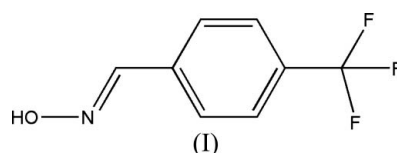
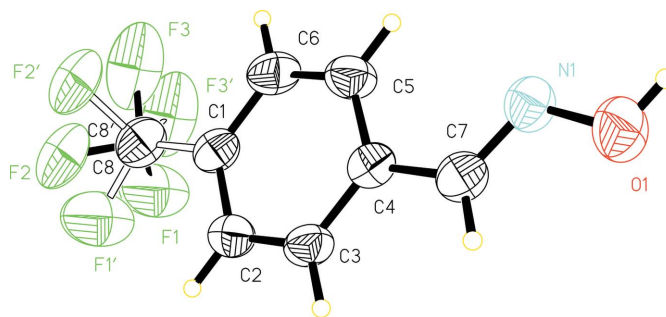


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Zhang and Jian-Wu Wang*School of Chemistry and Chemical Engineering,
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yugp2005@yahoo.com.cn**Key indicators**Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
Disorder in main residue
 R factor = 0.054
 wR factor = 0.148
Data-to-parameter ratio = 11.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**(E)-4-(Trifluoromethyl)benzaldehyde oxime**In the title compound, $\text{C}_8\text{H}_6\text{F}_3\text{NO}$, the trifluoromethyl group displays rotational disorder. The crystal packing is stabilized by intermolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds and van der Waals forces.Received 22 April 2006
Accepted 31 May 2006**Comment**

4-(Trifluoromethyl)benzaldehyde oxime is an important intermediate in organic synthesis, in particular in the formation of isoxazole (Sharghi & Sarvari, 2001). In this paper we report the crystal structure of the title compound, (I).

In (I), the bond lengths and angles are in agreement with values reported previously (Jerslev, 1983; Jensen, 1970). Atoms C1–C8, N1 and O1 are almost coplanar, the largest deviation being 0.050 (2) Å for atom N1. The crystal packing is stabilized by $\text{O}-\text{H}\cdots\text{N}$ intermolecular hydrogen bonds (Table 1) and van der Waals forces.**Experimental**

The title compound was synthesized by the reaction of 4-(trifluoromethyl)benzaldehyde (0.01 mol) with hydroxylamine hydrochloride (0.01 mol) in the presence of sodium carbonate (0.01 mol) in an aqueous methanol (water: methanol 1:1 v/v) solution (20 ml) at room temperature (5 h). After diluting with water, the aqueous solution

**Figure 1**
View of the title compound (I), with displacement ellipsoids drawn at the 40% probability level. Both disorder components are shown.

was extracted with dichloromethane, and the organic phase was dried and evaporated to afford the title product in 89% yield (Zhang & Li, 2004). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of a solution in a hexane/dichloromethane mixture (1:1 v/v) at room temperature over a period of one week.

Crystal data

C₈H₆F₃NO
M_r = 189.14
 Monoclinic, *P*₂₁/*c*
a = 7.543 (4) Å
b = 7.395 (4) Å
c = 15.058 (8) Å
 β = 99.278 (7)°
V = 829.0 (8) Å³

Z = 4
D_x = 1.515 Mg m⁻³
 Mo *K*α radiation
 μ = 0.15 mm⁻¹
T = 298 (2) K
 Block, colorless
 0.36 × 0.29 × 0.24 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.952, *T_{max}* = 0.961

4169 measured reflections
 1536 independent reflections
 1259 reflections with *I* > 2σ(*I*)
R_{int} = 0.050
θ_{max} = 25.5°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.054
wR (*F*²) = 0.148
S = 1.06
 1536 reflections
 130 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0725P)^2 + 0.1821P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δ/σ)_{max} < 0.001
 Δρ_{max} = 0.23 e Å⁻³
 Δρ_{min} = -0.27 e Å⁻³
 Extinction correction: SHELXL97
 Extinction coefficient: 0.73 (5)

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1—H1···N1 ⁱ	0.82	2.12	2.831 (3)	145

Symmetry code: (i) -*x* + 1, -*y*, -*z*.

All H atoms were placed in calculated positions, with C—H = 0.93 Å and O—H = 0.82 Å, and included in the final cycles of refinement using a riding model, with *U*_{iso}(H) = 1.2*U*_{eq}(C) for the aryl H atoms and 1.5*U*_{eq}(O) for the hydroxyl H atom. The trifluoromethyl group was found to be disordered; atoms C8, F1, F2 and F3 were refined over two positions [occupancies 0.093 (3) for the primed and 0.907 (3) for the unprimed atoms].

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1999); software used to prepare material for publication: SHELXTL.

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