

Methyl 2(*E*)-methoxyimino-2-[2-(2-methylphenoxy)methyl]phenyl]acetateDeepak Chopra,^{a*} T. P. Mohan,^b
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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ (C—C) = 0.003 Å
R factor = 0.050
wR factor = 0.149
Data-to-parameter ratio = 15.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The title compound (also known as kresoxim-methyl), C₁₈H₁₉NO₄, is an active agrochemical exhibiting fungicidal activity. The dihedral angle between the two rings is 65.9 (1)°. The crystal structure is stabilized by weak but highly directional C—H···O and C—H··· π intermolecular interactions.

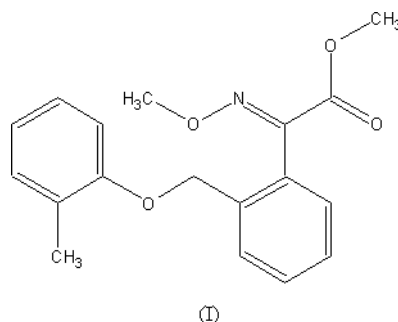
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Comment

An important aspect in the rational design of bioactive molecules involves relating chemical structure to biological activity (Lewis *et al.*, 1991). The conformation of the molecule is found to influence the levels of biological activity. Correlation of the results obtained from X-ray crystallography with biological activity has aided in the chemical design of few active agrochemicals. The activity of a series of triazolyl ketone herbicides (Anderson *et al.*, 1983) has been investigated along with the fungicidal activities of *N*-phenylsuccinamides (Zenei *et al.*, 1988). In this paper, we report the structure of the title compound, (I), which possesses fungicidal activity.



In (I), there is an intramolecular C8—H8B···O2 interaction (Fig. 1 and Table 2), forming a pseudo-seven-membered ring [Etter symbol *S*(7); Bernstein *et al.*, 1995]. Molecules are linked *via* C14—H14···O3ⁱⁱ hydrogen bond (see Table 2 for symmetry code), forming chains along the *b* axis. Furthermore, weak but highly directional C—H··· π interactions form molecular chains parallel to the *c* axis (Fig. 2 and Table 2).

Experimental

Compound (I) was obtained from Rallis India, Bangalore. Single crystals were grown by slow evaporation of an acetone solution at 278 K.

Crystal data

C₁₈H₁₉NO₄
M_r = 313.34
 Monoclinic, *C*2/*c*
a = 16.843 (16) Å
b = 15.480 (14) Å
c = 13.728 (13) Å
 β = 114.337 (14)°
V = 3261 (5) Å³
Z = 8

D_x = 1.276 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 865 reflections
 θ = 1.4–26.4°
 μ = 0.09 mm⁻¹
T = 293 (2) K
 Block, colorless
 0.28 × 0.25 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.933, *T_{max}* = 0.982
 16747 measured reflections

3315 independent reflections
 2332 reflections with *I* > 2σ(*I*)
R_{int} = 0.032
 θ_{max} = 26.4°
h = -21 → 20
k = -19 → 19
l = -17 → 16

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.050
wR (*F*²) = 0.149
S = 1.02
 3315 reflections
 211 parameters
 H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.0725*P*)² + 1.85*P*]
 where *P* = (*F_o*² + 2*F_c*²)/3
 (Δ/σ)_{max} < 0.001
 Δρ_{max} = 0.34 e Å⁻³
 Δρ_{min} = -0.23 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

O1–C5	1.365 (2)	O2–N1	1.379 (2)
O1–C8	1.428 (2)	N1–C15	1.287 (2)
C5–O1–C8–C9	179.98 (14)	C9–C10–C15–N1	72.0 (2)
C10–C9–C8–O1	63.6 (2)	C11–C10–C15–C18	71.6 (2)
C17–O4–C18–C15	178.73 (17)	C8–O1–C5–C4	2.8 (3)

Table 2

Hydrogen-bonding 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>
C8–H8B...O2	0.97	2.52	3.191 (3)	126
C17–H17B...Cg1 ⁱ	0.96	2.81	3.504 (4)	130
C14–H14...O3 ⁱⁱ	0.93	2.60	3.440 (4)	151

Symmetry codes: (i) *x*, -*y*, ½ + *z*; (ii) ½ - *x*, *y* - ½, ½ - *z*. Cg1 is the centroid of the C9–C14 benzene ring

All H atoms were constrained to ideal geometry, with C–H distances in the range 0.93–0.97 Å, and with *U*_{iso}(H) = 1.2*U*_{eq}(C) or 1.5*U*_{eq}(C_{methyl}). The methyl groups were allowed to rotate freely about the C–C bonds.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SIR92 (Altomare *et al.*, 1993); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: CAMERON (Watkin *et al.*, 1993); software used to prepare material for publication: PLATON (Spek, 2003).

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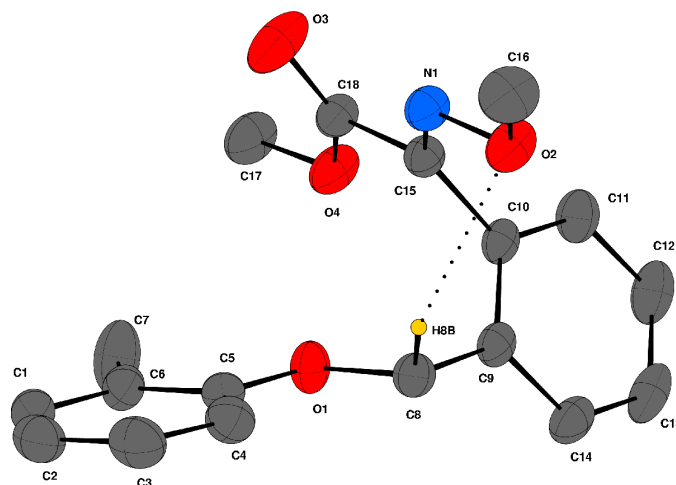


Figure 1

The molecular structure of (I), showing 50% probability ellipsoids. The dotted line indicates the C–H...O intramolecular interaction. Other H atoms have been omitted.

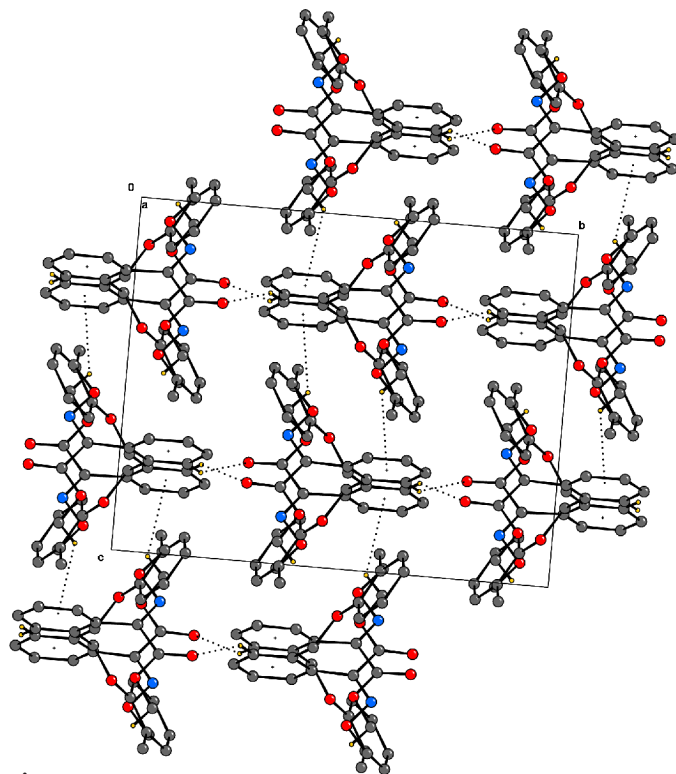


Figure 2

Packing diagram of (I), showing, by dotted lines, the C–H...O hydrogen bond and C–H...π intermolecular chains along the *b* and *c* axes, respectively.

IRHPA–DST program. D. Chopra thanks the CSIR, India, for a JRF.

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