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Methyl (*E,Z*)-α-(methoxyimino)-2-[({1-[3-(trifluoromethyl)phenyl]ethylidene}amino)oxymethyl]-benzeneacetate

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.036
wR factor = 0.073
Data-to-parameter ratio = 12.5

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

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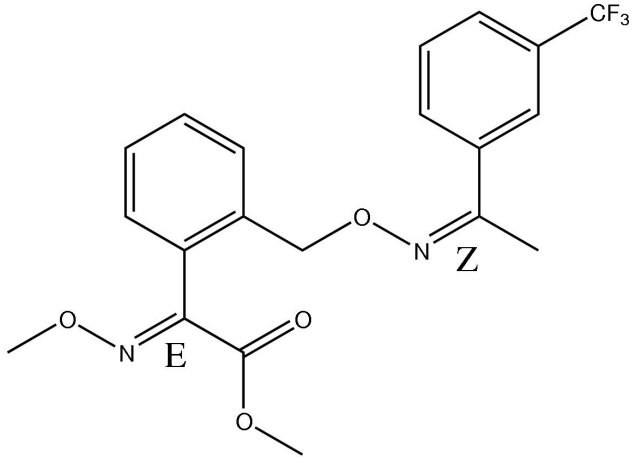
The crystal structure of the title compound, $C_{20}H_{19}F_3N_2O_4$, contains one molecule in the asymmetric unit. The CF_3 group is disordered over two positions. The important characteristics of the molecule are the two C=N bonds in an *E,Z*-configuration, *viz*. *E* in the β-methoxy system and *Z* in the oxymethyl chain between the two aromatic rings.

Comment

The title compound, (I), is an isomer of the fungicide trifloxystrobin (TFS). TFS exists in the *E,E*-configuration (Ebeling *et al.*, 2003) but, on exposure to the environment, it is susceptible to conversion to a mixture of four isomers. As part of our investigations on the isomerization of TFS in the environment, we have determined the crystal structure of (I). The important characteristics of the molecule are the two C=N bonds in an *E,Z*-configuration, *viz*. *E* in the β-methoxy system and *Z* in the oxymethyl chain between the two aromatic rings. The general synthesis route of TFS was described by Ziegler *et al.* (2003).



(I)

Experimental

Compound (I) was produced by illuminating a solution of TFS in acetone and purified by preparative HPLC by the method described in our earlier report (Banerjee *et al.*, 2004). Compound (I) eluted with a good baseline separation at a retention time of 24.3 min. The fraction corresponding to (I) was collected separately and evaporated to complete dryness at 303 K under vacuum. The purity of the white solid thus obtained was confirmed by IR, Raman, NMR and mass spectrometry. It was redissolved in a minimum quantity of methanol and kept inside a fume-hood at room temperature for slow evaporation. Compound (I) crystallized out over a period of a week.

Crystal data

$C_{20}H_{19}F_3N_2O_4$	D_x = 1.337 Mg m^{-3}
M_r = 408.37	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 14739 reflections
a = 8.0256 (12) Å	θ = 3.0–25.3°
b = 33.580 (5) Å	μ = 0.11 mm^{-1}
c = 8.0957 (11) Å	T = 291 (1) K
β = 111.566 (5)°	Block, colourless
V = 2029.1 (5) Å^3	0.24 × 0.24 × 0.22 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	R_{int} = 0.030
ω scans	θ_{max} = 25.3°
Absorption correction: none	$h = -9 \rightarrow 9$
14739 measured reflections	$k = -39 \rightarrow 39$
3658 independent reflections	$l = -9 \rightarrow 9$
1749 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.036	$w = 1/[\sigma^2(F_o^2) + (0.021P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.073	$(\Delta/\sigma)_{max}$ = 0.001
S = 0.98	$\Delta\rho_{max}$ = 0.11 e Å^{-3}
3658 reflections	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
293 parameters	

H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å, and were treated as riding, with $U_{iso} = 1.5U_{eq}$(C) for methyl groups and $1.2U_{eq}$(C) for others; the methyl groups were allowed to rotate but not to tip. Each F atom is disordered over two positions with occupancies of 0.45 (1) and 0.55 (1).

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*, *PARST95* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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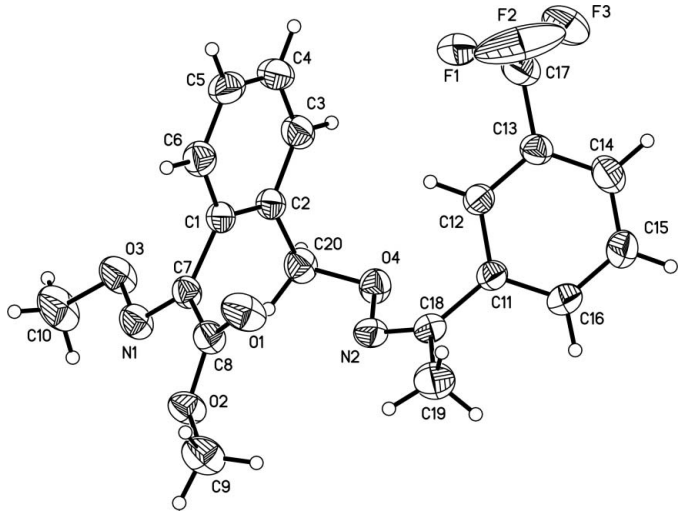

Figure 1
The molecular structure of the title compound, showing the labelling of all non-H atoms. Displacement ellipsoids are drawn at the 30% probability level. The F atoms are disordered, and for each F atom, only one of the two split positions is shown.

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