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2,6-Difluorobenzohydroxamic acid

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.041
wR factor = 0.115
Data-to-parameter ratio = 11.4

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

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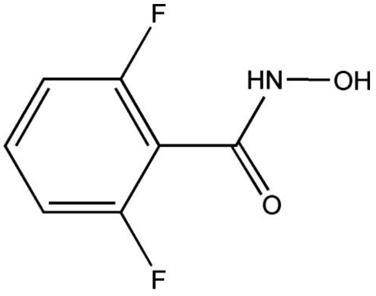
In the title compound, $C_7H_5F_2NO_2$, the two independent molecules are linked together by a combination of N—H···O, O—H···O and C—H···F hydrogen bonds, forming a one-dimensional structure along the *c* axis.

Comment

Continuing our study of of hydroxamic acid derivatives, we have recently reported the synthesis and crystal structure determination of two substituted hydroxamic acids (Shang *et al.*, 2005*a*,*b*). We describe here the structure of a fluoro-substituted benzohydroxamic acid, (I).



(I)

Compound (I) crystallizes in the centrosymmetric space group $P\overline{1}$ with Z' = 2. Because of the disorder of atoms F3 and F4, the two molecules in the asymmetric unit are similar but not identical. One molecule exhibit orientational disorder; atoms F3 and F4 have site-occupancy factors of 0.54 (3) and 0.46 (3) for the major and minor components, respectively.

Molecules are linked by a combination of N—H···O, O—H···O and weak C—H···F hydrogen bonds (Table 1), forming a one-dimensional structure along the *c* axis (Fig. 2), with an S-shaped supramolecular arrangement.

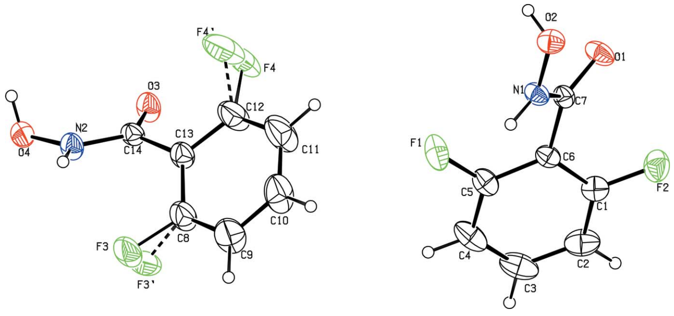


Figure 1
The asymmetric unit of (I), showing 30% probability displacement ellipsoids. Both disorder components are shown.

Experimental

Compound (I) was prepared by adding methyl 2,6-difluorobenzoate (1.72 g, 10 mmol) to a solution of NH_2OH (16 mmol) in methanol (30 ml) under N_2. The system was stirred at room temperature overnight. Under ice cooling, the pH of the solution was adjusted to *ca* 7 with concentrated HCl. A white precipitate formed and was filtered off. Single crystals of (I) suitable for X-ray analysis were obtained by recrystallization of this white precipitate from methanol.

Crystal data

$C_7H_5F_2NO_2$
$M_r = 173.12$
Triclinic, $P\bar{1}$
$a = 5.0742$ (5) Å
$b = 9.9436$ (11) Å
$c = 14.7249$ (16) Å
$\alpha = 97.982$ (2)°
$\beta = 96.684$ (2)°
$\gamma = 95.524$ (2)°
$V = 725.97$ (13) Å^3
$Z = 4$
$D_x = 1.584$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3254 reflections
$\theta = 2.3$–27.0°
$\mu = 0.15$ mm^{-1}
$T = 292$ (2) K
Prism, colorless
0.30 × 0.30 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{\min} = 0.943$, $T_{\max} = 0.971$
5689 measured reflections
2824 independent reflections
2364 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.018$
$\theta_{\max} = 26.0°$
$h = -6 \rightarrow 6$
$k = -12 \rightarrow 12$
$l = -16 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.115$
$S = 1.05$
2824 reflections
248 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0566P)^2 + 0.1612P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.20$ e Å^{-3}
$\Delta\rho_{\min} = -0.23$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···F4^{i}	0.93	2.48	3.361 (9)	158
O4—H4A···O2^{i}	0.83 (2)	2.57 (2)	3.005 (2)	114 (2)
O4—H4A···O1^{i}	0.83 (2)	1.93 (2)	2.742 (2)	165 (2)
O2—H2A···O3^{i}	0.83 (2)	1.96 (1)	2.783 (2)	171 (2)
N2—H2B···O3^{ii}	0.86 (2)	2.06 (2)	2.840 (2)	151 (2)
N1—H1A···O1^{ii}	0.86 (2)	2.09 (2)	2.845 (2)	147 (2)

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

It was apparent at an early stage that atoms F3 and F4 adopted an alternative orientation. The C—F bond distances were constrained using the SADI command (*SHELXL97*; Sheldrick, 1997). Refinement of the site-occupancy factors for the two components was constrained to sum to unity, giving values of 0.54 (3) and 0.46 (3) for the major and minor components, respectively. The benzene H atoms were placed at idealized postions, with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). The amine and hydroxyl H atoms were located in a difference map, and refined with restraints of N—H = 0.86 (1) Å and O—H = 0.82 (1) Å, the $U_{\rm iso}$(H) values being set at 1.5 times the $U_{\rm eq}$ value of their carrier atom.

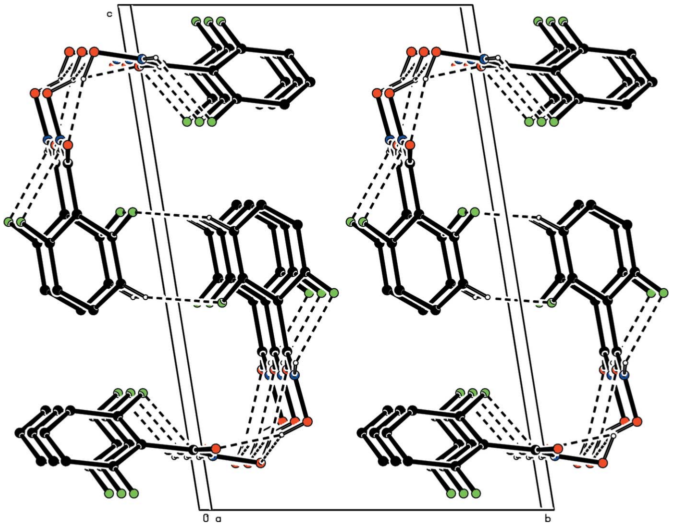


Figure 2
Plot of the crystal packing, viewed approximately along the *a* axis, showing the intermolecular hydrogen bonds (dashed lines). Only the major disorder component is shown. H atoms not involved in hydrogen bonding have been omitted.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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