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Nitronium tetrafluoroborate

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(O–N) = 0.001 Å
R factor = 0.019
wR factor = 0.061
Data-to-parameter ratio = 10.5

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

Commercially available nitronium tetrafluoroborate, $NO_2^+ \cdot BF_4^-$, has been recrystallized from CH_2Cl_2 as a side-product of a reaction in which it has been used as a starting material. Both the NO_2^+ cations and the BF_4^- anions are packed in considerably distorted cubic environments. The N═O distances of 1.1153 (8) and 1.1160 (7) Å as well as the O═N═O bond angle of 179.89 (7)° are similar to those found in other NO_2^+-containing salts described in the literature.

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Comment

The N═O distances in $[NO_2][BF_4]$ of 1.1153 (8) and 1.1160 (7) Å as well as the O═N═O bond angle of 179.89 (7)° are in good agreement with those found for other nitronium salts such as $[NO_2][Fe(NO_3)_4]$ ($d_{av.}$ = 1.116 Å) or $[NO_2][Zr(NO_3)_5]$ ($d_{av.}$ = 1.105 Å) (Tikhomirov *et al.*, 2002). In addition, the B—F distances (see Table 1) are typical for a tetrafluoroborate anion.

Weak bonding interactions shorter than the sum of the van der Waals radii [r(O + F) = 3.0 Å, r(N + F) = 3.1 Å; Holleman, 1995) are found between the cations and anions. The shortest are the N—F contacts which range from 2.474 (1) to 2.500 (1) Å (Fig. 1). Both the NO_2^+ cations and the BF_4^- anions are packed in considerably distorted cubic environments.

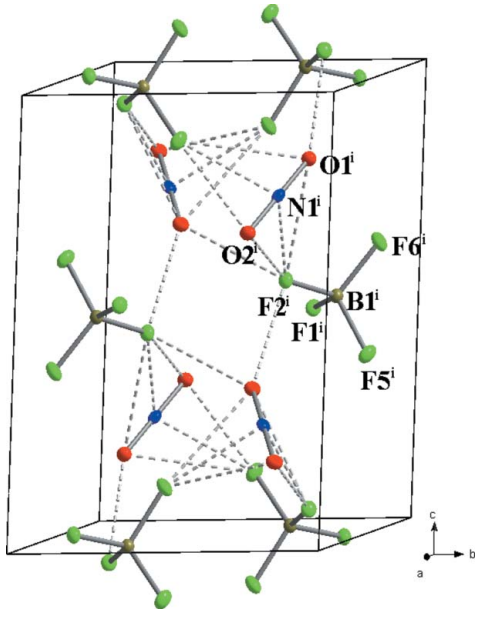

Figure 1
Packing diagram of $[NO_2][BF_4]$. Dashed lines represent cation–anion contacts shorter than the sum of the van der Waals radii. Displacement ellipsoids are drawn at the 25% probability level. [Symmetry code: (i) $1-x, \frac{1}{2}-x, \frac{1}{2}-z$.]

Experimental

Colourless block-shaped crystals of the title salt (Sigma–Aldrich) were fortuitously recrystallized from CH_2Cl_2 as a by-product of an attempted reaction with P_4.

Crystal data

$NO_2^+ \cdot BF_4^-$
M_r = 132.82
Monoclinic, $P2_1/c$
a = 6.5567 (13) Å
b = 6.8243 (14) Å
c = 9.1244 (18) Å
β = 104.40 (3)°
V = 395.44 (14) Å^3
Z = 4
D_x = 2.232 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 100 (2) K
Block, colourless
0.4 × 0.2 × 0.2 mm

Data collection

STOE IPDS-II diffractometer
φ scans
Absorption correction: none
2652 measured reflections
768 independent reflections
662 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.061
S = 1.16
768 reflections
73 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0289P)^2 + 0.0515P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.019
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

Table 1
Selected bond lengths (Å).

F1—B1	1.3885 (8)	F5—B1	1.3908 (9)
F2—B1	1.3907 (8)	F6—B1	1.3896 (9)

Data collection: *XPOSE* (Stoe, 2003); cell refinement: *CELL* (Stoe, 2003); data reduction: *X-RED32* (STtoe, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Crystal Impact, 2006); software used to prepare material for publication: *SHELXL97*.

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