

Ethyl (*E*)-2-methoxyimino-2-(4-nitrobenzoyl)acetate

Ignez Caracelli,^{a*} Paulo J. S. Moran,^b Luciana Hinoue,^b Julio Zukerman-Schpector^c and Edward R. T. Tiekink^d

^aBioMat-Physics Department, UNESP – Univ Estadual Paulista, 17033-360 Bauru, SP, Brazil, ^bInstituto de Química, Universidade Estadual de Campinas, CP 6154, 13083-970 Campinas, SP, Brazil, ^cDepartment of Chemistry, Universidade Federal de São Carlos, 13565-905 São Carlos, SP, Brazil, and ^dDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: ignez@fc.unesp.br

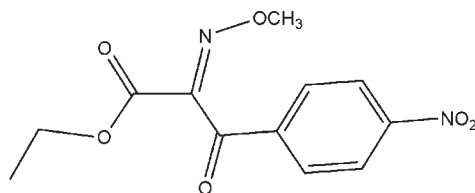
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.031; wR factor = 0.088; data-to-parameter ratio = 14.3.

The title molecule, $\text{C}_{12}\text{H}_{12}\text{N}_2\text{O}_6$, features an *E* conformation about the oxime group. The methoxyimino and ester residues are effectively coplanar with each other (r.m.s. deviation for the nine non-H atoms = 0.127 Å) and almost orthogonal [with dihedral angles of 99.44 (13) and -77.85 (13)°, respectively] to the carbonyl and nitrophenyl groups which lie to either side of this central plane. The crystal structure is consolidated by C—H···O contacts.

Related literature

For background to the synthesis of chiral hydroxyaminoacids and hydroxyaminoalcohols, see: Corrêa & Moran (1999); Kreutz *et al.* (1997, 2000). For related structures, see: Caracelli *et al.* (2010); Forsyth *et al.* (2006); Ramos Silva *et al.* (2004). For the synthesis of the title compound, see: Buehler (1967).



Experimental

Crystal data

$\text{C}_{12}\text{H}_{12}\text{N}_2\text{O}_6$
 $M_r = 280.24$
 Triclinic, $P\bar{1}$
 $a = 7.5197$ (1) Å
 $b = 7.5793$ (1) Å
 $c = 12.3338$ (2) Å
 $\alpha = 83.264$ (1)°
 $\beta = 73.731$ (1)°

$\gamma = 68.939$ (1)°
 $V = 629.62$ (2) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.12$ mm⁻¹
 $T = 100$ K
 $0.35 \times 0.25 \times 0.08$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.933$, $T_{\max} = 1.000$
 9325 measured reflections
 2614 independent reflections
 2310 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.088$
 $S = 1.05$
 2614 reflections
 183 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.28$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2···O4 ⁱ	0.93	2.56	3.3853 (14)	148
C3—H3···O2 ⁱⁱ	0.93	2.50	3.3950 (16)	162
C5—H5···O5 ⁱⁱⁱ	0.93	2.35	3.1856 (14)	150
C6—H6···O3 ^{iv}	0.93	2.46	3.3514 (16)	160

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997) and DIAMOND (Brandenburg, 2006); software used to prepare material for publication: WinGX (Farrugia, 1999), PARST (Nardelli, 1995) and publCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2157).

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supplementary materials

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Ethyl (*E*)-2-methoxyimino-2-(4-nitrobenzoyl)acetate

I. Caracelli, P. J. S. Moran, L. Hinoue, J. Zukerman-Schpector and E. R. T. Tiekink

Comment

In connection with studies involving the synthesis of chiral hydroxyaminoacids and hydroxyaminoalcohols, whereby α -ketomethoxyimino compounds are reduced by sodium borohydride (Corrêa & Moran, 1999) and enantioselectively bio-reduced by whole cells of yeast (Kreutz *et al.*, 1997; Kreutz *et al.*, 2000), the title compound was prepared as an intermediary.

The molecular structure of the title compound is illustrated in Fig. 1, and the geometrical parameters are given in the Supplementary information and the archived CIF. The conformation about the oxime bond [N2=C8 = 1.2790 (14) Å] is *E*. The methoxyimino moiety is effectively co-planar with the ester group, as seen in the sequence of O4-N2-C8-C9, N2-C8-C9-O5 and C8-C9-O6-C10 torsion angles of 177.54 (8), 6.76 (16) and 178.40 (9) °, respectively. While atom C7 lies in the mean plane of the ester group [O4-N2-C8-C7 = 2.17 (14) °], the carbonyl and nitrophenyl groups occupy positions almost orthogonal to the remaining atoms, as seen in the values of the N2-C8-C7-O3 and N2-C8-C7-C4 torsion angles of 99.44 (13) and -77.85 (13) °, respectively. The nitro group and the benzene ring to which it is attached are slightly twisted with respect to one another, with a dihedral angle of 8.54 (8)°. Globally, when viewed down the C7–C8 bond, the carbonyl-O3 atom lies to one side of the central plane and the nitrophenyl group to the other.

The crystal packing is dominated by C–H(aromatic)⋯O interactions involving the nitro-O2, carbonyl-O3 and oxime-O4 atoms to form layers in the *ab* plane (Table 1 and Fig. 2). These layers stack along [001] with interdigitation of the ethyl ester groups (Fig. 3), and C–H⋯O interactions involving the ester carbonyl-O5 atom.

The basic C(=O)C(=NOH)C(=O)OC framework in the title compound is comparatively rare with only three other structures reported, namely the recently described *Z*-isomer of the title compound (Caracelli *et al.*, 2010), 2-(hydroxyimino)-3-oxo-3-phenylpropionate, where *E*-conformations are found for each of the independent molecules (Ramos Silva *et al.*, 2004), and benzyl 2-(hydroxyimino)acetoacetate, for which a *Z* conformation is found (Forsyth *et al.*, 2006).

Experimental

The title compound was prepared following a modified literature method (Buehler, 1967). Silver oxide (1.3 mmol) was slowly added with stirring to a solution of a mixture of ethyl (*E*)- and (*Z*)-2-hydroximino-3-(4-nitrophenyl)-3-oxopropanoate (2.25 mmol) and methyl iodide (5.6 mmol) in CH₂Cl₂ (30 ml), and cooled in a ice-water bath. The temperature was then raised to 301 K and the stirring maintained for 1 h. The precipitate formed was filtered off and washed with CH₂Cl₂. The solvent was evaporated to afford yellow crystals of a mixture of *E*:*Z* (90:10) isomers in 86% yield. They were separated by TLC chromatography on silica gel with 5% ethyl acetate/hexane. The principal fraction was shown by crystallographic analysis to be the *E* isomer; m.p. 367.6–368.0 K.

Refinement

The H atoms were placed geometrically (C–H = 0.93–0.97 Å) and refined in the riding model approximation with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C-aromatic})$ and $1.5U_{\text{eq}}(\text{C-methyl})$.

Figures

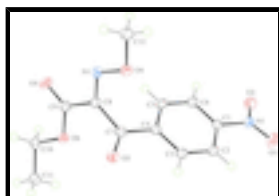


Fig. 1. Molecular structure of the title compound, showing the atom labelling scheme and displacement ellipsoids at the 50% probability level (arbitrary spheres for the H atoms).

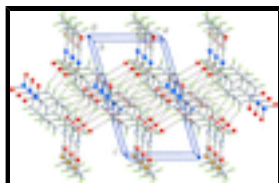


Fig. 2. A view of the layer structure in the title compound, sustained by C–H...O contacts [the C–H...O contacts are shown as brown dashed lines; colour code: O, red; N, blue; C, grey; H, green].

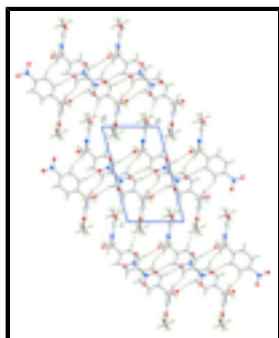


Fig. 3. A view along the *b* axis of the crystal packing of the title compound, highlighting the interdigitation of the ester groups [the C–H...O contacts are shown as brown dashed lines; colour code: O, red; N, blue; C, grey; H, green].

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Crystal data

$\text{C}_{12}\text{H}_{12}\text{N}_2\text{O}_6$

$M_r = 280.24$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 7.5197(1)\ \text{\AA}$

$b = 7.5793(1)\ \text{\AA}$

$c = 12.3338(2)\ \text{\AA}$

$\alpha = 83.264(1)^\circ$

$\beta = 73.731(1)^\circ$

$\gamma = 68.939(1)^\circ$

$V = 629.62(2)\ \text{\AA}^3$

$Z = 2$

$F(000) = 292$

$D_x = 1.478\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 5430 reflections

$\theta = 26.6\text{--}2.9^\circ$

$\mu = 0.12\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Block, pale-yellow

$0.35 \times 0.25 \times 0.08\ \text{mm}$

Data collection

Bruker APEXII CCD diffractometer	2614 independent reflections
Radiation source: fine-focus sealed tube graphite	2310 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.018$
Absorption correction: multi scan (SADABS; Sheldrick, 1996)	$\theta_{\text{max}} = 26.6^\circ$, $\theta_{\text{min}} = 1.7^\circ$
$T_{\text{min}} = 0.933$, $T_{\text{max}} = 1.000$	$h = -9 \rightarrow 9$
9325 measured reflections	$k = -9 \rightarrow 9$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.031$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.088$	H-atom parameters constrained
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 0.1834P]$
2614 reflections	where $P = (F_o^2 + 2F_c^2)/3$
183 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.28 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.24 \text{ e } \text{\AA}^{-3}$

Special details

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.95878 (16)	0.26376 (14)	0.48218 (9)	0.0180 (2)
C2	0.77279 (16)	0.24949 (15)	0.51100 (9)	0.0190 (2)
H2	0.7241	0.2000	0.5810	0.023*
C3	0.66149 (16)	0.31060 (15)	0.43316 (9)	0.0185 (2)
H3	0.5370	0.3003	0.4498	0.022*
C4	0.73587 (16)	0.38808 (14)	0.32919 (9)	0.0174 (2)

supplementary materials

C5	0.92289 (16)	0.40168 (15)	0.30321 (9)	0.0195 (2)
H5	0.9711	0.4539	0.2341	0.023*
C6	1.03760 (16)	0.33776 (15)	0.37975 (9)	0.0195 (2)
H6	1.1636	0.3444	0.3628	0.023*
C7	0.60888 (16)	0.45924 (14)	0.24893 (9)	0.0173 (2)
C8	0.67583 (15)	0.57310 (15)	0.14594 (9)	0.0175 (2)
C9	0.75507 (16)	0.49578 (15)	0.02915 (9)	0.0192 (2)
C10	0.81887 (17)	0.23916 (16)	-0.08355 (9)	0.0209 (2)
H10B	0.9588	0.2169	-0.1133	0.025*
H10A	0.7494	0.3237	-0.1353	0.025*
C11	0.78050 (19)	0.05568 (16)	-0.07074 (10)	0.0251 (3)
H11B	0.8255	-0.0029	-0.1430	0.038*
H11C	0.6416	0.0794	-0.0416	0.038*
H11A	0.8499	-0.0268	-0.0194	0.038*
C12	0.55476 (19)	1.00856 (16)	0.25880 (10)	0.0243 (3)
H12C	0.4759	1.0782	0.2084	0.036*
H12A	0.6827	1.0209	0.2336	0.036*
H12B	0.4920	1.0575	0.3336	0.036*
N2	0.65628 (13)	0.74693 (13)	0.15091 (8)	0.0189 (2)
N1	1.07936 (14)	0.19686 (13)	0.56457 (8)	0.0204 (2)
O6	0.74864 (12)	0.32311 (11)	0.02858 (6)	0.02006 (19)
O5	0.81359 (14)	0.58238 (12)	-0.05260 (7)	0.0283 (2)
O3	0.45219 (12)	0.43609 (11)	0.26469 (7)	0.02198 (19)
O4	0.57531 (12)	0.81146 (11)	0.26006 (6)	0.0221 (2)
O1	1.00183 (13)	0.15085 (13)	0.65930 (7)	0.0300 (2)
O2	1.25168 (13)	0.18865 (13)	0.53367 (7)	0.0285 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0223 (6)	0.0154 (5)	0.0157 (5)	-0.0056 (4)	-0.0047 (4)	-0.0012 (4)
C2	0.0233 (6)	0.0175 (5)	0.0144 (5)	-0.0084 (4)	-0.0006 (4)	0.0004 (4)
C3	0.0184 (5)	0.0185 (5)	0.0182 (5)	-0.0086 (4)	-0.0006 (4)	-0.0011 (4)
C4	0.0208 (5)	0.0153 (5)	0.0154 (5)	-0.0070 (4)	-0.0021 (4)	-0.0012 (4)
C5	0.0215 (5)	0.0202 (5)	0.0156 (5)	-0.0092 (4)	-0.0014 (4)	0.0021 (4)
C6	0.0180 (5)	0.0209 (5)	0.0194 (5)	-0.0087 (4)	-0.0020 (4)	0.0001 (4)
C7	0.0196 (5)	0.0155 (5)	0.0154 (5)	-0.0069 (4)	-0.0005 (4)	-0.0020 (4)
C8	0.0168 (5)	0.0200 (5)	0.0168 (5)	-0.0082 (4)	-0.0042 (4)	0.0016 (4)
C9	0.0192 (5)	0.0209 (5)	0.0182 (5)	-0.0079 (4)	-0.0048 (4)	0.0009 (4)
C10	0.0250 (6)	0.0227 (5)	0.0151 (5)	-0.0090 (4)	-0.0040 (4)	-0.0010 (4)
C11	0.0329 (7)	0.0234 (6)	0.0217 (6)	-0.0122 (5)	-0.0080 (5)	-0.0004 (5)
C12	0.0306 (6)	0.0174 (5)	0.0252 (6)	-0.0089 (5)	-0.0062 (5)	-0.0017 (4)
N2	0.0200 (5)	0.0212 (5)	0.0156 (5)	-0.0081 (4)	-0.0036 (4)	-0.0003 (4)
N1	0.0239 (5)	0.0198 (5)	0.0178 (5)	-0.0080 (4)	-0.0050 (4)	-0.0001 (4)
O6	0.0259 (4)	0.0197 (4)	0.0152 (4)	-0.0102 (3)	-0.0029 (3)	-0.0004 (3)
O5	0.0416 (5)	0.0267 (4)	0.0174 (4)	-0.0187 (4)	-0.0005 (4)	0.0013 (3)
O3	0.0217 (4)	0.0246 (4)	0.0219 (4)	-0.0121 (3)	-0.0051 (3)	0.0028 (3)
O4	0.0302 (4)	0.0188 (4)	0.0166 (4)	-0.0104 (3)	-0.0016 (3)	-0.0017 (3)

O1	0.0309 (5)	0.0414 (5)	0.0160 (4)	-0.0132 (4)	-0.0049 (4)	0.0057 (4)
O2	0.0245 (4)	0.0382 (5)	0.0269 (5)	-0.0153 (4)	-0.0094 (4)	0.0058 (4)

Geometric parameters (Å, °)

C1—C6	1.3839 (15)	C9—O5	1.2020 (14)
C1—C2	1.3839 (16)	C9—O6	1.3278 (13)
C1—N1	1.4753 (14)	C10—O6	1.4670 (13)
C2—C3	1.3798 (16)	C10—C11	1.5011 (16)
C2—H2	0.9300	C10—H10B	0.9700
C3—C4	1.4000 (15)	C10—H10A	0.9700
C3—H3	0.9300	C11—H11B	0.9600
C4—C5	1.3910 (16)	C11—H11C	0.9600
C4—C7	1.4889 (15)	C11—H11A	0.9600
C5—C6	1.3851 (16)	C12—O4	1.4442 (13)
C5—H5	0.9300	C12—H12C	0.9600
C6—H6	0.9300	C12—H12A	0.9600
C7—O3	1.2121 (14)	C12—H12B	0.9600
C7—C8	1.5194 (14)	N2—O4	1.3797 (12)
C8—N2	1.2790 (14)	N1—O1	1.2229 (12)
C8—C9	1.4965 (15)	N1—O2	1.2244 (13)
C6—C1—C2	123.25 (10)	O6—C9—C8	111.19 (9)
C6—C1—N1	118.25 (10)	O6—C10—C11	107.57 (9)
C2—C1—N1	118.51 (9)	O6—C10—H10B	110.2
C3—C2—C1	118.23 (10)	C11—C10—H10B	110.2
C3—C2—H2	120.9	O6—C10—H10A	110.2
C1—C2—H2	120.9	C11—C10—H10A	110.2
C2—C3—C4	120.00 (10)	H10B—C10—H10A	108.5
C2—C3—H3	120.0	C10—C11—H11B	109.5
C4—C3—H3	120.0	C10—C11—H11C	109.5
C5—C4—C3	120.30 (10)	H11B—C11—H11C	109.5
C5—C4—C7	121.09 (10)	C10—C11—H11A	109.5
C3—C4—C7	118.59 (10)	H11B—C11—H11A	109.5
C6—C5—C4	120.29 (10)	H11C—C11—H11A	109.5
C6—C5—H5	119.9	O4—C12—H12C	109.5
C4—C5—H5	119.9	O4—C12—H12A	109.5
C1—C6—C5	117.91 (10)	H12C—C12—H12A	109.5
C1—C6—H6	121.0	O4—C12—H12B	109.5
C5—C6—H6	121.0	H12C—C12—H12B	109.5
O3—C7—C4	122.79 (10)	H12A—C12—H12B	109.5
O3—C7—C8	119.12 (10)	C8—N2—O4	111.55 (9)
C4—C7—C8	118.03 (9)	O1—N1—O2	123.89 (10)
N2—C8—C9	114.45 (9)	O1—N1—C1	118.03 (9)
N2—C8—C7	122.66 (9)	O2—N1—C1	118.08 (9)
C9—C8—C7	122.72 (9)	C9—O6—C10	114.57 (8)
O5—C9—O6	125.40 (10)	N2—O4—C12	108.40 (8)
O5—C9—C8	123.40 (10)		
C6—C1—C2—C3	0.61 (16)	O3—C7—C8—C9	-75.55 (14)
N1—C1—C2—C3	-179.38 (9)	C4—C7—C8—C9	107.17 (12)

supplementary materials

C1—C2—C3—C4	-1.27 (15)	N2—C8—C9—O5	6.76 (16)
C2—C3—C4—C5	0.82 (16)	C7—C8—C9—O5	-177.87 (11)
C2—C3—C4—C7	-177.73 (9)	N2—C8—C9—O6	-172.26 (9)
C3—C4—C5—C6	0.35 (16)	C7—C8—C9—O6	3.10 (14)
C7—C4—C5—C6	178.85 (10)	C9—C8—N2—O4	177.54 (8)
C2—C1—C6—C5	0.52 (16)	C7—C8—N2—O4	2.17 (14)
N1—C1—C6—C5	-179.49 (9)	C6—C1—N1—O1	172.19 (10)
C4—C5—C6—C1	-0.99 (16)	C2—C1—N1—O1	-7.82 (14)
C5—C4—C7—O3	173.89 (10)	C6—C1—N1—O2	-8.63 (15)
C3—C4—C7—O3	-7.58 (16)	C2—C1—N1—O2	171.36 (10)
C5—C4—C7—C8	-8.93 (15)	O5—C9—O6—C10	-0.60 (16)
C3—C4—C7—C8	169.60 (9)	C8—C9—O6—C10	178.40 (9)
O3—C7—C8—N2	99.44 (13)	C11—C10—O6—C9	-173.74 (9)
C4—C7—C8—N2	-77.85 (13)	C8—N2—O4—C12	-179.06 (9)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 \cdots O4 ⁱ	0.93	2.56	3.3853 (14)	148
C3—H3 \cdots O2 ⁱⁱ	0.93	2.50	3.3950 (16)	162
C5—H5 \cdots O5 ⁱⁱⁱ	0.93	2.35	3.1856 (14)	150
C6—H6 \cdots O3 ^{iv}	0.93	2.46	3.3514 (16)	160

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

Fig. 1

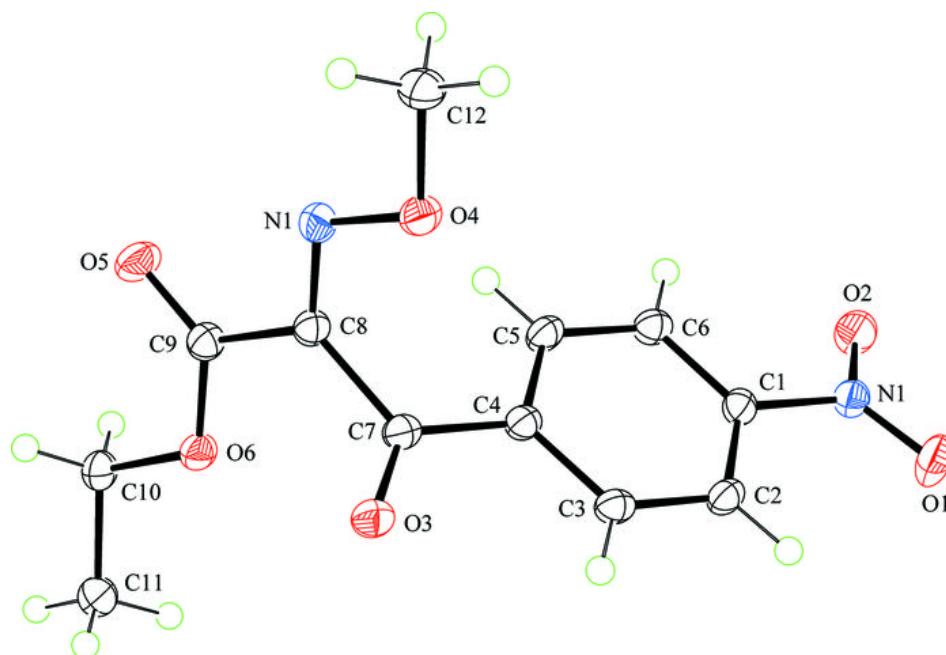


Fig. 2

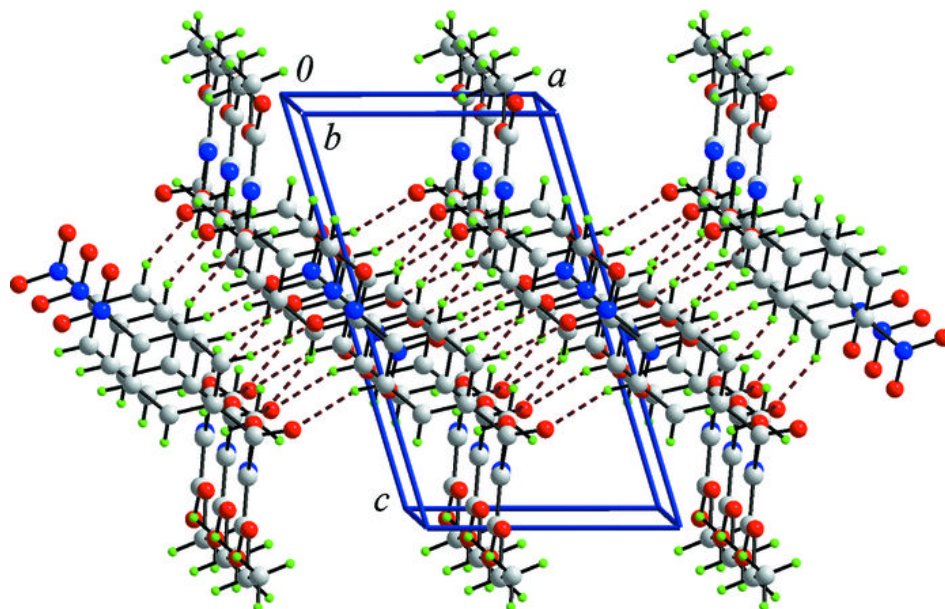


Fig. 3

