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# 1-(*N*,*N*-Diethylamino)-2,3-diphenylcyclopropenylium tetrafluoroborate

**Ewa Rozycka-Sokolowska, Tomasz Girek, Bernard Marciniak* and Volodymyr Pavlyuk**

Institute of Chemistry and Environment Protection, Jan Dlugosz Academy, al. Armii Krajowej 13/15, 42-200 Czestochowa, Poland

Correspondence e-mail: crystal@cz.onet.pl

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**Key indicators**

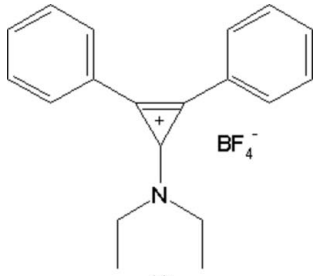
Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.003 Å
$R$ factor = 0.038
$wR$ factor = 0.121
Data-to-parameter ratio = 17.8

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

The asymmetric unit of the title compound, $C_{19}H_{20}N^{+}\cdot BF_4^{-}$, consists of an aminodiphenylcyclopropenylium cation and a tetrafluoroborate anion. The crystal packing is stabilized by C—H···F hydrogen bonds.

## Comment

Small unsaturated carbon fragments are important in fields ranging from organometallic chemistry (Bruce, 1998) to materials science (Dresselhaus *et al.*, 1996) and astrophysics (Weltner & Van Zee, 1989). The cyclopropenylium ion is a Hückel aromatic cation and would be a candidate for the cationic component of such unusual hydrocarbons (Kitagawa *et al.*, 2001). Although numerous derivatives of the cyclopropenylium ion have been prepared over the past decades (Komatsu & Yoshida, 1996), there are very few cyclopropenylium ions that are conjugated with amino groups (Yoshida *et al.*, 1985; Matsumoto *et al.*, 2002, 2003). Recently, we have synthesized and solved the crystal structure of the title compound, (I).




(I)

The asymmetric unit of (I) consists of an aminodiphenylcyclopropenylium cation and a tetrafluoroborate anion (Fig. 1). The F atoms of the anion revealed high displacement parameters. The plane of the cyclopropene ring makes angles of 12.14 (13) and 35.78 (14)°, respectively, with the C8–C13 and C14–C19 phenyl rings. The dihedral angle between the two phenyl rings is 45.23 (8)°. The N atom of the diethylamine group is displaced by 0.029 (1) Å from the plane defined by atoms C1–C3. In the crystal structure, each cation is linked to four anions *via* C—H···F hydrogen bonds (Table 1).

## Experimental

The title compound was prepared in 43% yield by the one-pot reaction of diphenylcyclopropenone with Meerwein reagent followed by diethylamine in dichloromethane at room temperature (Matsumoto *et al.*, 2002, 2003). Single crystals of (I) were obtained by slow cooling of a solution in dichloromethane.

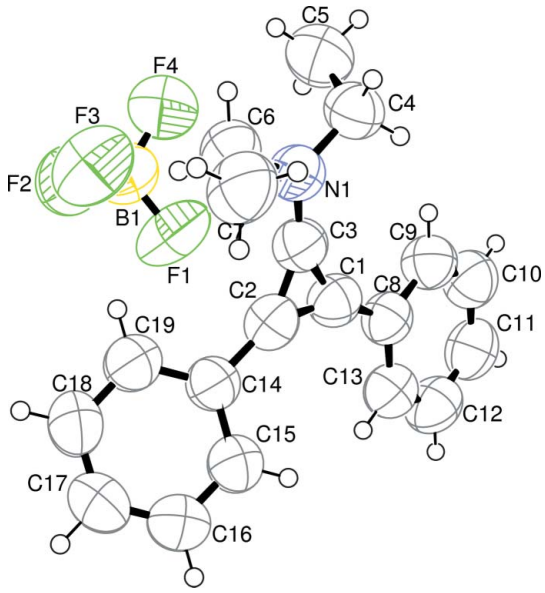



**Figure 1**
The constituent ions of (I), showing the atom numbering and with displacement ellipsoids drawn at the 50% probability level.

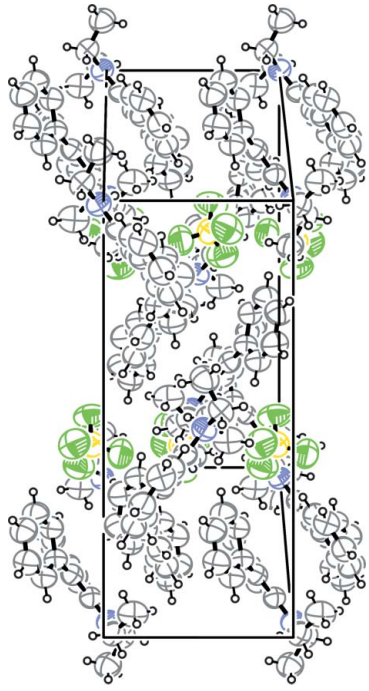


**Figure 2**
The crystal packing of (I).

*Crystal data*

$C_{19}H_{20}N^+\cdot BF_4^-$
$M_r$ = 349.17
Monoclinic, $P2_1/c$
$a$ = 14.216 (3) Å
$b$ = 8.004 (2) Å
$c$ = 18.501 (1) Å
$\beta$ = 121.19 (3)°
$V$ = 1800.9 (8) Å$^3$
$Z$ = 4
$D_x$ = 1.288 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 30 reflections
$\theta$ = 5–15°
$\mu$ = 0.10 mm$^{-1}$
$T$ = 293 (2) K
Tablet, colourless
0.50 × 0.34 × 0.08 mm

*Data collection*

Burevestnik DARCH-1 diffractometer
w/2$\theta$ scans
Absorption correction: refined from $\Delta F$ (*DIFABS*; Walker & Stuart, 1983)
$T_{min}$ = 0.979, $T_{max}$ = 0.997
4116 measured reflections
4116 independent reflections
2076 reflections with $I > 2\sigma(I)$
$\theta_{max}$ = 27.5°
$h = -18 \rightarrow 15$
$k = 0 \rightarrow 10$
$l = 0 \rightarrow 23$
3 standard reflections
every 100 reflections
intensity decay: 2.5%

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.121
$S$ = 0.81
4116 reflections
231 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.11 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.13 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C4—H4$B$···F2$^{i}$ | 0.97 | 2.51 | 3.373 (2) | 148 |
| C6—H6$B$···F3 | 0.97 | 2.45 | 3.293 (2) | 145 |
| C12—H12···F1$^{ii}$ | 0.93 | 2.54 | 3.443 (2) | 165 |
| C15—H15···F4$^{iii}$ | 0.93 | 2.52 | 3.343 (2) | 148 |

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

H atoms were treated in riding mode (C—H = 0.93–0.97 Å), with refined group $U_{iso}$(H) values.

Data collection: *DARCH Package* (Burevestnik, 1991); cell refinement: *DARCH Package*; data reduction: *DARCH Package*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia,1997); software used to prepare material for publication: *SHELXL97*.

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