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N′-(4-Methoxybenzylidene)methoxyformohydrazide

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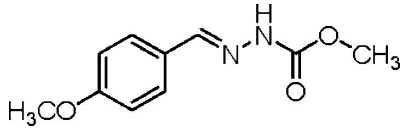
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.144; data-to-parameter ratio = 13.0.

There are two molecules in the asymmetric unit of the title compound, $C_{10}H_{12}N_2O_3$, with almost identical conformations. The crystal structure is stabilized by intermolecular N—H···O hydrogen bonds.

Related literature

For related literature, see: Borg *et al.* (1999); Goswami *et al.* (1984); Omar *et al.* (1996); Shang (2006); Shang *et al.* (2007); Tully *et al.* (1991); Yang & Dai (1993).



Experimental

Crystal data

$C_{10}H_{12}N_2O_3$
M_r = 208.22
Triclinic, $P\overline{1}$
a = 7.3738 (16) Å
b = 9.671 (2) Å
c = 14.689 (3) Å
α = 89.128 (4)°
β = 85.961 (4)°
γ = 87.693 (4)°
V = 1044.0 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
0.30 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.971, T_{max} = 0.984
5411 measured reflections
3674 independent reflections
2083 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.144
S = 1.00
3674 reflections
283 parameters
7 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O5^{i}	0.889 (10)	2.096 (13)	2.940 (2)	158 (2)
N4—H4A···O2	0.889 (10)	2.145 (14)	2.986 (2)	157 (2)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2470).

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supplementary materials

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N'-(4-Methoxybenzylidene)methoxyformohydrazide

Z.-H. Shang, H.-L. Zhang and Y. Ding

Comment

Symmetrical and unsymmetrical 1,3,4-oxadiazoles have been reported to be versatile compounds with many properties (Omar *et al.*, 1996; Goswami *et al.*, 1984; Tully *et al.*, 1991; Borg *et al.*, 1999). The most common synthetic approach to 1,3,4-oxadiazoles involves oxidative cyclization from the corresponding aldehyde *N*-acylhydrazones (Yang & Dai, 1993; Shang, 2006). The title compound, (I), as the oxidative precursor, was synthesized from 4-methoxybenzaldehyde and methyl hydrazinocarboxylate in ethanol under reflux.

Both asymmetric molecules of (I) adopt a *trans* configuration with respect to the C=N bond (Fig. 1) as discribed previously (Shang *et al.*, 2007). The crystal structure is stabilized mainly through intermolecular N—H··· O hydrogen bonds (Table 1).

Experimental

A mixture of 4-methoxybenzaldehyde (1.36 g, 10 mmol) and methyl hydrazinocarboxylate (0.90 g, 10 mmol) was refluxed in ethanol (30 ml) and monitored by thin-layer chromatography. After the reaction was complete, the resulting solid was filtered off and washed with a little cool methanol. 50 mg of (I) was dissolved in 20 ml e thanol and the solution was kept at room temperature for 10 d; natural evaporation gave colourless prisms of (I) suitable for X-ray analysis.

Refinement

The N-bound H atoms were located in a difference map and their positions and U_{iso} values were freely refined.

The C-bound H atoms were positioned geometrically, with C—H = 0.93–0.96Å and refined in a riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

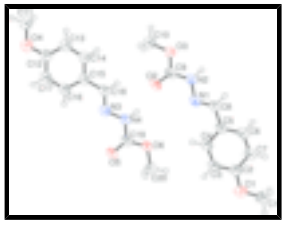

Fig. 1. The molecular structure of (I), drawn with 50% probability ellipsoids (arbitrary spheres for the H atoms).

Fig. 2. Reaction scheme for the formation of the title compound.

N'-(4-Methoxybenzylidene)methoxyformohydrazide

Crystal data

$C_{10}H_{12}N_2O_3$	$Z = 4$
$M_r = 208.22$	$F_{000} = 440$
Triclinic, $P\overline{1}$	$D_x = 1.325$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 464-466 K
$a = 7.3738$ (16) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 9.671$ (2) Å	Cell parameters from 1471 reflections
$c = 14.689$ (3) Å	$\theta = 2.5$–24.6º
$\alpha = 89.128$ (4)º	$\mu = 0.10$ mm^{-1}
$\beta = 85.961$ (4)º	$T = 293$ (2) K
$\gamma = 87.693$ (4)º	Prism, colorless
$V = 1044.0$ (4) Å^3	0.30 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD diffractometer	3674 independent reflections
Radiation source: fine-focus sealed tube	2083 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.025$
$T = 293$(2) K	$\theta_{max} = 25.0$º
ω scans	$\theta_{min} = 2.1$º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$h = -8 \rightarrow 8$
$T_{min} = 0.971$, $T_{max} = 0.984$	$k = -9 \rightarrow 11$
5411 measured reflections	$l = -12 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.144$	$w = 1/[\sigma^2(F_o^2) + (0.0721P)^2 + 0.0669P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
3674 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
283 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
7 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.0466 (3)	0.72191 (18)	−0.27347 (12)	0.0742 (6)
O2	0.4251 (3)	0.72508 (15)	0.24793 (12)	0.0739 (6)
O3	0.3898 (3)	0.92926 (15)	0.32026 (11)	0.0672 (5)
O4	0.1151 (3)	0.22590 (17)	0.70570 (12)	0.0740 (6)
O5	0.6009 (2)	0.21963 (15)	0.15450 (11)	0.0613 (5)
O6	0.6331 (2)	0.42596 (15)	0.08266 (11)	0.0609 (5)
N1	0.6155 (3)	0.85722 (18)	0.10837 (13)	0.0511 (5)
N2	0.5379 (3)	0.92379 (19)	0.18515 (14)	0.0543 (5)
N3	0.4456 (3)	0.35778 (19)	0.30239 (13)	0.0538 (5)
N4	0.5092 (3)	0.42285 (19)	0.22325 (14)	0.0554 (6)
C1	1.1315 (5)	0.8106 (3)	−0.34000 (18)	0.0860 (9)
H1A	1.0423	0.8755	−0.3620	0.129*
H1B	1.1851	0.7565	−0.3899	0.129*
H1C	1.2243	0.8598	−0.3131	0.129*
C2	0.9621 (3)	0.7807 (2)	−0.19683 (17)	0.0553 (6)
C3	0.8874 (4)	0.6903 (2)	−0.13273 (18)	0.0636 (7)
H3	0.8954	0.5958	−0.1440	0.076*
C4	0.8010 (3)	0.7373 (2)	−0.05229 (17)	0.0573 (7)
H4	0.7531	0.6744	−0.0094	0.069*
C5	0.7851 (3)	0.8790 (2)	−0.03477 (16)	0.0486 (6)
C6	0.8608 (4)	0.9673 (2)	−0.10001 (17)	0.0598 (7)
H6	0.8516	1.0620	−0.0895	0.072*
C7	0.9497 (4)	0.9210 (2)	−0.18051 (17)	0.0615 (7)
H7	1.0004	0.9834	−0.2229	0.074*
C8	0.6944 (3)	0.9342 (2)	0.04870 (16)	0.0511 (6)
H8	0.6943	1.0289	0.0586	0.061*
C9	0.4497 (4)	0.8480 (2)	0.24991 (17)	0.0543 (6)
C10	0.2883 (4)	0.8629 (3)	0.39364 (19)	0.0823 (9)
H10A	0.1935	0.8119	0.3699	0.123*
H10B	0.2354	0.9315	0.4351	0.123*
H10C	0.3677	0.8008	0.4253	0.123*
C11	0.0553 (4)	0.3160 (3)	0.77846 (17)	0.0767 (8)
H11A	0.1506	0.3770	0.7898	0.115*

H11B	0.0253	0.2623	0.8325	0.115*
H11C	−0.0503	0.3696	0.7621	0.115*
C12	0.1746 (3)	0.2837 (2)	0.62447 (17)	0.0555 (6)
C13	0.1735 (4)	0.4221 (3)	0.60634 (18)	0.0778 (9)
H13	0.1303	0.4850	0.6508	0.093*
C14	0.2377 (5)	0.4679 (3)	0.52072 (19)	0.0879 (10)
H14	0.2366	0.5627	0.5090	0.105*
C15	0.3028 (3)	0.3802 (2)	0.45221 (16)	0.0545 (6)
C16	0.3010 (4)	0.2401 (3)	0.47233 (18)	0.0685 (8)
H16	0.3434	0.1766	0.4281	0.082*
C17	0.2375 (4)	0.1938 (3)	0.55668 (19)	0.0776 (9)
H17	0.2369	0.0991	0.5685	0.093*
C18	0.3728 (4)	0.4349 (2)	0.36433 (16)	0.0616 (7)
H18	0.3635	0.5298	0.3535	0.074*
C19	0.5820 (3)	0.3447 (2)	0.15391 (16)	0.0486 (6)
C20	0.7034 (4)	0.3552 (3)	0.00160 (17)	0.0682 (8)
H20A	0.8084	0.2986	0.0149	0.102*
H20B	0.7369	0.4218	−0.0451	0.102*
H20C	0.6118	0.2978	−0.0192	0.102*
H2A	0.543 (3)	1.0150 (11)	0.1909 (16)	0.073 (8)*
H4A	0.496 (3)	0.5137 (11)	0.2144 (17)	0.075 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0931 (15)	0.0597 (11)	0.0668 (12)	0.0012 (10)	0.0165 (11)	−0.0158 (10)
O2	0.1020 (15)	0.0338 (9)	0.0830 (13)	−0.0088 (9)	0.0193 (11)	−0.0066 (9)
O3	0.0990 (15)	0.0413 (9)	0.0585 (11)	−0.0052 (9)	0.0160 (10)	−0.0047 (8)
O4	0.1010 (15)	0.0564 (11)	0.0617 (11)	−0.0050 (10)	0.0148 (10)	0.0021 (9)
O5	0.0861 (13)	0.0310 (9)	0.0655 (11)	0.0002 (8)	0.0045 (9)	−0.0051 (7)
O6	0.0915 (14)	0.0356 (9)	0.0533 (10)	−0.0021 (8)	0.0115 (9)	−0.0037 (8)
N1	0.0595 (13)	0.0370 (10)	0.0559 (12)	0.0019 (9)	0.0018 (10)	−0.0079 (10)
N2	0.0738 (15)	0.0313 (10)	0.0558 (13)	−0.0009 (10)	0.0090 (11)	−0.0035 (10)
N3	0.0657 (14)	0.0406 (10)	0.0544 (12)	−0.0047 (10)	0.0022 (11)	−0.0034 (10)
N4	0.0786 (16)	0.0330 (11)	0.0526 (12)	−0.0011 (10)	0.0099 (11)	−0.0041 (10)
C1	0.119 (3)	0.077 (2)	0.0587 (17)	0.0095 (18)	0.0152 (18)	−0.0035 (16)
C2	0.0609 (17)	0.0481 (14)	0.0563 (15)	0.0027 (12)	−0.0006 (13)	−0.0108 (12)
C3	0.0767 (19)	0.0371 (13)	0.0752 (18)	−0.0018 (12)	0.0103 (15)	−0.0145 (13)
C4	0.0639 (17)	0.0406 (13)	0.0663 (17)	−0.0026 (12)	0.0065 (13)	−0.0069 (12)
C5	0.0526 (15)	0.0370 (12)	0.0564 (15)	−0.0008 (10)	−0.0041 (12)	−0.0089 (11)
C6	0.0780 (19)	0.0373 (12)	0.0627 (16)	0.0030 (12)	0.0044 (14)	−0.0096 (12)
C7	0.079 (2)	0.0458 (14)	0.0581 (16)	−0.0003 (13)	0.0046 (14)	−0.0001 (12)
C8	0.0645 (17)	0.0321 (11)	0.0563 (15)	−0.0022 (11)	0.0001 (13)	−0.0065 (11)
C9	0.0671 (18)	0.0345 (13)	0.0608 (16)	0.0027 (11)	−0.0032 (13)	−0.0060 (12)
C10	0.106 (2)	0.0636 (17)	0.0737 (19)	−0.0154 (16)	0.0278 (17)	−0.0073 (15)
C11	0.096 (2)	0.0724 (18)	0.0594 (17)	−0.0045 (16)	0.0120 (16)	−0.0027 (15)
C12	0.0641 (17)	0.0472 (14)	0.0548 (15)	−0.0070 (12)	0.0001 (13)	0.0012 (12)
C13	0.122 (3)	0.0487 (16)	0.0600 (17)	−0.0051 (16)	0.0165 (17)	−0.0069 (13)

C14	0.149 (3)	0.0395 (15)	0.0697 (19)	0.0006 (16)	0.028 (2)	0.0000 (14)
C15	0.0658 (18)	0.0406 (13)	0.0562 (15)	−0.0022 (11)	0.0026 (13)	−0.0030 (11)
C16	0.092 (2)	0.0434 (14)	0.0676 (18)	−0.0036 (13)	0.0160 (16)	−0.0083 (13)
C17	0.112 (3)	0.0397 (14)	0.077 (2)	−0.0070 (14)	0.0239 (18)	−0.0012 (14)
C18	0.090 (2)	0.0355 (13)	0.0578 (16)	0.0018 (13)	0.0055 (15)	−0.0027 (12)
C19	0.0584 (17)	0.0338 (12)	0.0539 (15)	−0.0036 (11)	−0.0030 (12)	−0.0043 (11)
C20	0.093 (2)	0.0529 (15)	0.0558 (16)	0.0003 (14)	0.0123 (15)	−0.0101 (13)

Geometric parameters (Å, °)

O1—C2	1.368 (3)	C5—C6	1.377 (3)
O1—C1	1.419 (3)	C5—C8	1.453 (3)
O2—C9	1.211 (3)	C6—C7	1.383 (3)
O3—C9	1.347 (3)	C6—H6	0.9300
O3—C10	1.427 (3)	C7—H7	0.9300
O4—C12	1.361 (3)	C8—H8	0.9300
O4—C11	1.424 (3)	C10—H10A	0.9600
O5—C19	1.212 (2)	C10—H10B	0.9600
O6—C19	1.341 (3)	C10—H10C	0.9600
O6—C20	1.437 (3)	C11—H11A	0.9600
N1—C8	1.266 (3)	C11—H11B	0.9600
N1—N2	1.384 (3)	C11—H11C	0.9600
N2—C9	1.340 (3)	C12—C13	1.361 (3)
N2—H2A	0.889 (10)	C12—C17	1.375 (3)
N3—C18	1.262 (3)	C13—C14	1.385 (4)
N3—N4	1.375 (3)	C13—H13	0.9300
N4—C19	1.346 (3)	C14—C15	1.373 (3)
N4—H4A	0.889 (10)	C14—H14	0.9300
C1—H1A	0.9600	C15—C16	1.383 (3)
C1—H1B	0.9600	C15—C18	1.456 (3)
C1—H1C	0.9600	C16—C17	1.368 (3)
C2—C3	1.376 (3)	C16—H16	0.9300
C2—C7	1.380 (3)	C17—H17	0.9300
C3—C4	1.376 (3)	C18—H18	0.9300
C3—H3	0.9300	C20—H20A	0.9600
C4—C5	1.397 (3)	C20—H20B	0.9600
C4—H4	0.9300	C20—H20C	0.9600
C2—O1—C1	118.0 (2)	O3—C10—H10A	109.5
C9—O3—C10	116.03 (19)	O3—C10—H10B	109.5
C12—O4—C11	118.09 (19)	H10A—C10—H10B	109.5
C19—O6—C20	115.72 (17)	O3—C10—H10C	109.5
C8—N1—N2	115.66 (18)	H10A—C10—H10C	109.5
C9—N2—N1	118.34 (19)	H10B—C10—H10C	109.5
C9—N2—H2A	120.4 (17)	O4—C11—H11A	109.5
N1—N2—H2A	121.3 (17)	O4—C11—H11B	109.5
C18—N3—N4	116.34 (19)	H11A—C11—H11B	109.5
C19—N4—N3	118.58 (19)	O4—C11—H11C	109.5
C19—N4—H4A	118.6 (17)	H11A—C11—H11C	109.5
N3—N4—H4A	122.7 (17)	H11B—C11—H11C	109.5

O1—C1—H1A	109.5	C13—C12—O4	124.6 (2)
O1—C1—H1B	109.5	C13—C12—C17	118.8 (2)
H1A—C1—H1B	109.5	O4—C12—C17	116.6 (2)
O1—C1—H1C	109.5	C12—C13—C14	119.0 (3)
H1A—C1—H1C	109.5	C12—C13—H13	120.5
H1B—C1—H1C	109.5	C14—C13—H13	120.5
O1—C2—C3	116.0 (2)	C15—C14—C13	123.3 (2)
O1—C2—C7	124.5 (2)	C15—C14—H14	118.4
C3—C2—C7	119.5 (2)	C13—C14—H14	118.4
C2—C3—C4	121.2 (2)	C14—C15—C16	116.5 (2)
C2—C3—H3	119.4	C14—C15—C18	120.7 (2)
C4—C3—H3	119.4	C16—C15—C18	122.8 (2)
C3—C4—C5	120.2 (2)	C17—C16—C15	120.7 (2)
C3—C4—H4	119.9	C17—C16—H16	119.7
C5—C4—H4	119.9	C15—C16—H16	119.7
C6—C5—C4	117.4 (2)	C16—C17—C12	121.8 (2)
C6—C5—C8	120.0 (2)	C16—C17—H17	119.1
C4—C5—C8	122.5 (2)	C12—C17—H17	119.1
C5—C6—C7	122.7 (2)	N3—C18—C15	122.2 (2)
C5—C6—H6	118.6	N3—C18—H18	118.9
C7—C6—H6	118.6	C15—C18—H18	118.9
C2—C7—C6	118.8 (2)	O5—C19—O6	124.1 (2)
C2—C7—H7	120.6	O5—C19—N4	126.0 (2)
C6—C7—H7	120.6	O6—C19—N4	109.86 (19)
N1—C8—C5	122.0 (2)	O6—C20—H20A	109.5
N1—C8—H8	119.0	O6—C20—H20B	109.5
C5—C8—H8	119.0	H20A—C20—H20B	109.5
O2—C9—N2	126.7 (2)	O6—C20—H20C	109.5
O2—C9—O3	123.5 (2)	H20A—C20—H20C	109.5
N2—C9—O3	109.78 (19)	H20B—C20—H20C	109.5
C8—N1—N2—C9	178.8 (2)	C10—O3—C9—N2	178.3 (2)
C18—N3—N4—C19	−177.6 (2)	C11—O4—C12—C13	−3.1 (4)
C1—O1—C2—C3	−177.7 (2)	C11—O4—C12—C17	177.7 (2)
C1—O1—C2—C7	1.6 (4)	O4—C12—C13—C14	−179.9 (3)
O1—C2—C3—C4	179.1 (2)	C17—C12—C13—C14	−0.7 (4)
C7—C2—C3—C4	−0.3 (4)	C12—C13—C14—C15	0.1 (5)
C2—C3—C4—C5	1.0 (4)	C13—C14—C15—C16	0.4 (5)
C3—C4—C5—C6	−0.9 (4)	C13—C14—C15—C18	−178.4 (3)
C3—C4—C5—C8	179.6 (2)	C14—C15—C16—C17	−0.2 (4)
C4—C5—C6—C7	0.1 (4)	C18—C15—C16—C17	178.6 (3)
C8—C5—C6—C7	179.6 (2)	C15—C16—C17—C12	−0.4 (5)
O1—C2—C7—C6	−179.9 (2)	C13—C12—C17—C16	0.9 (5)
C3—C2—C7—C6	−0.5 (4)	O4—C12—C17—C16	−179.8 (2)
C5—C6—C7—C2	0.6 (4)	N4—N3—C18—C15	−178.8 (2)
N2—N1—C8—C5	178.8 (2)	C14—C15—C18—N3	174.7 (3)
C6—C5—C8—N1	176.5 (2)	C16—C15—C18—N3	−4.0 (4)
C4—C5—C8—N1	−4.0 (4)	C20—O6—C19—O5	4.0 (3)
N1—N2—C9—O2	−2.2 (4)	C20—O6—C19—N4	−176.4 (2)
N1—N2—C9—O3	177.75 (19)	N3—N4—C19—O5	−1.4 (4)

C10—O3—C9—O2	−1.8 (4)	N3—N4—C19—O6	178.99 (19)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O5^{i}	0.889 (10)	2.096 (13)	2.940 (2)	158 (2)
N4—H4A···O2	0.889 (10)	2.145 (14)	2.986 (2)	157 (2)

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

Fig. 1

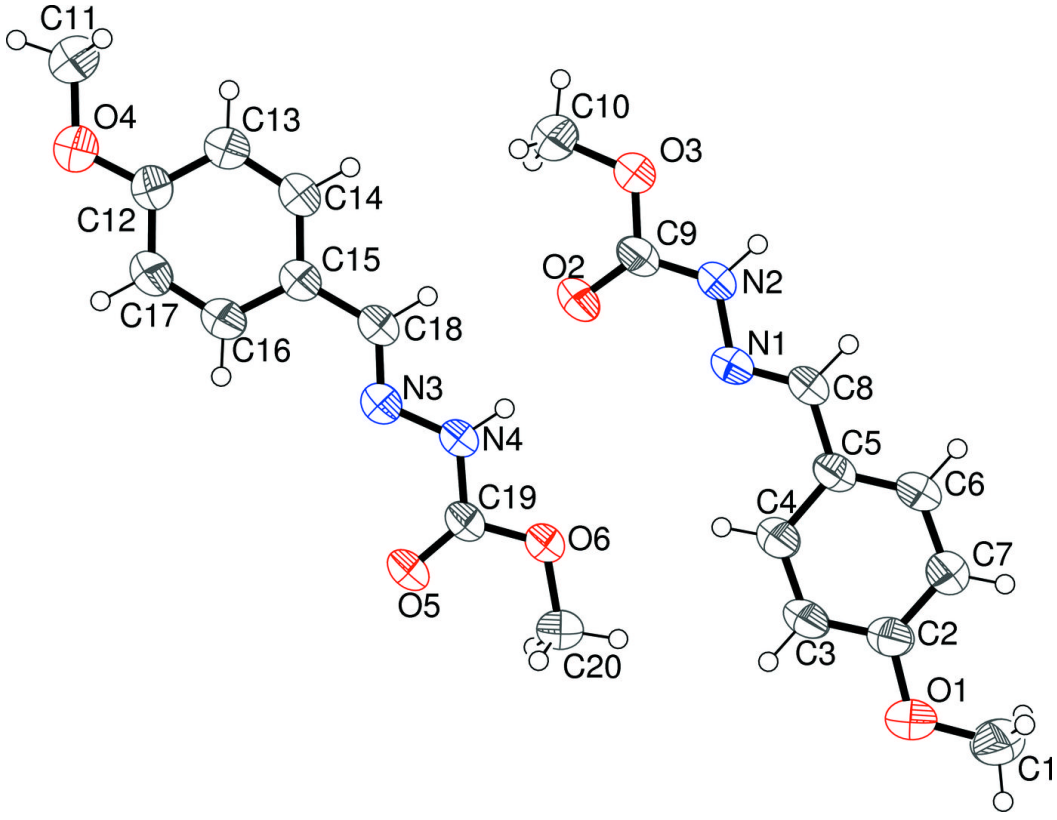
C11
O4
C13
C14
C12
C15
C17
C16
C18
N3
N4
C19
O6
O5
C20
C10
O3
C9
O2
N2
N1
C8
C5
C6
C4
C7
C3
C2
O1
C1

Fig. 2