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(E)-Methyl N'-(3-methoxybenzylidene)-hydrazinecarboxylateLu-Ping Lv,^a Wen-Bo Yu,^a Chun-Yu Huang,^b Wei-Wei Li^a and Xian-Chao Hu^{c*}^aDepartment of Chemical Engineering, Hangzhou Vocational and Technical College, Hangzhou 310018, People's Republic of China, ^bThe Children's Hospital of Zhejiang University, School of Medicine, Hangzhou 310003, People's Republic of China, and ^cResearch Center of Analysis and Measurement, Zhejiang University of Technology, Hangzhou 310014, People's Republic of China

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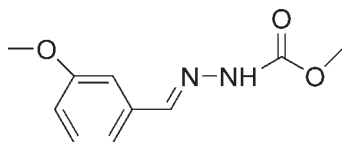
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Key indicators: single-crystal X-ray study; $T = 223$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.037; wR factor = 0.109; data-to-parameter ratio = 13.7.

The title compound, $\text{C}_{10}\text{H}_{12}\text{N}_2\text{O}_3$, crystallizes with two independent molecules in the asymmetric unit which differ in the orientation of the methoxy group. Each independent molecule adopts a *trans* configuration with respect to the $\text{C}=\text{N}$ bond. In the crystal structure, molecules are linked into chains running along [001] by $\text{N}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds. In addition, an intermolecular $\text{C}-\text{H}\cdots\pi$ interaction is observed.

Related literature

For general background to the properties of benzaldehyde-hydrazone derivatives, see: Parashar *et al.* (1988); Hadjoudis *et al.* (1987); Borg *et al.* (1999); Kahwa *et al.* (1986); Santos *et al.* (2001). For a related structure, see: Shang *et al.* (2007).



Experimental

Crystal data

$\text{C}_{10}\text{H}_{12}\text{N}_2\text{O}_3$
 $M_r = 208.22$
 Monoclinic, $P2_1/c$
 $a = 18.207$ (3) Å

$b = 7.3677$ (12) Å
 $c = 16.552$ (3) Å
 $\beta = 104.243$ (5)°
 $V = 2152.1$ (6) Å³

$Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹

$T = 223$ K
 $0.24 \times 0.21 \times 0.19$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
 $T_{\min} = 0.977$, $T_{\max} = 0.989$
 11364 measured reflections
 3790 independent reflections
 3033 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.109$
 $S = 1.07$
 3790 reflections

276 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.20$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.17$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H2}\cdots\text{O5}$	0.86	2.07	2.9188 (18)	172
$\text{N4}-\text{H4}\cdots\text{O2}^{\text{i}}$	0.86	2.25	2.8365 (17)	126
$\text{N4}-\text{H4}\cdots\text{N1}^{\text{i}}$	0.86	2.55	3.3883 (19)	164
$\text{C11}-\text{H11B}\cdots\text{Cg1}^{\text{ii}}$	0.96	2.91	3.776 (3)	150

Symmetry codes: (i) $x, -y + \frac{3}{2}, z + \frac{1}{2}$; (ii) $-x + 1, -y + 1, -z + 1$. Cg1 is the centroid of the C12-C17 ring.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); 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: CI2891).

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supplementary materials

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(*E*)-Methyl *N'*-(3-methoxybenzylidene)hydrazinecarboxylate

L.-P. Lv, W.-B. Yu, C.-Y. Huang, W.-W. Li and X.-C. Hu

Comment

Benzaldehydehydrazone derivatives have attracted much attention due to their pharmacological activity (Parashar *et al.*, 1988) and their photochromic properties (Hadjoudis *et al.*, 1987). They are important intermediates of 1,3,4-oxadiazoles, which have been reported to be versatile compounds with many interesting properties (Borg *et al.*, 1999). Metal complexes based on Schiff bases have received considerable attention because they can be utilized as model compounds of active centres in various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*, 2001). We report here the crystal structure of the title compound (Fig. 1).

The title compound contains two independent, but almost identical molecules in the asymmetric unit. Each independent molecule adopts a *trans* configuration with respect to the C=N bond. The N1/N2/O2/O3/C8/C9/C10 and N3/N4/O5/O6/C18/C19/C20 planes form dihedral angles of 4.51 (6)° and 13.80 (6)°, respectively, with the C2—C7 and C12—C17 planes. The dihedral angle between the two independent benzene rings is 59.18 (6)°. Bond lengths and angles are comparable to those observed for methyl *N'*-[(*E*)-4-methoxybenzylidene]hydrazinecarboxylate (Shang *et al.*, 2007).

In the crystal structure, molecules are linked into chains running along the [001] by N—H⋯O and N—H⋯N hydrogen bonds. In addition, an intermolecular C—H⋯π interaction is observed (Table 1).

Experimental

3-Methoxybenzaldehyde (1.36 g, 0.01 mol) and methyl hydrazinecarboxylate (0.90 g, 0.01 mol) were dissolved in stirred methanol (20 ml) and left for 2.5 h at room temperature. The resulting solid was filtered off and recrystallized from ethanol to give the title compound in 95% yield. Single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution at room temperature (m.p. 436–438 K).

Refinement

H atoms were positioned geometrically (N-H = 0.86 Å and C-H = 0.93 or 0.96 Å) and refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ and $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$. A rotating group model was used for the methyl groups.

Figures

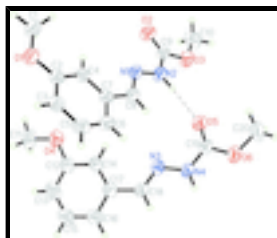


Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 40% probability level. The dashed line indicates a hydrogen bond.

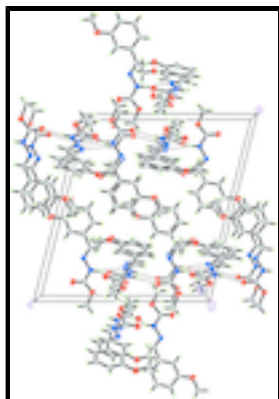


Fig. 2. Crystal packing of the title compound. Hydrogen bonds are shown as dashed lines.

(E)-Methyl N¹-(3-methoxybenzylidene)hydrazinecarboxylate

Crystal data

C₁₀H₁₂N₂O₃

M_r = 208.22

Monoclinic, *P*2₁/*c*

Hall symbol: -*P* 2ybc

a = 18.207 (3) Å

b = 7.3677 (12) Å

c = 16.552 (3) Å

β = 104.243 (5)°

V = 2152.1 (6) Å³

Z = 8

*F*₀₀₀ = 880

D_x = 1.285 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 3790 reflections

θ = 2.3–25.0°

μ = 0.10 mm⁻¹

T = 223 K

Block, colourless

0.24 × 0.21 × 0.19 mm

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 223 K

φ and ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2002)

T_{min} = 0.977, *T_{max}* = 0.989

11364 measured reflections

3790 independent reflections

3033 reflections with *I* > 2σ(*I*)

R_{int} = 0.020

θ_{max} = 25.0°

θ_{min} = 2.3°

h = -21→18

k = -8→8

l = -19→19

Refinement

Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2σ(*F*²)] = 0.037

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 0.3311P]$

where $P = (F_o^2 + 2F_c^2)/3$

$wR(F^2) = 0.109$	$(\Delta/\sigma)_{\max} = 0.004$
$S = 1.07$	$\Delta\rho_{\max} = 0.20 \text{ e } \text{\AA}^{-3}$
3790 reflections	$\Delta\rho_{\min} = -0.17 \text{ e } \text{\AA}^{-3}$
276 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0115 (12)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.68188 (7)	1.33813 (15)	-0.17091 (7)	0.0626 (3)
O2	0.86739 (7)	0.49630 (16)	-0.12622 (7)	0.0661 (3)
O3	0.92117 (7)	0.34574 (16)	-0.00794 (8)	0.0717 (4)
O4	0.55036 (7)	0.73143 (19)	-0.03581 (8)	0.0788 (4)
O5	0.90715 (7)	0.5763 (2)	0.18325 (7)	0.0792 (4)
O6	0.96333 (6)	0.64573 (18)	0.31586 (7)	0.0690 (4)
N1	0.82614 (7)	0.75999 (16)	-0.02931 (7)	0.0491 (3)
N2	0.86458 (7)	0.60387 (17)	0.00177 (8)	0.0545 (3)
H2	0.8769	0.5836	0.0546	0.065*
N3	0.77335 (7)	0.69523 (16)	0.21361 (7)	0.0492 (3)
N4	0.84157 (7)	0.68885 (19)	0.27209 (8)	0.0574 (4)
H4	0.8442	0.7210	0.3227	0.069*
C1	0.69744 (12)	1.2445 (3)	-0.23962 (10)	0.0724 (5)
H1A	0.6782	1.3132	-0.2896	0.109*
H1B	0.6735	1.1276	-0.2449	0.109*
H1C	0.7512	1.2294	-0.2309	0.109*
C2	0.70930 (8)	1.2656 (2)	-0.09344 (9)	0.0482 (4)
C3	0.70053 (9)	1.3743 (2)	-0.02757 (10)	0.0559 (4)
H3	0.6774	1.4873	-0.0382	0.067*
C4	0.74387 (8)	1.0972 (2)	-0.07774 (9)	0.0478 (4)
H4A	0.7500	1.0249	-0.1217	0.057*
C5	0.72602 (10)	1.3148 (2)	0.05299 (10)	0.0612 (4)
H5	0.7204	1.3879	0.0969	0.073*
C6	0.76013 (9)	1.1460 (2)	0.06930 (10)	0.0567 (4)

supplementary materials

H6	0.7768	1.1058	0.1240	0.068*
C7	0.76944 (8)	1.0368 (2)	0.00429 (9)	0.0475 (4)
C8	0.80804 (9)	0.8620 (2)	0.02498 (9)	0.0510 (4)
H8	0.8199	0.8239	0.0802	0.061*
C9	0.88263 (9)	0.4835 (2)	-0.05143 (10)	0.0522 (4)
C10	0.94571 (13)	0.2072 (3)	-0.05631 (15)	0.0888 (6)
H10A	0.9814	0.1291	-0.0201	0.133*
H10B	0.9694	0.2625	-0.0960	0.133*
H10C	0.9028	0.1373	-0.0853	0.133*
C11	0.47641 (11)	0.7249 (3)	-0.09038 (13)	0.0860 (6)
H11A	0.4804	0.7021	-0.1463	0.129*
H11B	0.4513	0.8388	-0.0885	0.129*
H11C	0.4478	0.6293	-0.0731	0.129*
C12	0.55619 (9)	0.7559 (2)	0.04734 (10)	0.0567 (4)
C13	0.49554 (11)	0.7833 (3)	0.08170 (14)	0.0777 (6)
H13	0.4464	0.7862	0.0480	0.093*
C14	0.62919 (9)	0.7513 (2)	0.09829 (10)	0.0518 (4)
H14	0.6700	0.7337	0.0747	0.062*
C15	0.50852 (12)	0.8064 (4)	0.16661 (15)	0.0962 (7)
H15	0.4676	0.8253	0.1899	0.115*
C16	0.58066 (11)	0.8024 (3)	0.21795 (13)	0.0812 (6)
H16	0.5882	0.8194	0.2751	0.097*
C17	0.64204 (9)	0.7725 (2)	0.18355 (10)	0.0531 (4)
C18	0.71842 (9)	0.7617 (2)	0.23885 (10)	0.0528 (4)
H18	0.7269	0.8041	0.2933	0.063*
C19	0.90395 (9)	0.6325 (2)	0.25016 (9)	0.0504 (4)
C20	1.03667 (10)	0.6043 (3)	0.30340 (14)	0.0839 (6)
H20A	1.0750	0.6610	0.3463	0.126*
H20B	1.0401	0.6489	0.2500	0.126*
H20C	1.0441	0.4752	0.3056	0.126*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0750 (8)	0.0619 (7)	0.0499 (6)	0.0148 (6)	0.0135 (5)	0.0052 (5)
O2	0.0832 (8)	0.0608 (7)	0.0546 (7)	0.0141 (6)	0.0177 (6)	0.0080 (5)
O3	0.0808 (9)	0.0605 (7)	0.0716 (8)	0.0215 (6)	0.0150 (6)	0.0188 (6)
O4	0.0582 (8)	0.1052 (10)	0.0640 (8)	0.0062 (7)	-0.0020 (6)	-0.0096 (7)
O5	0.0762 (9)	0.1133 (11)	0.0448 (7)	0.0302 (8)	0.0089 (6)	-0.0079 (7)
O6	0.0538 (7)	0.0895 (9)	0.0555 (7)	0.0082 (6)	-0.0021 (5)	-0.0090 (6)
N1	0.0505 (8)	0.0482 (7)	0.0468 (7)	0.0021 (6)	0.0085 (6)	0.0069 (5)
N2	0.0622 (8)	0.0538 (7)	0.0444 (7)	0.0074 (6)	0.0071 (6)	0.0094 (6)
N3	0.0509 (8)	0.0497 (7)	0.0434 (7)	-0.0003 (6)	0.0045 (6)	-0.0027 (5)
N4	0.0532 (8)	0.0758 (9)	0.0387 (7)	0.0044 (7)	0.0026 (6)	-0.0129 (6)
C1	0.0914 (14)	0.0770 (12)	0.0465 (9)	0.0169 (10)	0.0127 (9)	0.0039 (8)
C2	0.0458 (9)	0.0518 (8)	0.0477 (8)	-0.0018 (7)	0.0126 (6)	0.0009 (6)
C3	0.0568 (10)	0.0507 (8)	0.0629 (10)	0.0035 (7)	0.0201 (8)	-0.0039 (7)
C4	0.0493 (9)	0.0511 (8)	0.0437 (8)	-0.0004 (7)	0.0129 (6)	-0.0042 (6)

C5	0.0685 (11)	0.0645 (10)	0.0544 (10)	0.0014 (9)	0.0226 (8)	-0.0122 (8)
C6	0.0589 (10)	0.0689 (10)	0.0438 (8)	-0.0003 (8)	0.0157 (7)	-0.0013 (7)
C7	0.0432 (8)	0.0536 (8)	0.0468 (8)	-0.0038 (7)	0.0132 (6)	0.0006 (6)
C8	0.0519 (9)	0.0573 (9)	0.0431 (8)	-0.0014 (7)	0.0104 (7)	0.0057 (7)
C9	0.0507 (9)	0.0493 (8)	0.0546 (9)	0.0015 (7)	0.0091 (7)	0.0112 (7)
C10	0.0927 (15)	0.0646 (11)	0.1145 (17)	0.0286 (11)	0.0360 (13)	0.0127 (11)
C11	0.0681 (13)	0.0987 (15)	0.0760 (13)	-0.0005 (11)	-0.0113 (10)	-0.0085 (11)
C12	0.0513 (10)	0.0520 (9)	0.0634 (11)	-0.0023 (7)	0.0077 (8)	-0.0035 (7)
C13	0.0454 (10)	0.0951 (14)	0.0882 (15)	-0.0051 (10)	0.0079 (9)	-0.0067 (11)
C14	0.0457 (9)	0.0492 (8)	0.0596 (9)	-0.0009 (7)	0.0112 (7)	-0.0031 (7)
C15	0.0515 (12)	0.152 (2)	0.0911 (16)	-0.0039 (13)	0.0284 (11)	-0.0137 (15)
C16	0.0600 (12)	0.1185 (17)	0.0685 (12)	-0.0066 (11)	0.0224 (10)	-0.0107 (11)
C17	0.0496 (9)	0.0503 (8)	0.0601 (10)	-0.0052 (7)	0.0149 (7)	-0.0030 (7)
C18	0.0571 (10)	0.0539 (9)	0.0467 (8)	-0.0048 (7)	0.0116 (7)	-0.0053 (7)
C19	0.0565 (10)	0.0491 (8)	0.0414 (8)	0.0052 (7)	0.0044 (7)	0.0021 (6)
C20	0.0541 (12)	0.0970 (15)	0.0941 (15)	0.0160 (10)	0.0058 (10)	0.0073 (12)

Geometric parameters (Å, °)

O1—C2	1.3654 (18)	C5—C6	1.387 (2)
O1—C1	1.417 (2)	C5—H5	0.93
O2—C9	1.2039 (18)	C6—C7	1.387 (2)
O3—C9	1.3387 (18)	C6—H6	0.93
O3—C10	1.435 (2)	C7—C8	1.467 (2)
O4—C12	1.366 (2)	C8—H8	0.93
O4—C11	1.426 (2)	C10—H10A	0.96
O5—C19	1.1971 (18)	C10—H10B	0.96
O6—C19	1.3351 (18)	C10—H10C	0.96
O6—C20	1.433 (2)	C11—H11A	0.96
N1—C8	1.2757 (19)	C11—H11B	0.96
N1—N2	1.3785 (17)	C11—H11C	0.96
N2—C9	1.346 (2)	C12—C13	1.376 (3)
N2—H2	0.86	C12—C14	1.388 (2)
N3—C18	1.273 (2)	C13—C15	1.377 (3)
N3—N4	1.3749 (17)	C13—H13	0.93
N4—C19	1.341 (2)	C14—C17	1.381 (2)
N4—H4	0.86	C14—H14	0.93
C1—H1A	0.96	C15—C16	1.378 (3)
C1—H1B	0.96	C15—H15	0.93
C1—H1C	0.96	C16—C17	1.391 (2)
C2—C4	1.386 (2)	C16—H16	0.93
C2—C3	1.393 (2)	C17—C18	1.467 (2)
C3—C5	1.372 (2)	C18—H18	0.93
C3—H3	0.93	C20—H20A	0.96
C4—C7	1.396 (2)	C20—H20B	0.96
C4—H4A	0.93	C20—H20C	0.96
C2—O1—C1	117.64 (12)	O3—C10—H10A	109.5
C9—O3—C10	115.68 (14)	O3—C10—H10B	109.5
C12—O4—C11	118.03 (15)	H10A—C10—H10B	109.5

supplementary materials

C19—O6—C20	117.62 (14)	O3—C10—H10C	109.5
C8—N1—N2	115.11 (12)	H10A—C10—H10C	109.5
C9—N2—N1	119.26 (12)	H10B—C10—H10C	109.5
C9—N2—H2	120.4	O4—C11—H11A	109.5
N1—N2—H2	120.4	O4—C11—H11B	109.5
C18—N3—N4	115.39 (13)	H11A—C11—H11B	109.5
C19—N4—N3	119.91 (12)	O4—C11—H11C	109.5
C19—N4—H4	120.0	H11A—C11—H11C	109.5
N3—N4—H4	120.0	H11B—C11—H11C	109.5
O1—C1—H1A	109.5	O4—C12—C13	124.38 (16)
O1—C1—H1B	109.5	O4—C12—C14	115.73 (15)
H1A—C1—H1B	109.5	C13—C12—C14	119.90 (16)
O1—C1—H1C	109.5	C12—C13—C15	119.10 (17)
H1A—C1—H1C	109.5	C12—C13—H13	120.4
H1B—C1—H1C	109.5	C15—C13—H13	120.4
O1—C2—C4	124.80 (13)	C17—C14—C12	120.93 (16)
O1—C2—C3	115.07 (13)	C17—C14—H14	119.5
C4—C2—C3	120.13 (14)	C12—C14—H14	119.5
C5—C3—C2	120.02 (15)	C13—C15—C16	121.65 (19)
C5—C3—H3	120.0	C13—C15—H15	119.2
C2—C3—H3	120.0	C16—C15—H15	119.2
C2—C4—C7	119.68 (14)	C15—C16—C17	119.41 (19)
C2—C4—H4A	120.2	C15—C16—H16	120.3
C7—C4—H4A	120.2	C17—C16—H16	120.3
C3—C5—C6	120.27 (15)	C14—C17—C16	119.00 (16)
C3—C5—H5	119.9	C14—C17—C18	121.84 (15)
C6—C5—H5	119.9	C16—C17—C18	119.15 (16)
C7—C6—C5	120.23 (15)	N3—C18—C17	121.13 (14)
C7—C6—H6	119.9	N3—C18—H18	119.4
C5—C6—H6	119.9	C17—C18—H18	119.4
C6—C7—C4	119.66 (14)	O5—C19—O6	124.39 (15)
C6—C7—C8	118.10 (13)	O5—C19—N4	126.52 (14)
C4—C7—C8	122.22 (14)	O6—C19—N4	109.08 (13)
N1—C8—C7	123.03 (13)	O6—C20—H20A	109.5
N1—C8—H8	118.5	O6—C20—H20B	109.5
C7—C8—H8	118.5	H20A—C20—H20B	109.5
O2—C9—O3	124.75 (15)	O6—C20—H20C	109.5
O2—C9—N2	126.11 (14)	H20A—C20—H20C	109.5
O3—C9—N2	109.14 (13)	H20B—C20—H20C	109.5
C8—N1—N2—C9	176.68 (14)	N1—N2—C9—O3	178.40 (12)
C18—N3—N4—C19	-175.58 (14)	C11—O4—C12—C13	-3.2 (3)
C1—O1—C2—C4	-7.6 (2)	C11—O4—C12—C14	176.59 (15)
C1—O1—C2—C3	172.35 (15)	O4—C12—C13—C15	180.0 (2)
O1—C2—C3—C5	179.99 (15)	C14—C12—C13—C15	0.2 (3)
C4—C2—C3—C5	-0.1 (2)	O4—C12—C14—C17	-179.29 (14)
O1—C2—C4—C7	-179.72 (14)	C13—C12—C14—C17	0.5 (2)
C3—C2—C4—C7	0.4 (2)	C12—C13—C15—C16	-0.2 (4)
C2—C3—C5—C6	-0.4 (3)	C13—C15—C16—C17	-0.6 (4)
C3—C5—C6—C7	0.7 (3)	C12—C14—C17—C16	-1.3 (2)

C5—C6—C7—C4	-0.4 (2)	C12—C14—C17—C18	177.79 (14)
C5—C6—C7—C8	178.06 (15)	C15—C16—C17—C14	1.3 (3)
C2—C4—C7—C6	-0.1 (2)	C15—C16—C17—C18	-177.8 (2)
C2—C4—C7—C8	-178.51 (13)	N4—N3—C18—C17	-178.49 (13)
N2—N1—C8—C7	177.72 (13)	C14—C17—C18—N3	-15.0 (2)
C6—C7—C8—N1	-172.84 (15)	C16—C17—C18—N3	164.04 (17)
C4—C7—C8—N1	5.6 (2)	C20—O6—C19—O5	5.5 (2)
C10—O3—C9—O2	0.7 (2)	C20—O6—C19—N4	-175.48 (15)
C10—O3—C9—N2	-178.90 (15)	N3—N4—C19—O5	-3.8 (3)
N1—N2—C9—O2	-1.2 (2)	N3—N4—C19—O6	177.20 (13)

Hydrogen-bond geometry (\AA , $^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N2—H2 \cdots O5	0.86	2.07	2.9188 (18)	172
N4—H4 \cdots O2 ⁱ	0.86	2.25	2.8365 (17)	126
N4—H4 \cdots N1 ⁱ	0.86	2.55	3.3883 (19)	164
C11—H11B \cdots Cg1 ⁱⁱ	0.96	2.91	3.776 (3)	150

Symmetry codes: (i) $x, -y+3/2, z+1/2$; (ii) $-x+1, -y+1, -z+1$.

Fig. 1

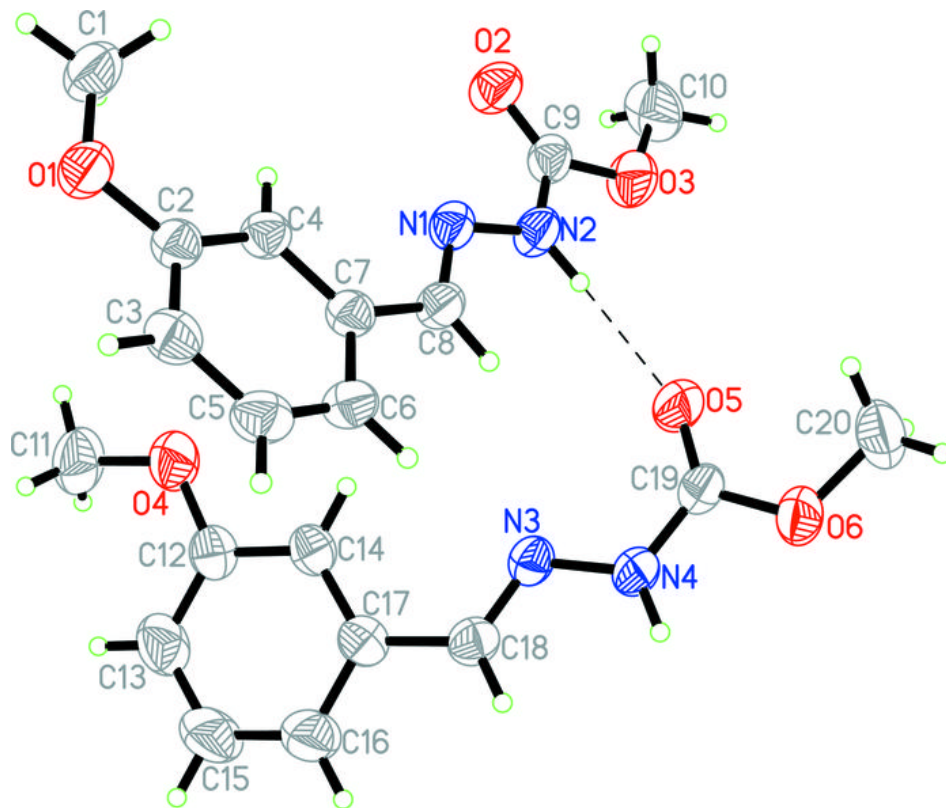


Fig. 2

