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3-Fluorophenylboronic acid

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.007 Å
R factor = 0.084
wR factor = 0.189
Data-to-parameter ratio = 13.0

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

The title compound, $C_6H_6BFO_2$, is a versatile building block in organic synthesis. In the crystal structure, intermolecular O—H···O hydrogen bonds link the molecules into dimers, which may be effective in the stabilization of the crystal structure.

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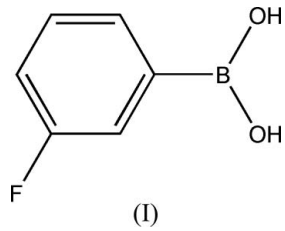
Comment

The title compound, (I), is a versatile building block in organic synthesis and an important intermediate in the synthesis of active compounds in the agrochemical and pharmaceutical industries (Meudt *et al.*, 2002).



(I)

In the molecule of the title compound, (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987).

As can be seen from the packing diagram (Fig. 2), intermolecular O—H···O hydrogen bonds (Table 2) link the molecules into dimers, which may be effective in the stabilization of the crystal structure. Dipole–dipole and van der Waals interactions are also effective in the molecular packing.

Experimental

Compound (I) was prepared according to the reported procedure of Meudt *et al.* (2002). Single crystals suitable for X-ray diffraction were

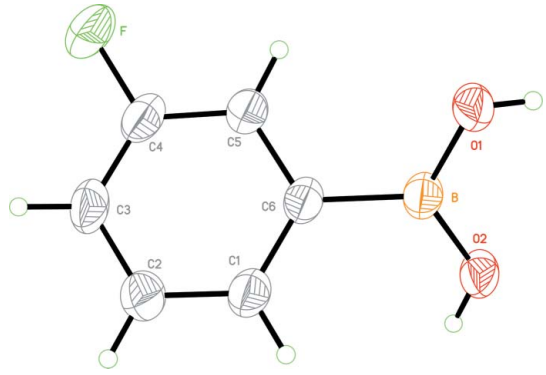


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

obtained by slow evaporation of an acetonitrile (25 ml) solution of (I) (1.0 g).

Crystal data

$C_6H_6BFO_2$
M_r = 139.92
Monoclinic, $P2_1/c$
a = 5.7560 (12) Å
b = 5.027 (1) Å
c = 22.402 (5) Å
β = 91.19 (3)°
V = 648.1 (2) Å^3
Z = 4
D_x = 1.434 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 294 (2) K
Block, white
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.965, T_{max} = 0.988
1265 measured reflections
1265 independent reflections
868 reflections with $I > 2\sigma(I)$
θ_{max} = 26.0°
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.084
$wR(F^2)$ = 0.189
S = 0.97
1265 reflections
97 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.03P)^2 + 2P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.85 (3)	2.06 (4)	2.796 (5)	144 (4)
O2—H2···O1^{ii}	0.86 (3)	2.08 (3)	2.831 (5)	145 (4)

Symmetry codes: (i) $-x, -y, -z$; (ii) $x, y+1, z$.

The H atoms of OH groups were located in difference syntheses and refined [O—H = 0.851 (19)–0.855 (19) Å, with U_{iso}(H) = 1.2U_{eq}(O)]. The remaining H atoms were positioned geometrically, with C—H = 0.93 Å for aromatic H atoms, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

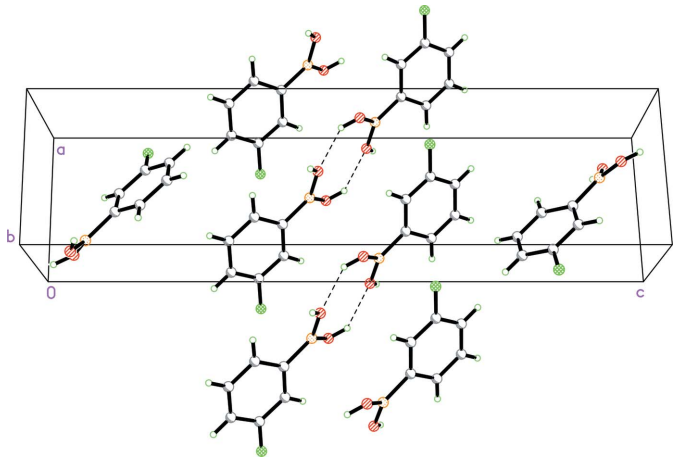


Figure 2
A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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