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

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The title compound, $C_{20}H_{19}F_3N_2O_4$, crystallizes with two molecules in the asymmetric unit. The important characteristics of the molecule are the two C═N bonds in *Z,E* configuration, one in the *β*-methoxy-system and the other in the oxymethyl side chain between the two aromatic rings.

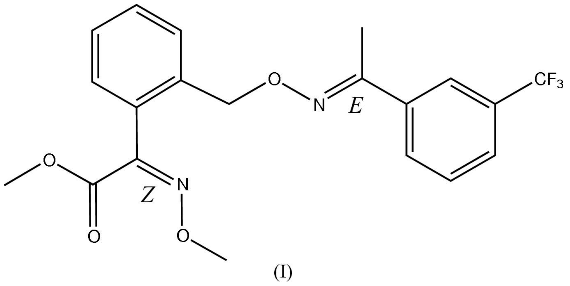
Key indicators

Single-crystal X-ray study
T = 173 K
Mean *σ*(C–C) = 0.005 Å
R factor = 0.033
wR factor = 0.050
Data-to-parameter ratio = 7.2

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

Comment

The title compound, (I), is an isomer of the fungicide trifloxystrobin (TFS). TFS appears in the *E,E* configuration (Ebeling *et al.*, 2003), but, on exposure to the environment, 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 general synthesis route of TFS was described by Ziegler *et al.* (2003). The title compound crystallizes with two molecules in the asymmetric unit. The dihedral angle between the two rings is 75.86 (8)° in the molecule containing atom C1 and 62.51 (8)° in the molecule containing C1′.



(I)

Experimental

Compound (I) was produced by illuminating a solution of TFS in acetone and was purified by preparative HPLC according to the method described in our earlier report (Banerjee *et al.*, 2004). It eluted with a good baseline separation at a retention time of 18.9 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

$C_{20}H_{19}F_3N_2O_4$	Mo *Kα* radiation
M_r = 408.37	Cell parameters from 27239 reflections
Orthorhombic, $Pna2_1$	θ = 2.9–25.4°
a = 22.4800 (14) Å	μ = 0.12 mm^{-1}
b = 22.1594 (15) Å	*T* = 173 (1) K
c = 7.7029 (6) Å	Needle, colourless
V = 3837.1 (5) Å^3	0.34 × 0.12 × 0.10 mm
Z = 8	
D_x = 1.414 Mg m^{-3}	

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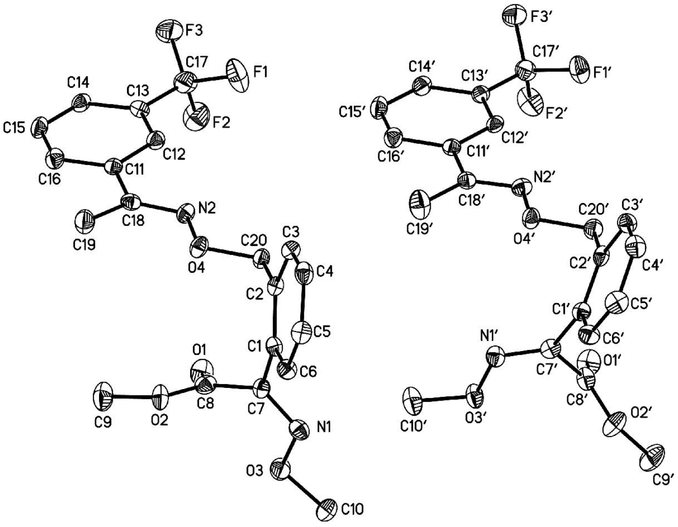

Figure 1

The structure of the asymmetric unit of the title compound, showing the labelling of all non-H atoms. Displacement ellipsoids are shown at the 30% probability level. H atoms have been omitted.

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: none
27239 measured reflections
3790 independent reflections
2109 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.040$
$\theta_{\rm max} = 25.4°$
$h = -27 \rightarrow 27$
$k = -26 \rightarrow 26$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.050$
$S = 0.86$
3790 reflections
529 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.005P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.14$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.15$ e Å^{-3}

H atoms were placed in calculated positions (C—H = 0.93–0.97 Å) and were treated as riding [$U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for methyl groups and 1.2$U_{\rm eq}$(C) for others; the methyl groups were allowed to rotate but not to tip]. In the absence of significant anomalous dispersion effects, Friedel pairs were averaged and the absolute configuration was arbitrarily assigned.

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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