

## 3,3'-(1,4-Naphthalenedimethylene)bis(1-methylimidazolium) diiodide monohydrate

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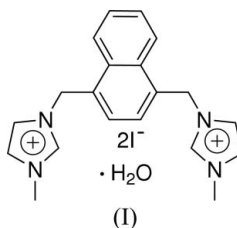
## Key indicators

Single-crystal X-ray study  
 $T = 292$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å  
 $R$  factor = 0.032  
 $wR$  factor = 0.083  
Data-to-parameter ratio = 15.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title compound,  $\text{C}_{20}\text{H}_{22}\text{N}_4^{2+} \cdot 2\text{I}^- \cdot \text{H}_2\text{O}$ , the two imidazolium rings are twisted away from the central naphthalene plane by  $76.6$  (1) and  $74.5$  (1)°. The crystal packing is stabilized by  $\text{O}-\text{H} \cdots \text{I}$ ,  $\text{C}-\text{H} \cdots \text{O}$  and  $\text{C}-\text{H} \cdots \text{I}$  hydrogen bonds.

## Comment

Numerous flexible or rigid *N*-heterocyclic carbene precursors have been synthesized and studied. They attract considerable attention because of their diverse coordination capabilities and the important catalytic properties of their metal complexes (Herrmann, 2002; Herrmann & Kocher, 1997). We report here the crystal structure of the title compound, (I).



Bond lengths and angles in (I) are normal (Table 1). The naphthalene ring system is planar, with a maximum deviation of  $0.022$  (4) Å for C9. The dihedral angle between the N1/C12/N2/C13/C14 and C1–C10 planes is  $76.6$  (1)° and that between the N3/C17/N4/C18/C19 and C1–C10 planes is  $74.5$  (1)°. The dihedral angle between the two imidazolium rings is  $6.6$  (4)°. In the crystal structure, the water molecule and iodide ions are involved in  $\text{O}-\text{H} \cdots \text{I}$  hydrogen bonds (Fig. 1). In addition, the crystal packing is stabilized by  $\text{C}-\text{H} \cdots \text{O}$  and  $\text{C}-\text{H} \cdots \text{I}$  hydrogen bonds.

## Experimental

Compound (I) was synthesized by the reaction of 1,4-bis-(imidazolymethyl)naphthalene with iodomethane in dichloromethane at room temperature, according to the reported procedure of Baker *et al.* (2001). Yellow single crystals of (I) were obtained by recrystallization from methanol and diethyl ether.

## Crystal data

 $\text{C}_{20}\text{H}_{22}\text{N}_4^{2+} \cdot 2\text{I}^- \cdot \text{H}_2\text{O}$   
 $M_r = 590.23$   
Triclinic,  $P\bar{1}$   
 $a = 8.563$  (3) Å  
 $b = 9.572$  (3) Å  
 $c = 14.684$  (6) Å  
 $\alpha = 102.97$  (3)°  
 $\beta = 103.66$  (3)°  
 $\gamma = 98.24$  (3)°  
 $V = 1114.9$  (7) Å<sup>3</sup> $Z = 2$   
 $D_x = 1.758$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
Cell parameters from 18 reflections  
 $\theta = 4.4-7.4$ °  
 $\mu = 2.84$  mm<sup>-1</sup>  
 $T = 292$  (2) K  
Block, yellow  
 $0.25 \times 0.15 \times 0.08$  mm

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## Data collection

Enraf–Nonius CAD-4  
diffractometer  
 $\omega/2\theta$  scans  
Absorption correction:  $\psi$  scan  
(North *et al.*, 1968)  
 $T_{\min} = 0.583$ ,  $T_{\max} = 0.797$   
3927 measured reflections  
3900 independent reflections  
2850 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.016$   
 $\theta_{\text{max}} = 25.0^\circ$   
 $h = -10 \rightarrow 9$   
 $k = -2 \rightarrow 11$   
 $l = -17 \rightarrow 17$   
3 standard reflections  
every 300 reflections  
intensity decay: 2.1%

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.032$   
 $wR(F^2) = 0.083$   
 $S = 1.00$   
3900 reflections  
254 parameters

H-atom parameters treated by a  
mixture of independent and  
constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.48 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.51 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

N1—C12	1.324 (5)	N3—C19	1.366 (5)
N1—C14	1.381 (6)	N3—C16	1.483 (5)
N1—C11	1.462 (5)	N4—C17	1.325 (5)
N2—C12	1.313 (5)	N4—C18	1.370 (5)
N2—C13	1.361 (6)	N4—C20	1.468 (6)
N2—C15	1.475 (5)	C4—C16	1.510 (6)
N3—C17	1.314 (5)		
N1—C11—C1	114.7 (3)	N3—C16—C4	111.6 (3)

Table 2

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W $\cdots$ I2	0.85 (4)	2.76 (4)	3.578 (6)	164 (6)
O1W—H2W $\cdots$ I1	0.85 (9)	2.87 (9)	3.649 (7)	154 (6)
C17—H17 $\cdots$ I2 <sup>i</sup>	0.93	2.90	3.799 (5)	162
C18—H18 $\cdots$ O1W <sup>ii</sup>	0.93	2.52	3.327 (8)	145
C19—H19 $\cdots$ I2 <sup>ii</sup>	0.93	2.93	3.830 (4)	163

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

The H atoms of the water molecule were located in a difference Fourier map and refined with O—H and H $\cdots$ H distance restraints of 0.84 (1) and 1.37 (2)  $\text{\AA}$ , respectively. All other H atoms were placed in calculated positions [C—H = 0.93–0.97  $\text{\AA}$ ], and included in the final cycles of refinement using a riding-model approximation, with  $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5U_{\text{eq}}(\text{carrier atom})$ .

Data collection: *DIFRAC* (Gabe & White, 1993); cell refinement: *DIFRAC*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s)

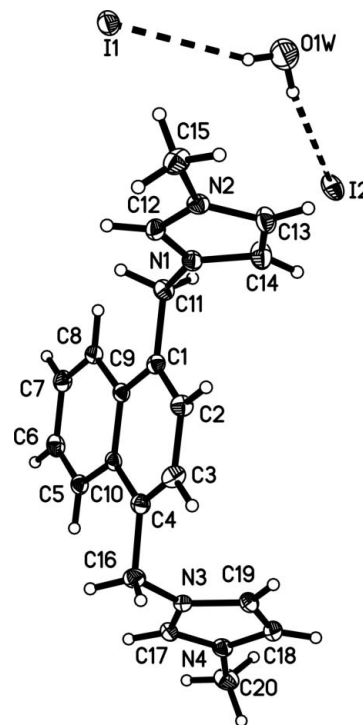


Figure 1

The structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering. Dashed lines indicate hydrogen bonds.

used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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