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## Key indicators

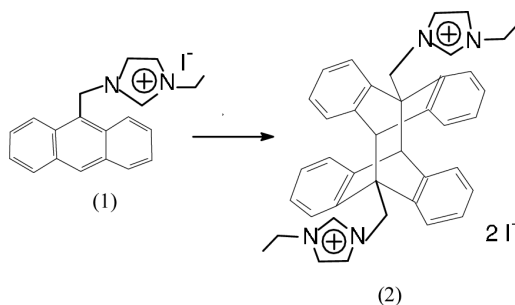
Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$   
 $R$  factor = 0.031  
 $wR$  factor = 0.069  
Data-to-parameter ratio = 13.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.The photodimer of 1-(anthracen-9-yl-  
methyl)-3-ethylimidazolium iodide

The title compound, 9,10'-bis(3-ethylimidazolium-1-ylmethyl)-9,9':10,10'-bianthracenyl diiodide, was obtained by the photodimerization of 1-(9-anthracenylmethyl)-3-ethylimidazolium iodide. The centrosymmetric crystal structure confirms that the compound is a head-to-tail dimer.

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## Comment

Many photodimers derived from substituted anthracenes in solution and in the solid state have been reported (Bouas-Laurent *et al.*, 2000). Considerable interest is now focused on the development of multifunctional spin systems with synergic properties. Successful studies have recently been carried out on photofunctional magnetic materials derived from some organic spin systems with photofunctionality (Matsuda *et al.*, 2001) and organomagnetic materials with a variety of properties have also been developed (Tyson *et al.*, 2002). The chromophoric system of anthracene is a promising system for investigating the change of magnetic properties in a spin system by the structural change produced upon irradiation. Photodimerizations of 9-substituted anthracenes in solution are efficient, usually giving rise to head-to-tail dimers (Becker & Langer, 1993).



We have synthesized the photodimer 9,10'-bis(3-ethylimidazolium-1-ylmethyl)-9,9':10,10'-bianthracenyl diiodide, (2), by intermolecular [4 + 4]-cycloaddition of 1-(9-anthracenylmethyl)-3-ethylimidazolium iodide. The centrosymmetric crystal structure confirms that the compound is a head-to-tail dimer. In (2), the bond lengths and angles of the imidazole ring are similar to those in 1-(9-anthracenylmethyl)-3-ethylimidazolium iodide dichloromethane solvate hydrate, (3) (Liu *et al.*, 2003). However, in (2), C4—C5 [1.541 (4) Å] is somewhat longer than that in (3) [1.483 (1) Å], perhaps due to larger steric hindrance in the former. In (2), C5—C12A is 1.636 (4) Å, similar to that in the bi(anthracene-9,10-dimethylene) photoisomer [1.644 (3) Å; Dougherty *et al.*, 1986]. The bond lengths and angles of the central six-membered ring in (2) are also similar to those in di-*para*-anthracene (Choi & Marinkas, 1980).

## Experimental

An acetonitrile solution (20 ml) of 1-(9-anthracenylmethyl)-3-ethylimidazolium iodide, (1) (0.400 g, 0.984 mmol), was exposed to sunlight for 10 d at room temperature, yielding a pale-yellow precipitate. The precipitate was filtered off and washed with diethyl ether to give a pale-yellow powder (0.120 g, yield 15%). Compound (2) is soluble in DMSO and insoluble in chloroform.  $^1\text{H}$  NMR (300 MHz, DMSO):  $\delta$  1.19 (*t*,  $J = 7.2$  Hz, 6H,  $\text{CH}_3$ ), 4.06 (*q*,  $J = 7.2$  Hz, 4H,  $\text{CH}_2$ ), 4.21 (*s*, 2H, CH), 5.74 (*s*, 4H,  $\text{CH}_2\text{An}$ ), 6.79 (*d*,  $J = 7.2$  Hz, 8H, AnH; An = anthracene), 6.75 and 7.49 (*s*, 4H, 4 or 5-imiH; imi = imidazole), 6.90 (*m*,  $J = 8.4$  Hz, 8H, AnH), 7.13 (*d*,  $J = 7.2$  Hz, 4H, AnH), 8.61 (*s*, 2H, 2-imiH).  $^{13}\text{C}$  NMR (75 MHz, DMSO):  $\delta$  15.7 ( $\text{CH}_2\text{CH}_3$ ), 44.3 ( $\text{NCH}_2\text{CH}_3$ ), 50.9 ( $\text{NCH}_2\text{An}$ ), 59.6 and 55.3 ( $\text{C}_{\text{quaternary}}$  or CH), 121.2, 123.7, 125.9, 126.3, 128.1, 136.7, 140.5, 141.8 (imiC or AnC); m.p. 512 K. Analysis calculated for  $\text{C}_{30}\text{H}_{24}$ : C 57.99, H 4.62, N 3.38%; found: C 57.52, H 4.92, N 3.78%.

### Crystal data

$\text{C}_{40}\text{H}_{38}\text{N}_4^{2+}\cdot 2\text{I}^-$   
 $M_r = 828.54$   
 Monoclinic,  $P2_1/c$   
 $a = 7.696$  (5) Å  
 $b = 21.230$  (13) Å  
 $c = 11.005$  (7) Å  
 $\beta = 106.404$  (10)°  
 $V = 1724.9$  (18) Å<sup>3</sup>  
 $Z = 2$

$D_x = 1.595$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 937 reflections  
 $\theta = 2.7\text{--}24.6^\circ$   
 $\mu = 1.86$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Prism, yellow  
 $0.48 \times 0.42 \times 0.24$  mm

### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\text{min}} = 0.449$ ,  $T_{\text{max}} = 0.640$   
 7030 measured reflections

2903 independent reflections  
 2215 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.030$   
 $\theta_{\text{max}} = 25.0^\circ$   
 $h = -6 \rightarrow 9$   
 $k = -25 \rightarrow 25$   
 $l = -7 \rightarrow 13$

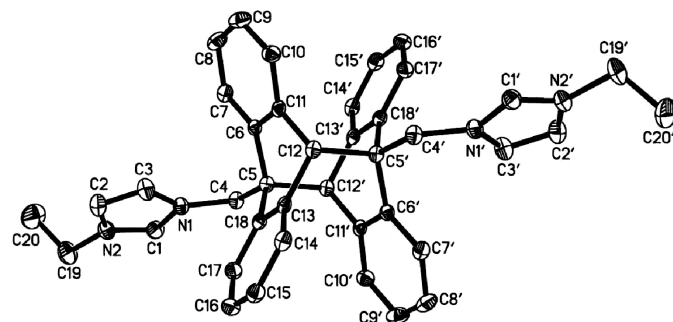
### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.031$   
 $wR(F^2) = 0.069$   
 $S = 1.02$   
 2903 reflections  
 210 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0239P)^2 + 1.4667P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.002$   
 $\Delta\rho_{\text{max}} = 0.47$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.63$  e Å<sup>-3</sup>  
 Extinction correction: SHELXL97  
 Extinction coefficient: 0.0041 (3)

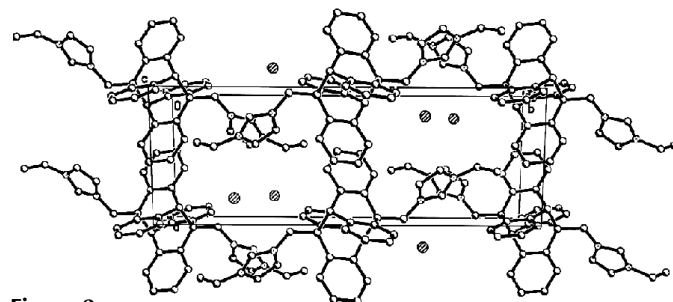
All H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry, with C—H distances of 0.96 Å and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ , but each group was allowed to rotate freely about its C—C bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances in the range 0.93–0.98 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: SMART (Bruker, 1998); cell refinement: SMART; data reduction: SAINT (Bruker, 1998); program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine



**Figure 1**

A view of (2), together with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted. Atoms marked with a prime (') are at the symmetry position ( $2 - x, 1 - y, -z$ ).



**Figure 2**

A view, down the  $c$  axis, of the packing arrangement in the crystal structure of (2). H atoms have been omitted.

structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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