Acta Crystallographica Section E
**Structure Reports**
**Online**

ISSN 1600-5368

# 2-[(2,6-Diisopropylphenyl)iminio]propyl bromide

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**Key indicators**

Single-crystal X-ray study
$T$ = 100 K
Mean $\sigma$(C–C) = 0.002 Å
$R$ factor = 0.023
$wR$ factor = 0.049
Data-to-parameter ratio = 22.5

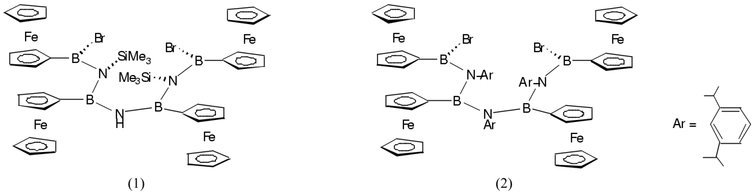
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title structure, $C_{15}H_{24}N^+\cdot Br^-$, there is an N—H···Br hydrogen bond [H···Br = 2.35 (2) Å] and several short C—H···Br contacts.

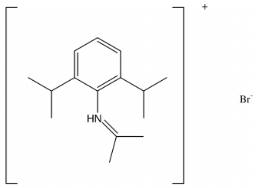
Received 9 July 2003
Accepted 16 July 2003
Online 24 July 2003

## Comment

Oligonuclear aggregates of organometallic compounds are currently attracting growing attention. Useful applications can be anticipated in the fields of magnetic and electronic materials (Henry, 1992). In this context, a variety of systems containing ferrocenyl moieties, *e.g.* the complex (1) (see Scheme below), have been synthesized (Ma *et al.*, 2002).



The properties of complex (2) are of particular interest to us, but in an attempt to crystallize complex (2), crystals of the title compound, (I), were grown from the reaction solution.



(I)

The geometric parameters of the title compound may be regarded as normal. The plane consisting of the iminium bond and the two attached methyl C atoms is nearly perpendicular to the phenyl ring; the two planes enclose an angle of 84.87 (5)°. As well as the N—H···Br hydrogen bond, there are several other short C—H···Br contacts (see Table 2).

## Experimental

Crystals of (I) were grown from a hexane solution of the products of reaction of dibromoferrocenylborane with 2,6-diisopropylaniline (yield 10%). The NMR spectra were recorded on a Bruker DPX 250 spectrometer. $^1$H NMR ($CDCl_3$, internal TMS): $\delta$ 1.17 (*d*; $CH_3$, $^3J$ = 6.88 Hz), 1.30 (*d*; $CH_3$, $^3J$ = 6.73 Hz), 2.15 (*s*; $CH_3$), 2.77 (*m*; 2CH), 3.09 (*s*; $CH_3$), 7.28 (*m*), 7.42(*m*).

### *Crystal data*

$C_{15}H_{24}N^{+}\cdot Br^{-}$
$M_r = 298.26$
Monoclinic, $P2_1/c$
$a = 13.0623$ (9) Å
$b = 10.9266$ (5) Å
$c = 11.6561$ (8) Å
$\beta = 111.958$ (5)°
$V = 1542.95$ (17) Å$^3$
$Z = 4$

$D_x = 1.284$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 30660 reflections
$\theta = 3.5$–27.5°
$\mu = 2.65$ mm$^{-1}$
$T = 100$ (2) K
Block, colourless
0.39 × 0.33 × 0.27 mm

### *Data collection*

Stoe IPDS-II two-circle diffractometer
$\omega$ scans
Absorption correction: multi-scan (*MULABS*; Spek, 1990; Blessing, 1995)
$T_{\min} = 0.389$, $T_{\max} = 0.489$
34535 measured reflections

3605 independent reflections
3047 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.043$
$\theta_{\max} = 27.7°$
$h = -16 \rightarrow 17$
$k = -14 \rightarrow 14$
$l = -15 \rightarrow 15$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.049$
$S = 1.01$
3605 reflections
160 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0295P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.35$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.39$ e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| N1—C9 | 1.2900 (18) | C9—C11 | 1.482 (2) |
| N1—C1 | 1.4521 (17) | C9—C10 | 1.4888 (19) |
| | | | |
| C9—N1—C1 | 125.98 (12) | N1—C9—C10 | 119.10 (13) |
| N1—C9—C11 | 122.17 (13) | C11—C9—C10 | 118.73 (13) |

**Table 2**
Hydrogen-bonding geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···Br1 | 0.85 (2) | 2.35 (2) | 3.1957 (12) | 177 (2) |
| C10—H10$C$···Br1 | 0.98 | 3.09 | 3.9088 (16) | 143 |
| C7—H7···Br1$^{\rm i}$ | 1.00 | 3.12 | 3.8356 (14) | 130 |
| C8—H8···Br1$^{\rm ii}$ | 1.00 | 3.05 | 3.9015 (13) | 144 |
| C10—H10$B$···Br1$^{\rm ii}$ | 0.98 | 3.03 | 3.6806 (15) | 125 |
| C11—H11$A$···Br1$^{\rm ii}$ | 0.98 | 2.99 | 3.7391 (16) | 134 |
| C11—H11$B$···Br1$^{\rm iii}$ | 0.98 | 3.08 | 4.0109 (15) | 159 |

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

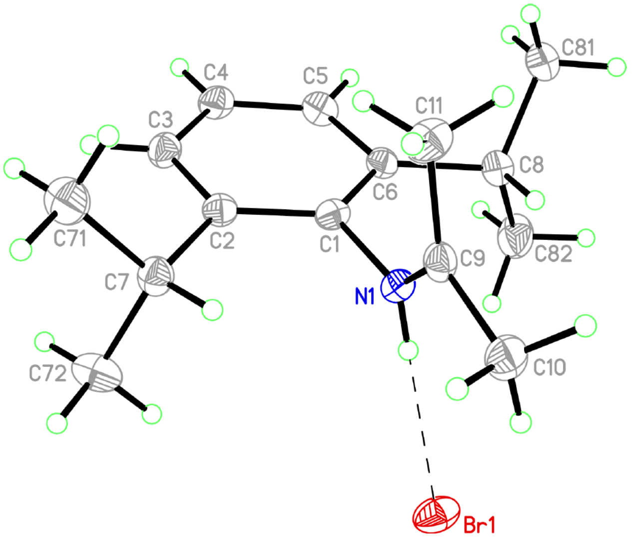


**Figure 1**
Perspective view of the title compound, with the atom numbering scheme; displacement ellipsoids are drawn at the 50% probability level.

H atoms bonded to C atoms were refined with fixed individual displacement parameters [$U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ or 1.5 $U_{\rm eq}$(methyl C)], using a riding model with aromatic C—H = 0.95 Å, tertiary C—H = 1.00 Å or methyl C—H = 0.98 Å and methyl groups C10 and C11 were allowed to rotate but not to tip. The H atom bonded to the N atom was refined isotropically.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97.

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