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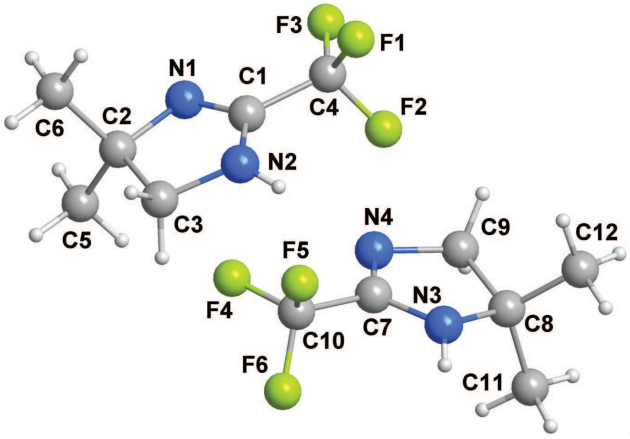
Crystal structure of 4,4-dimethyl-2-(trifluoromethyl)-4,5-dihydro-1*H*-imidazole, $C_6H_9F_3N_2$



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Abstract

$C_6H_9F_3N_2$, monoclinic, $P2_1/n$ (no. 14), $a = 10.6224(9)$ Å, $b = 11.8639(9)$ Å, $c = 13.3139(11)$ Å, $\beta = 105.903(3)°$, $V = 1613.6(2)$ Å^3, $Z = 8$, $R_{gt}(F) = 0.0618$, $wR_{ref}(F^2) = 0.1629$, $T = 102(2)$ K [1–3].

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The 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.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.40 × 0.20 × 0.18 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.13 mm^{-1}
Diffractometer, scan mode:	Bruker Venture Photon, φ and ω
θ_{max}, completeness:	27.6°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	25043, 3722, 0.029
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3126
$N(param)_{refined}$:	211
Programs:	Bruker [1], SHELX [2, 3]

Source of material

Stoichiometric amount of 2-methylpropane-1,2-diamine (1.68 g, 19.06 mmol) was dissolved in 50 mL of dioxone in one neck round bottom flask equipped with a reflux condenser and magnetic stirring bar. Ethyl 2,2,2-trifluoroacetate (2.71 mL, 3.97 g, 38.12 mmol) was added dropwise and the mixture was stirred at moderate heating (50 °C) overnight. The solvent was completely removed and viscous colorless product was obtained. The product was further purified by distillation under reduced pressure (0.1 mm Hg, RT), (Yield 79%). M.P. 55−57 °C.

Experimental details

Hydrogen atoms were placed at the calculated positions and included using a riding model with $U_{iso}(H) = 1.2U_{eq}$ or $1.5U_{eq}$ of the adjacent non-hydrogen atom.

Comment

The development of imidazole-based molecules has speedily increased recently, since it can be used extensively in medicinal chemistry as man-made drugs, agrochemicals, artificial acceptors, biomimetic catalysts, supramolecular material [4–6]. Several imidazole medicinal drugs have been used for treatment of broad types of diseases, imidazole derivatives demonstrated anti-inflammatory, analgesic, antiviral, antitubercular, antimicrobial, antimalarial, anti-diabetic and anticancer activity [7–10].

The molecule $C_6H_9F_3N_2$ crystallizes in the space group $P2_1/n$. The asymmetric unit of the title structure contains

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.6367(2)	0.27964(17)	0.58791(15)	0.0254(4)
C2	0.73966(18)	0.44033(16)	0.63748(15)	0.0220(4)
C3	0.6742(2)	0.40100(18)	0.72269(16)	0.0281(4)
H3A	0.739069	0.395447	0.791899	0.034*
H3B	0.603163	0.452885	0.727600	0.034*
C4	0.5809(3)	0.1758(2)	0.52623(18)	0.0413(6)
C5	0.6921(2)	0.55617(19)	0.59481(18)	0.0333(5)
H5A	0.729385	0.574908	0.537231	0.050*
H5B	0.719890	0.612439	0.650379	0.050*
H5C	0.596356	0.555871	0.569313	0.050*
C6	0.8882(2)	0.4379(2)	0.67844(19)	0.0346(5)
H6A	0.916767	0.361909	0.703466	0.052*
H6B	0.916464	0.491723	0.736064	0.052*
H6C	0.927006	0.458485	0.622156	0.052*
C7	0.40653(17)	0.18527(15)	0.85401(14)	0.0181(4)
C8	0.22696(18)	0.08125(16)	0.77486(14)	0.0214(4)
C9	0.31326(19)	0.11170(18)	0.70118(15)	0.0241(4)
H9A	0.349257	0.042471	0.678059	0.029*
H9B	0.260652	0.152188	0.638705	0.029*
C10	0.49772(19)	0.25035(17)	0.94148(14)	0.0232(4)
C11	0.0969(2)	0.1437(2)	0.74606(18)	0.0326(5)
H11A	0.052868	0.132647	0.801053	0.049*
H11B	0.041604	0.114349	0.679815	0.049*
C12	0.2065(2)	−0.04492(18)	0.78123(18)	0.0350(5)
H12A	0.291734	−0.082610	0.804080	0.053*
H12B	0.158469	−0.073403	0.712299	0.053*
H12C	0.156267	−0.060202	0.831429	0.053*
F1	0.6175(4)	0.08556(15)	0.57764(17)	0.1328(15)
F2	0.4514(2)	0.1738(2)	0.5063(2)	0.1104(11)
F3	0.6078(2)	0.16886(14)	0.43734(13)	0.0660(6)
F4	0.58725(15)	0.30726(13)	0.90982(10)	0.0436(4)
F5	0.56104(13)	0.18335(11)	1.01875(10)	0.0353(3)
F6	0.43133(14)	0.32464(12)	0.98252(11)	0.0413(4)
N1	0.69927(17)	0.35430(14)	0.55252(13)	0.0246(4)
H1N	0.567(3)	0.259(3)	0.706(2)	0.051(9)*
N2	0.6232(2)	0.2912(17)	0.68486(15)	0.0371(5)
H2N	0.283(3)	0.137(2)	0.928(2)	0.036(7)*
N3	0.31069(16)	0.12340(15)	0.87538(13)	0.0252(4)
N4	0.42054(16)	0.18443(13)	0.76162(12)	0.0207(3)

two independent molecules (figure), with a high similarity in their structural parameters like bond lengths and angles. The similarity of these two structures extends to their hydrogen-bonding motifs. The molecules in the title structure are connected *via* intermolecular hydrogen bonds, of N—H···N type (N2···N4: 2.91 Å; N1···N3′: 2.93 Å; ′ = 0.5 + *x*, 0.5 − *y*, −0.5 + *z*).

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