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(*E,E*)-α-(Methoxyimino)-2-[({1-[3-(trifluoromethyl)-phenyl]ethylidene}amino)oxymethyl]benzeneacetic acid

Kaushik Banerjee,[a]‡ Axel Patrick Ligon,[a] Markus Schürmann,[b] Hans Preut[b]* and Michael Spiteller[a]

[a]Institut für Umweltforschung, Universität Dortmund, Otto-Hahn-Straße 6, 44221 Dortmund, Germany, and [b]Fachbereich Chemie, Universität Dortmund, Otto-Hahn-Straße 6, 44221 Dortmund, Germany

‡ Current address: National Research Centre for Grapes, Pune 412307, India

Correspondence e-mail: uch002@uxp1.hrz.uni-dortmund.de

Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.036
wR factor = 0.094
Data-to-parameter ratio = 12.2

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

The crystal structure of the title compound, $C_{19}H_{17}F_3N_2O_4$, a metabolite of the fungicide trifloxystrobin (TFS), 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,E* configuration, one in the β-methoxy system and the other in the oxymethyl side chain between the two aromatic rings. The molecules are linked *via* an O—H···N hydrogen bond and an infinite spiral is formed along the *b*-axis direction.

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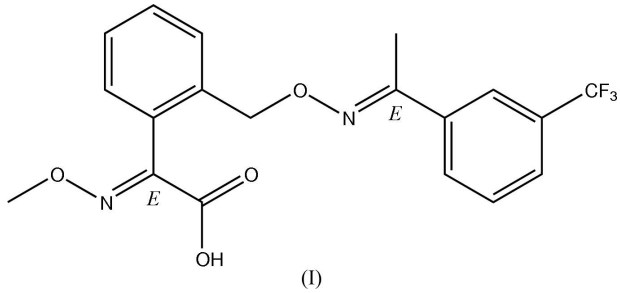

(I)

Experimental

Compound (I) was produced by alkaline hydrolysis of TFS with 0.05 *M* NaOH in a medium of acetone–water (50:50 *v*/*v*) at 293 K with continuous stirring with a magnetic stirrer. The white solid thus obtained was dissolved in a minimum quantity of *n*-hexane and kept inside a fume-hood at room temperature for slow evaporation.

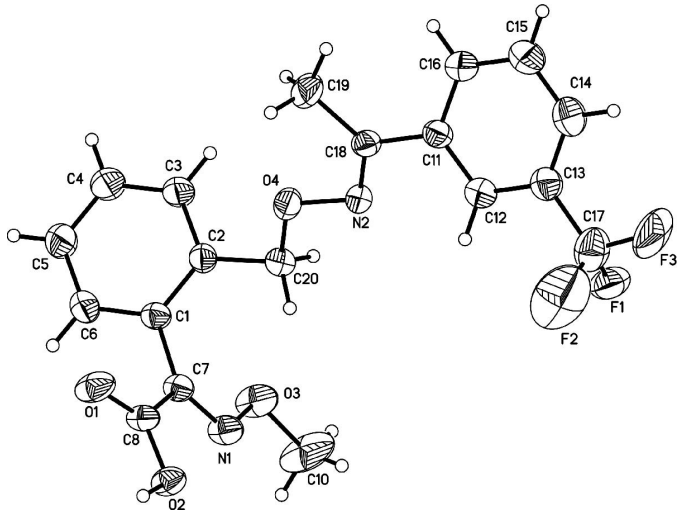

Figure 1
The molecular structure of the title compound, showing the labelling of all non-H atoms. Displacement ellipsoids are shown at the 30% probability level. The F atoms are disordered over two positions; one of the two split positions is shown.

Compound (I) crystallized out over a period of a week. In soil, in the absence of light, TFS is converted to (I) by microbial hydrolysis (Ebeling *et al.*, 2003).

Crystal data

$C_{19}H_{17}F_3N_2O_4$
M_r = 394.35
Monoclinic, $P2_1/c$
a = 13.6953 (14) Å
b = 9.0282 (15) Å
c = 16.302 (2) Å
β = 106.983 (7)°
V = 1927.7 (5) Å^3
Z = 4
D_x = 1.359 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10 735 reflections
θ = 3.1–25.4°
μ = 0.12 mm^{-1}
T = 291 (1) K
Plate, colourless
0.10 × 0.08 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: none
10 735 measured reflections
3500 independent reflections
1216 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 25.4°
$h = -16 \rightarrow 16$
$k = -10 \rightarrow 10$
$l = -19 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.094
S = 1.05
3500 reflections
288 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = [\exp(4.20(\sin\theta/\lambda)^2)]/[\sigma^2(F_o^2)]$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0061 (5)

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N2^{i}	0.97 (4)	1.81 (4)	2.761 (3)	164 (3)

Symmetry code: (i) $1-x, \frac{1}{2}+y, \frac{1}{2}-z$.

H atoms, except those on O2, 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. The H atom on O2 was refined isotropically. The F atoms are disordered over two positions with site-occupation factors of 0.56:0.44 (2).

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*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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