\cdots$ O1 <sup>iii</sup>	0.85	2.02	2.751 (3)	143
O3—H2 $\cdots$ O4 <sup>iv</sup>	0.82	1.84	2.658 (3)	173
O2—H6 $\cdots$ N2 <sup>v</sup>	0.82	1.84	2.636 (3)	164
O1—H4 $\cdots$ N4 <sup>vi</sup>	0.82	1.79	2.596 (3)	170

Symmetry codes: (iii)  $x, y+1, z$ ; (iv)  $x-1, y-1, z$ ; (v)  $-x+2, -y+1, -z+1$ ; (vi)  $x, y-1, z$ .



Fig. 1

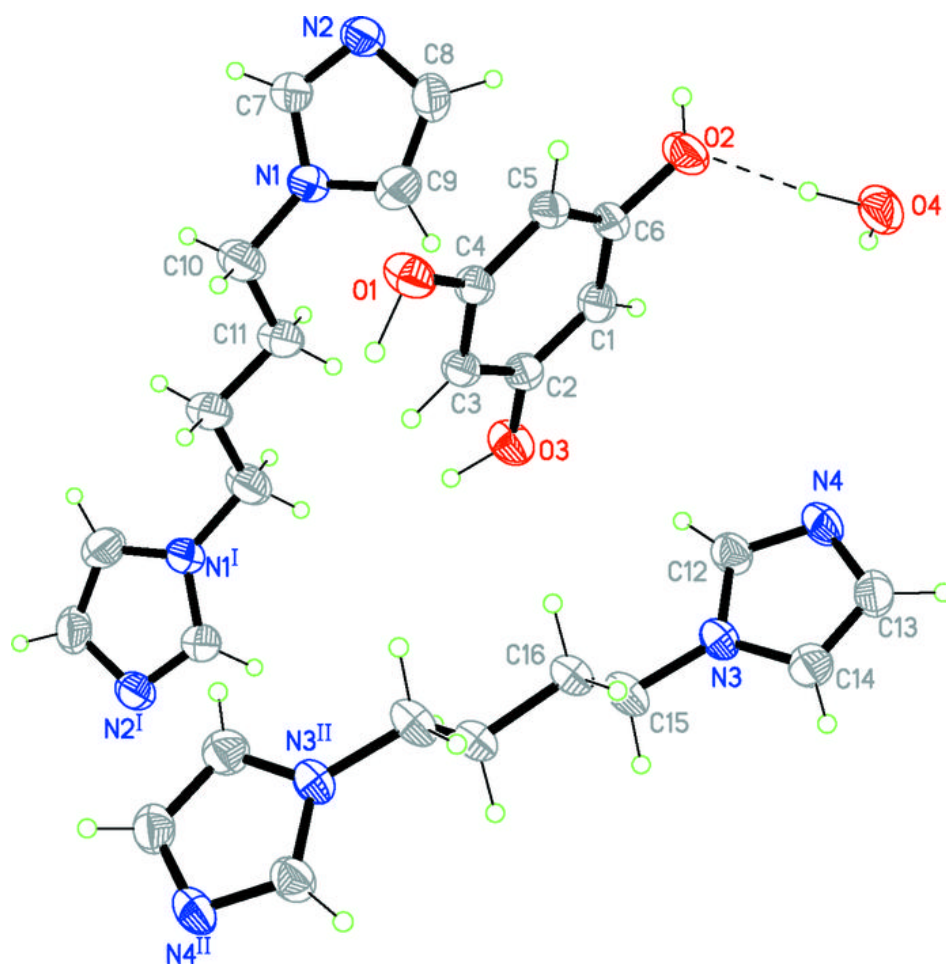


Fig. 2

