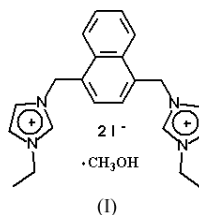


3,3'-(1,4-Naphthalenedimethylene)bis-(1-ethylimidazolium) diiodide methanol solvate**Ru-Yi Zou, Feng-Bo Xu,
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People's Republic of ChinaCorrespondence e-mail:
zzzhang@public.tpt.tj.cn**Key indicators**Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.015\text{ \AA}$
 R factor = 0.068
 wR factor = 0.184
Data-to-parameter ratio = 16.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The title compound, $\text{C}_{22}\text{H}_{26}\text{I}_2\text{N}_4$, (I), was synthesized by reaction of 1,4-bis(imidazolymethyl)naphthalene with iodoethane. The X-ray structure of (I) reveals the presence of discrete hydrogen-bond interactions and π - π -stacking interactions of naphthalene rings, resulting in a three-dimensional structure. A methanol solvent molecule is also found in the asymmetric unit.

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Numerous flexible or rigid *N*-heterocyclic carbene precursors have been synthesized and studied. They attract considerable attention due to their diverse coordination capabilities and the important catalysis properties of their metal complexes (Bourissou *et al.*, 2000; Herrmann, 2002; Herrmann & Kocher, 1997). In addition, the photophysical properties of these complexes have also been studied. For example, a luminescent silver(I) stair polymer has been reported by our group (Liu *et al.*, 2003), though this type of property has rarely been described. As a continuation of our systematic studies of the various *N*-heterocyclic carbene ligands and the photophysical properties of their polymeric metal complexes, a new bis-carbene precursor with the naphthyl fluorescence group, *viz.* 3,3'-(1,4-naphthalenedimethylene)bis(1-ethylimidazolium) diiodide methanol solvate, (I), has been synthesized.



As shown in Fig. 1, the 3,3'-(1,4-naphthalenedimethylene)-bis(1-ethylimidazolium) cation unit has two terminal ethyl-imidazolium groups bound in a *cis* arrangement, with their ring least-squares planes having a dihedral angle of $98.9(3)^\circ$. The dihedral angles between the central naphthalene plane and the two imidazolium groups are $100.0(8)$ and $86.0(7)^\circ$, respectively. A methanol solvent molecule is also found in the asymmetric unit.

Experimental

The title compound was synthesized by the reaction of 1,4-bis-(imidazolymethyl)naphthalene with iodoethane in dioxane at 373 K, according to a literature method (Baker *et al.*, 2001). Yellow single crystals of the title compound were obtained by recrystallization from methanol and diethyl ether (yield: 87%, m.p. 475–477 K). Analysis calculated for $\text{C}_{22}\text{H}_{26}\text{I}_2\text{N}_4$: C 44.02, H 4.37, N 9.33%; found: C 44.31,

H 4.46, N 8.98%. ^1H NMR (300 MHz, $\text{DMSO}-d_6$): δ 1.39 (*t*, 6H), 4.19(*m*, 4H), 5.96 (*s*, 4H), 7.53 (*s*, 2H), 7.71 (*m*, 2H), 7.78 (*s*, 2H), 7.84 (*s*, 2H), 8.22 (*m*, 2H), 9.31 (*s*, 2H).

Crystal data

$\text{C}_{22}\text{H}_{26}\text{N}_4^{2+}\cdot 2\text{I}^-\cdot \text{CH}_4\text{O}$
 $M_r = 632.31$
 Triclinic, $P\bar{1}$
 $a = 9.959$ (5) Å
 $b = 10.770$ (5) Å
 $c = 13.407$ (7) Å
 $\alpha = 98.340$ (11)°
 $\beta = 104.132$ (12)°
 $\gamma = 105.691$ (12)°
 $V = 1307.7$ (11) Å³

$Z = 2$
 $D_x = 1.606$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 715 reflections
 $\theta = 3.1\text{--}22.8^\circ$
 $\mu = 2.43$ mm⁻¹
 $T = 293$ (2) K
 Block, yellow
 $0.20 \times 0.18 \times 0.14$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.608$, $T_{\max} = 0.712$
 6446 measured reflections

4417 independent reflections
 2512 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.059$
 $\theta_{\text{max}} = 25.0^\circ$
 $h = -11 \rightarrow 11$
 $k = -12 \rightarrow 12$
 $l = -15 \rightarrow 8$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.068$
 $wR(F^2) = 0.184$
 $S = 0.95$
 4417 reflections
 276 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0555P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 1.73$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.75$ e Å⁻³

H atoms were included at idealized positions, constrained to ride on the atom to which they are bonded ($\text{C-H} = 0.95$ or 0.98 Å) and given displacement parameters equal to 1.2 or 1.5 times U_{eq} of the carrier atom.

Data collection: SMART (Bruker, 1998); cell refinement: SMART; data reduction: SAINT (Bruker, 1998); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.

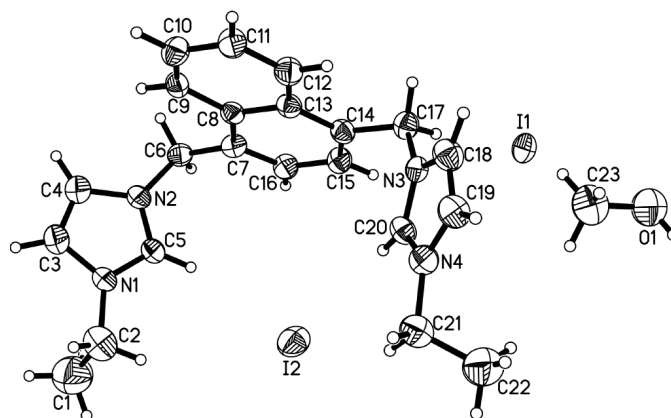


Figure 1
 View of the title compound, with displacement ellipsoids drawn at the 30% probability level.

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