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Retraction of articles

This article reports the retraction of 39 articles published in *Acta Crystallographica Section E* between 2004 and 2009.

After thorough investigation (see Harrison *et al.*, 2010), 39 additional articles are retracted as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	Retracted by	DOI	Refcode
trans-Bis{1-[3-(cyclohexylamino)propyliminomethyl]-2-naphtholato}copper(II) dichloride dihydrate	Zhang (2004)	Journal	10.1107/S1600536804028296	BIPDUA
Bis(4-bromo-2-formylphenolato-κ^2O,O')copper(II)	Sun & Gao (2005)	Author	10.1107/S160053680500187X	FEYSUY
Bis(salicylaldehydo)zinc(II)	Xiong & Liu (2005)	Journal	10.1107/S1600536805010913	GAMDUU
Bis(4-bromo-2-formylphenolato-κ^2O,O')zinc(II)	Chen (2006)	Journal	10.1107/S1600536805040432	SAZCUS
Bis(2-formylphenolato-κ^2O,O')nickel(II)	Li & Chen (2006)	Journal	10.1107/S1600536806012931	IDAZAP
Bis(2-formylphenolato)cobalt(II)	Qiu (2006)	Journal	10.1107/S1600536806015704	GEJDUV
Bis(2-formylphenolato-κ^2O,O')manganese(II)	Wang & Fang (2006)	Journal	10.1107/S1600536806021039	IDOVED
Tetraaqua(1,10-phenanthroline-κ^2N,N')copper(II) naphthalene-1,5-disulfonate dihydrate	Liu *et al.* (2006)	Author	10.1107/S1600536806030637	GENYOO
Tetraaqua(1,10-phenanthroline-κ^2N,N')nickel(II) naphthalene-1,5-disulfonate dihydrate	Liu & Fan (2006)	Author	10.1107/S1600536806035410	KERBEP
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratolutetium(III)copper(II)	Sui *et al.* (2006)	Journal	10.1107/S160053680604565X	HESPEP
Bis(2-formylphenolato-κ^2O,O')iron(II)	Yang *et al.* (2007)	Author	10.1107/S1600536807021721	PIFCAJ
2,6-Dimethoxybenzohydrazide	Qadeer *et al.* (2007*a*)	Journal	10.1107/S1600536807022593	PIFHES
2-(2,4-Dichlorophenylsulfanyl)acetohydrazide	Qadeer *et al.* (2007*b*)	Journal	10.1107/S1600536807022891	YIFSOW
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoeuropium(III)zinc(II)	Hu *et al.* (2007)	Author	10.1107/S1600536807031121	WIHKEE
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratocerium(III)zinc(II)	Sui, Zhang, Hu & Yin (2007)	Author	10.1107/S1600536807032564	WIHREL
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)zinc(II)	Chen *et al.* (2007)	Author	10.1107/S1600536807032540	WIHRIP
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)nickel(II)	Sui, Li *et al.* (2007)	Author	10.1107/S1600536807032618	UFACUA
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(methanol-1κO)-μ-nitrato-1:2κ^2O:O′-dinitrato-1κ^4O,O'-cerium(III)zinc(II)	Sui, Fang, Hu & Lin (2007)	Author	10.1107/S1600536807033314	UDUYIC
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratosamarium(III)nickel(II)	Sui, Zhang, Hu & Jiang (2007)	Author	10.1107/S1600536807037130	AFECEU
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratopraseodymium(III)zinc(II)	Sui, Fang & Yuan (2007)	Author	10.1107/S1600536807037488	AFICEY
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratolutetium(III)zinc(II)	Sui, Sui *et al.* (2007)	Author	10.1107/S1600536807037737	AFEFOH
catena-Poly[[chloridonickel(II)]-di-μ-chlorido-[chloridonickel(II)]-μ-4,4′-methylenebis(3,5-dimethylpyrazole)-κ^2N^2:$N^{2'}$]	Huang & Chen (2007)	Author	10.1107/S1600536807039384	VIJYOD
{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}zinc(II)	Liu *et al.* (2007*a*)	Author	10.1107/S1600536807040640	DIKYUS
trans-Bis(ethylenediamine-κ^2N,N')bis(nitrato-κO)zinc(II)	Liu, Zeng & Chen (2007)	Author	10.1107/S1600536807042390	XIKYEW
[N,N′-(o-Phenylene)bis(picolinamido)-κ^4N,N',N'',N''']cobalt(II)	Liu & Zeng (2007*a*)	Author	10.1107/S1600536807044571	XILFII
[N,N′-(o-Phenylene)dipicolinamide-κ^4N]nickel(II)	Liu & Zeng (2007*b*)	Author	10.1107/S1600536807048386	WINWEW
{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}manganese(II)	Liu *et al.* (2007*b*)	Author	10.1107/S1600536807052993	VIQPIV
N-(2-Amino-3-pyridyl)urea monohydrate	Li *et al.* (2007)	Author	10.1107/S1600536807047526	SIMFEA
N-(2-Fluorophenyl)carbamic acid monohydrate	Yang (2007)	Author	10.1107/S1600536807052464	WINMOW
Aqua(dimethylglyoxime-κ^2N,N')(3,5-dinitro-2-oxidobenzoato-κ^2O^1,O^2)-copper(II)	Liu & Wen (2007)	Author	10.1107/S1600536807054244	HIQCAM
μ-Acetato-tri-μ-ferrocenecarboxylatobis[(N,N-dimethylformamide)-copper(II)]	Liu, Lin *et al.* (2007)	Journal	10.1107/S1600536807059041	HIQQEE

 doi:10.1107/S1600536809054300

Table 1 (continued)

Title	Reference	Retracted by	DOI	Refcode
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoeuropium(III)zinc(II)	Hu *et al.* (2008)	Author	10.1107/S160053680706151X	MIRPAF
Bis(4-chloro-2-formylphenolato)nickel(II)	Li *et al.* (2008)	Author	10.1107/S1600536807056309	RISTET
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoterbium(III)zinc(II)	Chen *et al.* (2008)	Author	10.1107/S1600536808006958	QIXHIP
Bis(2-ethoxy-6-formylphenolato-κ^2O^1,O^6)nickel(II)	Han (2008)	Journal	10.1107/S160053680800809X	QIXLIT
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoholmium(III)zinc(II)	Xiao, Sui *et al.* (2008)	Author	10.1107/S1600536808013743	BIZTUA
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoholmium(III)nickel(II)	Xiao, Fu *et al.* (2008)	Author	10.1107/S1600536808013755	BIZVAI
Hydrogen-bonding patterns in the cocrystal terephthalic acid–4,4′-bipyridine (2/1)	Wang *et al.* (2009)	Journal	10.1107/S160053680903236X	DUCZEH
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(ethanol-1κO)-μ-nitrato-1:2κ^2O:O′-dinitrato-1κ^4O,O′-samarium(III)zinc(II)	Huang *et al.* (2009)	Journal	10.1107/S1600536809033558	YUCWAV

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2,6-Dimethoxybenzohydrazide

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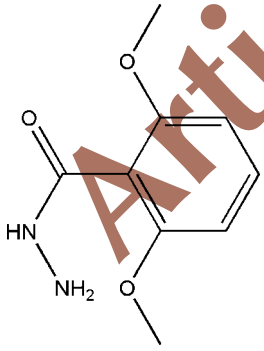
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.066; wR factor = 0.109; data-to-parameter ratio = 20.4.

The title compound, $C_9H_{12}N_2O_3$, is an important intermediate for the synthesis of biologically active heterocyclic compounds. The planar hydrazide group is oriented with respect to the benzene ring at a dihedral angle of 82.93 (3)°.

Related literature

For general background, see: Zheng *et al.* (2003); Al-Talib *et al.* (1990); Yousif *et al.* (1986); Ahmad *et al.* (2001); Al-Soud *et al.* (2004); El-Emam *et al.* (2004); Allen *et al.* (1987); Furniss *et al.* (1978).



Experimental

Crystal data

$C_9H_{12}N_2O_3$
M_r = 196.21
Orthorhombic, *Pbca*
a = 7.2598 (5) Å
b = 14.2558 (11) Å
c = 20.0412 (11) Å
V = 2074.1 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
0.16 × 0.14 × 0.06 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.981, T_{max} = 0.993
14489 measured reflections
2615 independent reflections
1044 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.109
S = 1.99
2615 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); 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, 1999); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2245).

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supplementary materials

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2,6-Dimethoxybenzohydrazide

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Comment

Aromatic hydrazides are important intermediates in heterocyclic chemistry and have been used for the synthesis of various biologically active five-membered heterocycles such as 2,5-disubstituted-1,3,4-oxadiazoles (Zheng *et al.*, 2003; Al-Talib *et al.*, 1990) and 5-substituted-2-mercapto-1,3,4-oxadiazoles (Yousif *et al.*, 1986; Ahmad *et al.*, 2001; Al-Soud *et al.*, 2004; El-Emam *et al.*, 2004). In view of the versatility of these compounds, we have synthesized the title compound, (I), and reported its crystal structure.

In the molecule of the title compound, (I), (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The dihedral angle between the planar hydrazidic group (C9/O3/N1/N2) and benzene ring (C1—C6) is 97.07 (3)°.

Experimental

The title compound, (I), is synthesized by reaction of the methyl ester of 3,5-difluorobenzoic acid with hydrazine hydrate using a reported procedure (Furniss *et al.*, 1978). For the preparation of (I), a mixture of methyl-2,6-dimethoxybenzoate (1.96 g, 10 mmol) and hydrazine hydrate (80%, 15 ml) in absolute ethanol (50 ml) was refluxed for 5 h at 413-423 K. The excess solvent was removed by distillation. The solid residue was filtered off, washed with water and recrystallized from ethanol (30%) to give the title compound (yield 1.78 g, 91%; m.p. 517-519 K). Colorless single crystals of (I) were obtained by slow evaporation of an ethanol solution at room temperature.

Refinement

H atoms were positioned geometrically, with N—H = 0.86 Å (for NH and NH_2) and C—H = 0.93 and 0.96 Å for aromatic and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C,N)$, where x = 1.5 for methyl H, and x = 1.2 for all other H atoms.

Figures

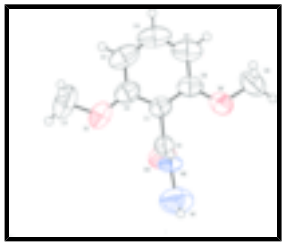


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

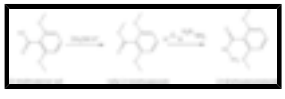


Fig. 2. The formation of the title compound.

2,6-Dimethoxybenzohydrazide

Crystal data

$C_9H_{12}N_2O_3$

$M_r = 196.21$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 7.2598$ (5) Å

$b = 14.2558$ (11) Å

$c = 20.0412$ (11) Å

$V = 2074.1$ (2) Å^3

$Z = 8$

$F_{000} = 832$

$D_x = 1.257$ Mg m^{-3}

Melting point: 244(2) K

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 1520 reflections

$\theta = 2.7$–24.9^o

$\mu = 0.10$ mm^{-1}

$T = 294$ (2) K

Block, colourless

0.16 × 0.14 × 0.06 mm

Data collection

Bruker APEXII diffractometer

Radiation source: rotating-anode generator

Monochromator: graphite

$T = 294$(2) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{min} = 0.981$, $T_{max} = 0.993$

14489 measured reflections

2615 independent reflections

1044 reflections with $I > 2\sigma(I)$

$R_{int} = 0.043$

$\theta_{max} = 28.7^o$

$\theta_{min} = 2.9^o$

$h = -9\rightarrow9$

$k = -19\rightarrow19$

$l = -26\rightarrow26$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.066$

$wR(F^2) = 0.109$

$S = 1.99$

2615 reflections

128 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + 0.1639P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.37$ e Å^{-3}

$\Delta\rho_{min} = -0.40$ e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick,1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0102 (7)

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 $F^2 > 2\text{sigma}(F^2)$ 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	−0.0885 (3)	0.45612 (13)	0.41648 (11)	0.0982 (7)
O2	0.4159 (3)	0.29139 (14)	0.33521 (9)	0.0827 (6)
O3	−0.0195 (3)	0.24193 (13)	0.37742 (10)	0.0873 (6)
N1	0.1159 (4)	0.1846 (2)	0.49375 (14)	0.1344 (12)
H1A	0.0378	0.1475	0.4751	0.161*
H1B	0.1633	0.1701	0.5317	0.161*
N2	0.1671 (3)	0.27065 (13)	0.46145 (9)	0.0542 (5)
H2A	0.2450	0.3082	0.4796	0.065*
C1	0.1691 (4)	0.37920 (17)	0.37441 (12)	0.0623 (7)
C2	0.0721 (5)	0.4629 (2)	0.38130 (15)	0.0787 (9)
C3	0.1419 (6)	0.5447 (2)	0.35300 (17)	0.1006 (11)
H3A	0.0796	0.6014	0.3575	0.121*
C4	0.3060 (6)	0.5399 (3)	0.31813 (17)	0.1075 (13)
H4A	0.3530	0.5945	0.2994	0.129*
C5	0.4017 (5)	0.4583 (3)	0.31005 (15)	0.0969 (11)
H5A	0.5103	0.4572	0.2855	0.116*
C6	0.3336 (4)	0.3771 (2)	0.33932 (13)	0.0713 (8)
C7	−0.1954 (5)	0.5395 (2)	0.42662 (18)	0.1352 (15)
H7A	−0.3034	0.5246	0.4522	0.203*
H7B	−0.2314	0.5648	0.3842	0.203*
H7C	−0.1230	0.5850	0.4503	0.203*
C8	0.5861 (4)	0.2843 (2)	0.29912 (15)	0.1081 (11)
H8A	0.6286	0.2205	0.3001	0.162*
H8B	0.6766	0.3243	0.3194	0.162*
H8C	0.5670	0.3034	0.2537	0.162*
C9	0.0935 (4)	0.29037 (18)	0.40452 (14)	0.0637 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1089 (17)	0.0674 (13)	0.1182 (17)	0.0212 (13)	0.0054 (15)	−0.0019 (12)
O2	0.0755 (14)	0.0910 (15)	0.0816 (13)	−0.0016 (12)	0.0144 (11)	0.0078 (11)

O3	0.0909 (15)	0.0748 (13)	0.0963 (15)	−0.0186 (12)	−0.0211 (12)	0.0075 (11)
N1	0.128 (3)	0.142 (3)	0.133 (3)	−0.016 (2)	−0.016 (2)	0.043 (2)
N2	0.0614 (13)	0.0551 (12)	0.0461 (11)	−0.0188 (11)	−0.0156 (11)	0.0142 (10)
C1	0.0708 (19)	0.0545 (16)	0.0617 (17)	−0.0057 (16)	−0.0072 (16)	−0.0024 (14)
C2	0.096 (2)	0.0639 (19)	0.077 (2)	−0.0052 (19)	−0.0124 (19)	−0.0016 (17)
C3	0.137 (3)	0.060 (2)	0.104 (3)	−0.011 (2)	−0.031 (2)	0.0052 (19)
C4	0.139 (4)	0.082 (3)	0.102 (3)	−0.043 (3)	−0.019 (3)	0.024 (2)
C5	0.109 (3)	0.092 (2)	0.090 (2)	−0.032 (2)	−0.007 (2)	0.016 (2)
C6	0.082 (2)	0.0689 (19)	0.0632 (18)	−0.0172 (18)	−0.0092 (17)	0.0040 (16)
C7	0.149 (4)	0.092 (3)	0.164 (4)	0.052 (3)	−0.001 (3)	−0.017 (2)
C8	0.082 (2)	0.138 (3)	0.104 (2)	−0.002 (2)	0.027 (2)	0.016 (2)
C9	0.0566 (17)	0.0564 (17)	0.078 (2)	0.0001 (14)	0.0090 (16)	−0.0064 (15)

Geometric parameters (Å, °)

O1—C2	1.366 (3)	C2—C3	1.393 (4)
O1—C7	1.434 (3)	C3—C4	1.383 (4)
O2—C6	1.362 (3)	C3—H3A	0.9300
O2—C8	1.436 (3)	C4—C5	1.364 (4)
O3—C9	1.202 (3)	C4—H4A	0.9300
N1—N2	1.436 (3)	C5—C6	1.390 (4)
N1—H1A	0.8600	C5—H5A	0.9300
N1—H1B	0.8600	C7—H7A	0.9600
N2—C9	1.291 (3)	C7—H7B	0.9600
N2—H2A	0.8600	C7—H7C	0.9600
C1—C6	1.386 (3)	C8—H8A	0.9600
C1—C2	1.393 (3)	C8—H8B	0.9600
C1—C9	1.506 (3)	C8—H8C	0.9600
C2—O1—C7	118.4 (3)	C4—C5—H5A	120.7
C6—O2—C8	118.1 (2)	C6—C5—H5A	120.7
N2—N1—H1A	120.0	O2—C6—C5	124.5 (3)
N2—N1—H1B	120.0	O2—C6—C1	115.3 (3)
H1A—N1—H1B	120.0	C5—C6—C1	120.2 (3)
C9—N2—N1	118.5 (2)	O1—C7—H7A	109.5
C9—N2—H2A	120.7	O1—C7—H7B	109.5
N1—N2—H2A	120.7	H7A—C7—H7B	109.5
C6—C1—C2	120.3 (3)	O1—C7—H7C	109.5
C6—C1—C9	119.9 (2)	H7A—C7—H7C	109.5
C2—C1—C9	119.7 (3)	H7B—C7—H7C	109.5
O1—C2—C3	125.5 (3)	O2—C8—H8A	109.5
O1—C2—C1	115.0 (3)	O2—C8—H8B	109.5
C3—C2—C1	119.5 (3)	H8A—C8—H8B	109.5
C2—C3—C4	118.5 (3)	O2—C8—H8C	109.5
C2—C3—H3A	120.7	H8A—C8—H8C	109.5
C4—C3—H3A	120.7	H8B—C8—H8C	109.5
C5—C4—C3	122.8 (3)	O3—C9—N2	123.8 (3)
C5—C4—H4A	118.6	O3—C9—C1	123.4 (3)
C3—C4—H4A	118.6	N2—C9—C1	112.7 (2)
C4—C5—C6	118.6 (3)		

Fig. 1

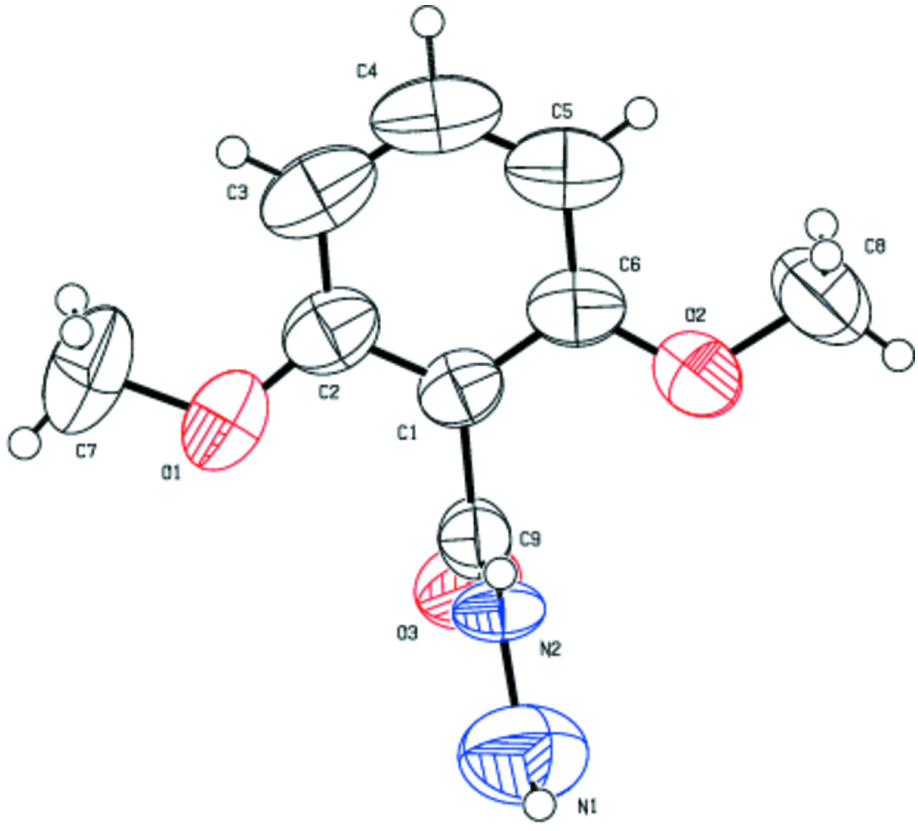
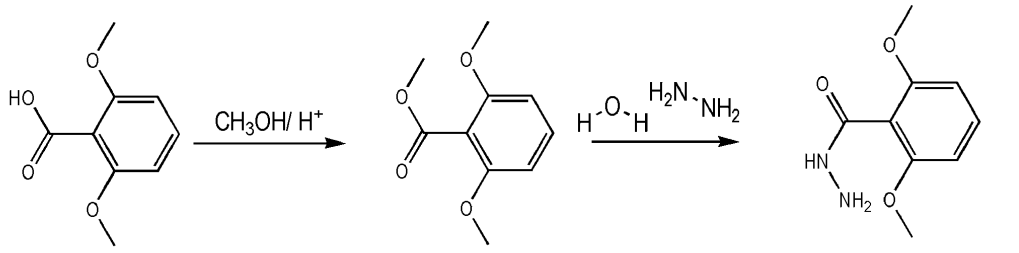


Fig. 2



2,6-dimethoxybenzoic acid methyl 2,6-dimethoxybenzoate 2,6-dimethoxybenzohydrazide