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The crystal structure of [6-methoxy-2-(2,2,2-trifluoroacetyl)-3,4-dihydronaphthalen-1(2H)-one]difluoroborane, $C_{13}H_{10}BF_5O_3$

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	$0.28 \times 0.26 \times 0.24$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	1.6 cm^{-1}
Diffractometer, scan mode:	Xcalibur, ω -scans
$2\theta_{\text{max}}$, completeness:	59.6° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	5444, 3261, 0.014
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2390
$N(\text{param})_{\text{refined}}$:	200
Programs:	CrysAlis ^{PRO} [1], SHELX [2]

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Abstract

$C_{13}H_{10}BF_5O_3$, triclinic, $P\bar{1}$ (no. 2), $a = 7.737(2)$ Å, $b = 7.8600(19)$ Å, $c = 11.803(3)$ Å, $\alpha = 82.03(2)^\circ$, $\beta = 76.91(2)^\circ$, $\gamma = 69.69(2)^\circ$, $V = 654.2(3)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0471$, $wR_{\text{ref}}(F^2) = 0.1203$, $T = 293$ K.

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The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

[6-methoxy-2-(2,2,2-trifluoroacetyl)-3,4-dihydronaphthalen-1(2H)-one]difluoroborane was synthesized by a representative means of the reference paper [3]. Boron trifluoride diethyl etherate (0.9 mL, 4.5 mmol) was added to a solution of

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O3	1.27975(16)	0.64622(17)	0.18252(10)	0.0447(3)
O2	1.27631(15)	0.66809(17)	0.38618(10)	0.0440(3)
F1	1.54142(15)	0.50139(17)	0.26436(10)	0.0632(3)
F2	1.44395(16)	0.80795(16)	0.23748(10)	0.0627(3)
F3	1.13462(17)	0.6912(2)	0.00592(9)	0.0780(4)
C7	1.0947(2)	0.7234(2)	0.40694(13)	0.0333(3)
C6	0.9995(2)	0.7440(2)	0.52610(13)	0.0350(3)
C8	0.9934(2)	0.7570(2)	0.31505(13)	0.0344(3)
F4	0.89597(18)	0.89960(17)	0.08623(10)	0.0687(4)
F5	0.90317(18)	0.62390(17)	0.11558(10)	0.0680(4)
O1	0.7459(2)	0.7796(2)	0.87210(11)	0.0624(4)
C4	0.7181(2)	0.7771(2)	0.67251(14)	0.0412(4)
H4	0.5910	0.7900	0.6933	0.049*
C11	1.0965(2)	0.7117(2)	0.20787(13)	0.0358(3)
C5	0.8070(2)	0.7643(2)	0.55668(13)	0.0350(3)
C1	1.0988(2)	0.7362(2)	0.61380(14)	0.0425(4)
H1	1.2264	0.7207	0.5942	0.051*
C10	0.7042(2)	0.7612(2)	0.46317(14)	0.0395(4)
H10A	0.5724	0.8307	0.4860	0.047*
H10B	0.7134	0.6368	0.4559	0.047*
C3	0.8187(3)	0.7707(2)	0.75780(14)	0.0451(4)
C9	0.7827(2)	0.8397(2)	0.34558(14)	0.0414(4)
H9A	0.7273	0.8167	0.2858	0.050*
H9B	0.7490	0.9703	0.3478	0.050*
C12	1.0076(3)	0.7301(3)	0.10214(14)	0.0464(4)
C2	1.0094(3)	0.7511(3)	0.72725(15)	0.0485(4)
H2	1.0756	0.7482	0.7845	0.058*

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
B1	1.3926(3)	0.6553(3)	0.26566(17)	0.0423(4)
C13	0.5527(3)	0.7938(3)	0.91341(17)	0.0670(6)
H13A	0.4742	0.9037	0.8798	0.101*
H13B	0.5236	0.7962	0.9968	0.101*
H13C	0.5308	0.6911	0.8913	0.101*

6-methoxy-2-(2,2,2-trifluoroacetyl)-3,4-dihydronaphthalen-1(2*H*)-one (0.8 g, 3 mmol) in 25 mL CH₂Cl₂ at room temperature under N₂. The mixture was stirred for 12 h. The solvent was removed in vacuo. The residue was recrystallized from hexanes/acetone (4:1) to give the title compound as a yellow powder: 538 mg, (56%). Crystals suitable for X-ray diffraction were obtained by evaporation from CH₂Cl₂ at room temperature.

Experimental details

All H atoms on C atoms were placed in idealized positions [C—H = 0.96 (methyl), 0.97(methylene) and 0.93 Å(aromatic)] and included in the refinement using the riding-model approximation, with *U*_{iso}(H) = 1.5*U*_{eq}(methyl) and 1.2*U*_{eq}(methylene and aromatic).

Discussion

Difluoroboron compounds have applications in sensors, optoelectronic devices, probes, and catalysis in the past few years [4–6]. Herein, we report the crystal structure of [6-methoxy-2-(2,2,2-trifluoroacetyl)-3,4-dihydronaphthalen-1(2*H*)-one]difluoroborane.

The structural analysis reveals that the complex crystallizes in the triclinic space group *P* $\bar{1}$. There is one complete molecule in the asymmetric unit. There are no classic hydrogen bonds found in the title crystal structure, but there are weak C—H...F hydrogen bonds. The plane of BF₂ moieties is nearly perpendicular to the plane of six-membered ring which contains the boron atom. All of the bond distances and angles of the complex are in normal range.

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