

## Retraction of articles by T. Liu *et al.*

T. Liu,<sup>a\*</sup> Y.-X. Wang,<sup>b</sup> Z.-W. Wang,<sup>a</sup> Z.-P. Xie<sup>a,c</sup> and J. Y. Zhu<sup>d</sup>

<sup>a</sup>College of Engineering, Jinggangshan University, Jian 343009, People's Republic of China, <sup>b</sup>College of Mathematics and Physics, Jinggangshan University, Jian

343009, People's Republic of China, <sup>c</sup>Department of Chemistry, Jiangxi University of Science and Technology, Ganzhou 341000, People's Republic of China, and

<sup>d</sup>Department of Information Engineering, Jiangxi University of Science and Technology, Nanchang 330013, People's Republic of China

Correspondence e-mail: taoliu07@126.com

Received 20 November 2009; accepted 15 December 2009

A series of 29 papers by Liu *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 29 papers by Liu *et al.* are retracted. 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	DOI	Refcode
<i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)</i> <i>(Dihydroxyglyoxime-κ<sup>2</sup>N,N')bis(I,10-phenanthroline-κ<sup>2</sup>N,N')copper(II) dinitrate dihydrate</i>	Liu & Xie (2007a) Liu, Wang, Wang & Xie (2007b)	10.1107/S1600536807026852 10.1107/S1600536807028255	EDUMAS EDUVAB
<i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)</i>	Liu & Xie (2007b)	10.1107/S1600536807028735	RIGQAA
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(I,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]</i>	Liu, Wang, Wang & Xie (2007c)	10.1107/S1600536807030917	UDUMIQ
<i>Polymeric KNO<sub>2</sub></i> <i>(Dihydroxyglyoxime-κ<sup>2</sup>N,N')bis(I,10-phenanthroline-κ<sup>2</sup>N,N')cobalt(II) dinitrate dihydrate</i>	Liu Wang, Wang & Xie (2007a) Liu, Wang, Wang & Xie (2007d)	10.1107/S1600536807027195 10.1107/S1600536807031224	ICSD 240891 WIHIED
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(I,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]</i>	Liu, Wang, Wang & Xie (2007e)	10.1107/S1600536807032679	WIHQEK
<i>Tetrakis[μ-(2-pyridyloxyacetato-κ<sup>2</sup>O:O')bis(I,10-phenanthroline-κ<sup>2</sup>N,N')-(2-pyridyloxyacetato-κO)neodymium(III)]</i>	Liu, Wang, Wang & Xie (2007f)	10.1107/S1600536807035349	TIGDAP
<i>(Dihydroxyglyoxime-κ<sup>2</sup>N,N')bis(I,10-phenanthroline-κ<sup>2</sup>N,N')manganese(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007g)	10.1107/S1600536807035076	TIGDET
<i>2-Amino-3,5-dinitrobenzoic acid-ammonium (I/I)</i>	Liu & Zhu (2007j)	10.1107/S1600536807040068	KIKQAX
<i>2-Hydroxy-3,5-dinitrobenzamide monohydrate</i>	Liu & Zhu (2007k)	10.1107/S1600536807039712	KIKQEB
<i>2-(1-Hydroxy-2-pyridyl)acetamide monohydrate</i>	Liu & Zhu (2007l)	10.1107/S1600536807040652	CIKQOD
<i>Bis(2,2'-bipyridine-κN,N')bis(thiocyanato-κN)iron(II)</i>	Liu & Zhu (2007a)	10.1107/S1600536807043486	XIFXOA
<i>catena-Poly[hexakis(μ<sub>2</sub>-anilinoacetamide)bis(I,10-phenanthroline)disamarium(III)]</i>	Liu & Zhu (2007b)	10.1107/S1600536807045485	XILNAI
<i>3-Hydroxy-2,4,6-trinitropyridine monohydrate</i>	Liu & Zhu (2007m)	10.1107/S1600536807045230	PILNOO
<i>catena-Poly[hexakis(μ<sub>2</sub>-anilinoacetamide)bis(I,10-phenanthroline)-dipraseodymium(III)]</i>	Liu & Zhu (2007c)	10.1107/S1600536807047733	SILZET
<i>catena-Poly[[tetra-μ-anilinoacetamido-bis(I,10-phenanthroline)dicerium(III)-di-μ-anilinoacetamido]</i>	Liu & Zhu (2007d)	10.1107/S1600536807050969	GIMZOS
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)chromium(II)</i>	Liu & Zhu (2007e)	10.1107/S1600536807051756	WINFAB
<i>2-Ammonio-3-carboxy-5-nitrobenzoate monohydrate</i>	Liu & Zhu (2007n)	10.1107/S1600536807048477	GINFEP
<i>2-(Benzoylhydrazinocarbonyl)benzoic acid</i>	Liu & Zhu (2007o)	10.1107/S160053680705204X	TINZIA
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)vanadium(II)</i>	Liu & Zhu (2007f)	10.1107/S1600536807054529	HIPZIQ
<i>catena-Poly[[nitrato-κO](I,10-phenanthroline-κ<sup>2</sup>N,N')nickel(II)-μ-acetamido-κ<sup>2</sup>O:N]</i>	Liu & Zhu (2007g)	10.1107/S1600536807056504	XIRGIP
<i>catena-Poly[[nitrato-κO](I,10-phenanthroline-κ<sup>2</sup>N,N')copper(II)-μ-acetamido-κ<sup>2</sup>O:N]</i>	Liu & Zhu (2007h)	10.1107/S1600536807059077	HIQROP
<i>catena-Poly[[nitrato-κO](I,10-phenanthroline-κ<sup>2</sup>N,N')cobalt(II)-μ-acetamido-κ<sup>2</sup>O:N]</i>	Liu & Zhu (2007i)	10.1107/S1600536807060631	YIQMER
<i>N'-Benzoyl-4-nitronicotinohydrazide</i>	Liu & Zhu (2007p)	10.1107/S1600536807053068	CIPVON
<i>N'-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide</i>	Liu & Zhu (2007q)	10.1107/S1600536807054876	RIRWEV

# addenda and errata

**Table 1 (continued)**

Title	Reference	DOI	Refcode
Ethylenediammonium sulfate	Liu & Zhu (2007r)	10.1107/S1600536807056280	ETDAMS03
Ethylenediammonium perchlorate	Liu & Zhu (2007s)	10.1107/S1600536807059909	HIRYEN
catena-Poly[ $\mu$ (nitro- $\kappa O$ )(1,10-phenanthroline- $\kappa^2 N,N'$ )manganese(II)]- $\mu$ -nitroato- $\kappa^2 O:O'$ ]	Liu & Zhu (2008)	10.1107/S160053680706254X	MIRROV

## References

- Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007a). *Acta Cryst.* E63, i170.  
Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007b). *Acta Cryst.* E63, m1887–m1888.  
Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007c). *Acta Cryst.* E63, m2020–m2021.  
Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007d). *Acta Cryst.* E63, m2027–m2028.  
Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007e). *Acta Cryst.* E63, m2080–m2081.  
Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007f). *Acta Cryst.* E63, m2196–m2197.  
Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007g). *Acta Cryst.* E63, m2198–m2199.  
Liu, T. & Xie, Z.-P. (2007a). *Acta Cryst.* E63, m1820.  
Liu, T. & Xie, Z.-P. (2007b). *Acta Cryst.* E63, m1908.  
Liu, T. & Zhu, J. Y. (2007a). *Acta Cryst.* E63, m2506–m2507.  
Liu, T. & Zhu, J.-Y. (2007b). *Acta Cryst.* E63, m2592–m2593.  
Liu, T. & Zhu, J. Y. (2007c). *Acta Cryst.* E63, m2659–m2660.  
Liu, T. & Zhu, J. Y. (2007d). *Acta Cryst.* E63, m2775–m2776.  
Liu, T. & Zhu, J. Y. (2007e). *Acta Cryst.* E63, m2809.  
Liu, T. & Zhu, J. Y. (2007f). *Acta Cryst.* E63, m2912.  
Liu, T. & Zhu, J.-Y. (2007g). *Acta Cryst.* E63, m2977–m2978.  
Liu, T. & Zhu, J. Y. (2007h). *Acta Cryst.* E63, m3108.  
Liu, T. & Zhu, J. Y. (2007i). *Acta Cryst.* E63, m3144.  
Liu, T. & Zhu, J.-Y. (2007j). *Acta Cryst.* E63, o3829.  
Liu, T. & Zhu, J. Y. (2007k). *Acta Cryst.* E63, o3830.  
Liu, T. & Zhu, J.-Y. (2007l). *Acta Cryst.* E63, o3860.  
Liu, T. & Zhu, J. Y. (2007m). *Acta Cryst.* E63, o4112.  
Liu, T. & Zhu, J. Y. (2007n). *Acta Cryst.* E63, o4267.  
Liu, T. & Zhu, J. Y. (2007o). *Acta Cryst.* E63, o4441.  
Liu, T. & Zhu, J. Y. (2007p). *Acta Cryst.* E63, o4527.  
Liu, T. & Zhu, J. Y. (2007q). *Acta Cryst.* E63, o4574.  
Liu, T. & Zhu, J.-Y. (2007r). *Acta Cryst.* E63, o4660.  
Liu, T. & Zhu, J. Y. (2007s). *Acta Cryst.* E63, o4874.  
Liu, T. & Zhu, J. Y. (2008). *Acta Cryst.* E64, m28.

## N'-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide

T. Liu<sup>a\*</sup> and J. Y. Zhu<sup>b</sup>

<sup>a</sup>College of Engineering, Jinggangshan University, Jian 343009, People's Republic of China, and <sup>b</sup>Department of Information Engineering, Jiangxi University of Science and Technology, Nanchang 330013, People's Republic of China  
Correspondence e-mail: taoliu07@126.com

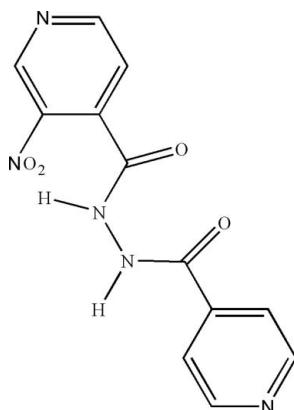
Received 28 October 2007; accepted 31 October 2007

Key indicators: single-crystal X-ray study;  $T = 273\text{ K}$ ; mean  $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$ ;  $R$  factor = 0.050;  $wR$  factor = 0.144; data-to-parameter ratio = 14.2.

In the molecule of the title compound,  $\text{C}_{12}\text{H}_9\text{N}_5\text{O}_4$ , the rings are oriented at a dihedral angle of  $8.00(2)^\circ$ . In the crystal structure, intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds result in the formation of a supramolecular network.

### Related literature

For general background, see: Desiraju (1995, 1997); Braga *et al.* (1998); Li *et al.* (2005); Liu *et al.* (2004); Pan & Xu (2004); Wu *et al.* (2003). For bond-length data, see: Allen *et al.* (1987).



### Experimental

#### Crystal data

$\text{C}_{12}\text{H}_9\text{N}_5\text{O}_4$   
 $M_r = 287.24$

Monoclinic,  $P2_1/n$   
 $a = 8.2027(12)\text{ \AA}$

$b = 12.8813(17)\text{ \AA}$   
 $c = 12.970(2)\text{ \AA}$   
 $\beta = 92.491(7)^\circ$   
 $V = 1369.1(3)\text{ \AA}^3$   
 $Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 0.11\text{ mm}^{-1}$   
 $T = 273(2)\text{ K}$   
 $0.27 \times 0.17 \times 0.16\text{ mm}$

#### Data collection

Bruker SMART CCD area-detector diffractometer  
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  
 $R_{\text{int}} = 0.043$   
 $T_{\text{min}} = 0.971$ ,  $T_{\text{max}} = 0.983$

8849 measured reflections  
2718 independent reflections  
1360 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.043$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$   
 $wR(F^2) = 0.144$   
 $S = 1.02$   
2718 reflections

191 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.40\text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.26\text{ e \AA}^{-3}$

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N1—H1A $\cdots$ O2 <sup>i</sup>	0.86	1.97	2.823 (3)	170
N2—H2A $\cdots$ O1 <sup>ii</sup>	0.86	2.07	2.862 (3)	152

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

We thank the Youth Program of Jinggangshan University for financial support of this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2357).

### References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Braga, D., Grepioni, F. & Desiraju, G. R. (1998). *Chem. Rev.* **98**, 1375–1386.
- Desiraju, G. R. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 2311–2315.
- Desiraju, G. R. (1997). *J. Chem. Soc. Chem. Commun.* pp. 1475–1476.
- Li, H., Yin, K.-L. & Xu, D.-J. (2005). *Acta Cryst. C* **61**, m19–m21.
- Liu, B.-X., Su, J.-R. & Xu, D.-J. (2004). *Acta Cryst. C* **60**, m183–m185.
- Pan, T.-T. & Xu, D.-J. (2004). *Acta Cryst. E* **60**, m56–m58.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Siemens (1996). *SMART*, *SAINT* and *SHELXTL*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Wu, Z.-Y., Xue, Y.-H. & Xu, D.-J. (2003). *Acta Cryst. E* **59**, m809–m811.

**supplementary materials**

Article retracted

*Acta Cryst.* (2007). E63, o4574 [doi:10.1107/S1600536807054876]

### **N'-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide**

**T. Liu and J. Y. Zhu**

#### **Comment**

In the synthesis of crystal structures by design, the assembly of molecular units in predefined arrangements is a key goal (Desiraju, 1995, 1997; Braga *et al.*, 1998). Due to pyridine groups are one of the most important classes of biological ligands, the coordination of metal-pyridine groups complexes are of critical importance in biological systems, organic materials and coordination chemistry. Recently, pyridine groups with variable coordination modes have been used to construct metal-organic supramolecular structures (Wu *et al.*, 2003; Pan & Xu, 2004; Liu *et al.*, 2004; Li *et al.*, 2005). We originally attempted to synthesize complexes featuring Cu metal chains by the reaction of copper(II) ion with 3-nitro-4-[*N*-(4-carbonylhydrazinopyridyl)- carbonyl]pyridine ligand. Unfortunately, we obtained only the title compound, (I), and we report herein its crystal structure.

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The rings A (N3/C1—C5) and B (N4/C8—C12) are, of course, planar and they are oriented at a dihedral angle of 8.00 (2) $^{\circ}$ .

In the crystal structure, intermolecular N—H···O hydrogen bonds (Table 1) result in the formation of a supramolecular network structure.

#### **Experimental**

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb. Copper dinitrate hexahydrate (147.8 mg, 0.5 mmol), 3-nitro-4-[*N*-(4-carbonylhydrazinopyridyl)- carbonyl]pyridine (278.4 mg, 1 mmol) and distilled water (6 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 453 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small colorless crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

#### **Refinement**

H atoms were positioned geometrically, with N—H = 0.86 Å (for NH) and C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ .

# supplementary materials

---

## Figures

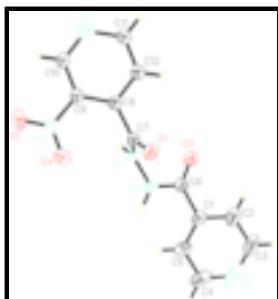
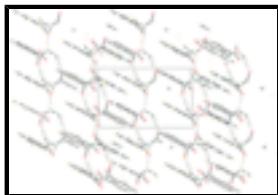


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.



## *N'*-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide

### Crystal data

$C_{12}H_9N_5O_4$

$M_r = 287.24$

Monoclinic,  $P2_1/n$

Hall symbol: -p 2yn

$a = 8.2027(12)$  Å

$b = 12.8813(17)$  Å

$c = 12.970(2)$  Å

$\beta = 92.491(7)^\circ$

$V = 1369.1(3)$  Å<sup>3</sup>

$Z = 4$

$F_{000} = 592$

$D_x = 1.393$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 2003 reflections

$\theta = 2.4\text{--}20.9^\circ$

$\mu = 0.11$  mm<sup>-1</sup>

$T = 273(2)$  K

Prism, colorless

$0.27 \times 0.17 \times 0.16$  mm

### Data collection

Bruker SMART CCD area-detector diffractometer

2718 independent reflections

Radiation source: fine-focus sealed tube

1360 reflections with  $I > 2\sigma(I)$

Monochromator: graphite

$R_{\text{int}} = 0.043$

$T = 273(2)$  K

$\theta_{\max} = 26.5^\circ$

$\varphi$  and  $\omega$  scans

$\theta_{\min} = 2.2^\circ$

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

$h = -10 \rightarrow 10$

$T_{\min} = 0.971$ ,  $T_{\max} = 0.983$

$k = -16 \rightarrow 16$

8849 measured reflections

$l = -16 \rightarrow 15$

*Refinement*Refinement on  $F^2$ 

Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full

H-atom parameters constrained

$$R[F^2 > 2\sigma(F^2)] = 0.050$$

$$w = 1/[\sigma^2(F_o^2) + (0.0601P)^2 + 0.155P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$wR(F^2) = 0.144$$

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

$$S = 1.02$$

$$\Delta\rho_{\text{max}} = 0.40 \text{ e \AA}^{-3}$$

2718 reflections

$$\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$$

191 parameters

$$\begin{aligned} \text{Extinction correction: SHELXL,} \\ F_c^* = k F_c [1 + 0.001 x F_c^2 \lambda^3 / \sin(2\theta)]^{1/4} \end{aligned}$$

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.0065 (15)

Secondary atom site location: difference Fourier map

*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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.9294 (2)	-0.01082 (13)	0.62609 (13)	0.0612 (5)
O2	0.5681 (2)	0.15846 (13)	0.51252 (15)	0.0660 (5)
O3	0.7545 (4)	-0.37731 (18)	0.5472 (2)	0.1294 (10)
O4	0.8681 (3)	-0.23389 (16)	0.51340 (15)	0.0835 (7)
N1	0.7077 (3)	-0.02937 (16)	0.51883 (17)	0.0614 (6)
H1A	0.6179	-0.0622	0.5058	0.074*
N2	0.7559 (3)	0.04917 (15)	0.45297 (16)	0.0611 (6)
H2A	0.8306	0.0381	0.4098	0.073*
N3	0.8478 (5)	0.3838 (3)	0.2666 (4)	0.1365 (15)
N4	0.5791 (3)	-0.2646 (2)	0.8124 (2)	0.0876 (8)
N5	0.7828 (3)	-0.28597 (18)	0.56574 (19)	0.0696 (7)
C1	0.7452 (3)	0.22485 (19)	0.38874 (19)	0.0549 (7)
C2	0.7185 (4)	0.3276 (2)	0.4150 (2)	0.0773 (9)
H2	0.6631	0.3429	0.4741	0.093*
C3	0.7725 (5)	0.4065 (3)	0.3550 (3)	0.1009 (12)
H3	0.7577	0.4752	0.3745	0.121*

## supplementary materials

---

C4	0.8753 (4)	0.2817 (3)	0.2375 (3)	0.0889 (10)
H4	0.9278	0.2668	0.1771	0.107*
C5	0.8225 (3)	0.2021 (2)	0.3006 (2)	0.0683 (8)
H5	0.8399	0.1333	0.2825	0.082*
C6	0.6826 (3)	0.14377 (19)	0.45812 (19)	0.0521 (6)
C7	0.8009 (3)	-0.05374 (18)	0.6022 (2)	0.0502 (6)
C8	0.7259 (3)	-0.13277 (17)	0.67218 (18)	0.0484 (6)
C9	0.7149 (3)	-0.23985 (17)	0.65642 (18)	0.0505 (6)
C10	0.6410 (3)	-0.30405 (19)	0.7257 (2)	0.0590 (7)
H10	0.6338	-0.3749	0.7127	0.071*
C11	0.5878 (3)	-0.1582 (2)	0.8306 (2)	0.0645 (8)
H11	0.5439	-0.1305	0.8896	0.077*
C12	0.6613 (3)	-0.0937 (2)	0.7616 (2)	0.0600 (7)
H12	0.6677	-0.0229	0.7751	0.072*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0632 (12)	0.0470 (10)	0.0741 (12)	-0.0084 (9)	0.0107 (9)	-0.0013 (8)
O2	0.0679 (13)	0.0583 (12)	0.0729 (12)	-0.0038 (10)	0.0167 (10)	0.0012 (9)
O3	0.207 (3)	0.0549 (14)	0.132 (2)	-0.0219 (16)	0.0728 (18)	-0.0345 (14)
O4	0.1065 (17)	0.0721 (14)	0.0751 (14)	0.0053 (12)	0.0420 (12)	-0.0020 (11)
N1	0.0625 (14)	0.0513 (13)	0.0708 (15)	-0.0114 (11)	0.0078 (12)	0.0203 (11)
N2	0.0683 (15)	0.0504 (13)	0.0664 (14)	-0.0034 (11)	0.0216 (11)	0.0176 (11)
N3	0.144 (3)	0.117 (3)	0.144 (3)	-0.050 (3)	-0.038 (3)	0.066 (3)
N4	0.099 (2)	0.0762 (19)	0.088 (2)	0.0024 (15)	0.0108 (15)	0.0131 (15)
N5	0.0926 (19)	0.0477 (15)	0.0704 (16)	0.0033 (13)	0.0237 (14)	-0.0032 (12)
C1	0.0558 (17)	0.0486 (16)	0.0599 (17)	-0.0075 (12)	-0.0019 (13)	0.0120 (12)
C2	0.091 (2)	0.0503 (18)	0.089 (2)	-0.0082 (16)	-0.0111 (17)	0.0083 (15)
C3	0.146 (4)	0.0531 (19)	0.101 (3)	-0.024 (2)	-0.018 (3)	0.020 (2)
C4	0.088 (2)	0.096 (3)	0.083 (2)	-0.017 (2)	0.0013 (17)	0.037 (2)
C5	0.0700 (19)	0.0669 (18)	0.0683 (19)	-0.0063 (15)	0.0055 (15)	0.0214 (15)
C6	0.0555 (17)	0.0466 (16)	0.0540 (16)	-0.0052 (13)	0.0017 (13)	0.0015 (12)
C7	0.0579 (17)	0.0346 (13)	0.0592 (17)	0.0020 (13)	0.0157 (13)	0.0002 (12)
C8	0.0540 (15)	0.0379 (13)	0.0540 (15)	0.0010 (12)	0.0094 (12)	0.0037 (11)
C9	0.0586 (16)	0.0396 (14)	0.0539 (15)	0.0043 (12)	0.0096 (12)	0.0012 (11)
C10	0.0768 (19)	0.0381 (14)	0.0630 (17)	0.0033 (13)	0.0134 (14)	0.0045 (12)
C11	0.084 (2)	0.0541 (17)	0.0574 (16)	0.0052 (15)	0.0219 (14)	0.0011 (13)
C12	0.0736 (19)	0.0454 (15)	0.0624 (17)	-0.0006 (13)	0.0194 (14)	-0.0014 (13)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

O1—C7	1.218 (3)	C1—C6	1.485 (3)
O2—C6	1.213 (3)	C2—C3	1.365 (4)
O3—N5	1.221 (3)	C2—H2	0.9300
O4—N5	1.201 (3)	C3—H3	0.9300
N1—C7	1.334 (3)	C4—C5	1.392 (4)
N1—N2	1.392 (3)	C4—H4	0.9300
N1—H1A	0.8600	C5—H5	0.9300

N2—C6	1.362 (3)	C7—C8	1.512 (3)
N2—H2A	0.8600	C8—C12	1.391 (3)
N3—C3	1.357 (6)	C8—C9	1.397 (3)
N3—C4	1.390 (6)	C9—C10	1.380 (3)
N4—C10	1.353 (4)	C10—H10	0.9300
N4—C11	1.392 (3)	C11—C12	1.379 (3)
N5—C9	1.450 (3)	C11—H11	0.9300
C1—C5	1.363 (4)	C12—H12	0.9300
C1—C2	1.386 (4)		
C7—N1—N2	120.0 (2)	C1—C5—H5	119.9
C7—N1—H1A	120.0	C4—C5—H5	119.9
N2—N1—H1A	120.0	O2—C6—N2	121.5 (2)
C6—N2—N1	118.9 (2)	O2—C6—C1	122.7 (2)
C6—N2—H2A	120.6	N2—C6—C1	115.8 (2)
N1—N2—H2A	120.6	O1—C7—N1	123.9 (2)
C3—N3—C4	121.2 (3)	O1—C7—C8	121.5 (2)
C10—N4—C11	119.5 (2)	N1—C7—C8	114.3 (2)
O4—N5—O3	122.5 (2)	C12—C8—C9	117.0 (2)
O4—N5—C9	118.9 (2)	C12—C8—C7	115.9 (2)
O3—N5—C9	118.6 (2)	C9—C8—C7	127.0 (2)
C5—C1—C2	119.7 (2)	C10—C9—C8	121.6 (2)
C5—C1—C6	122.9 (2)	C10—C9—N5	118.5 (2)
C2—C1—C6	117.4 (3)	C8—C9—N5	119.9 (2)
C3—C2—C1	120.8 (3)	N4—C10—C9	120.5 (2)
C3—C2—H2	119.6	N4—C10—H10	119.8
C1—C2—H2	119.6	C9—C10—H10	119.8
N3—C3—C2	119.5 (3)	C12—C11—N4	120.2 (2)
N3—C3—H3	120.3	C12—C11—H11	119.9
C2—C3—H3	120.3	N4—C11—H11	119.9
N3—C4—C5	118.6 (3)	C11—C12—C8	121.1 (2)
N3—C4—H4	120.7	C11—C12—H12	119.4
C5—C4—H4	120.7	C8—C12—H12	119.4
C1—C5—C4	120.2 (3)		

*Hydrogen-bond geometry (Å, °)*

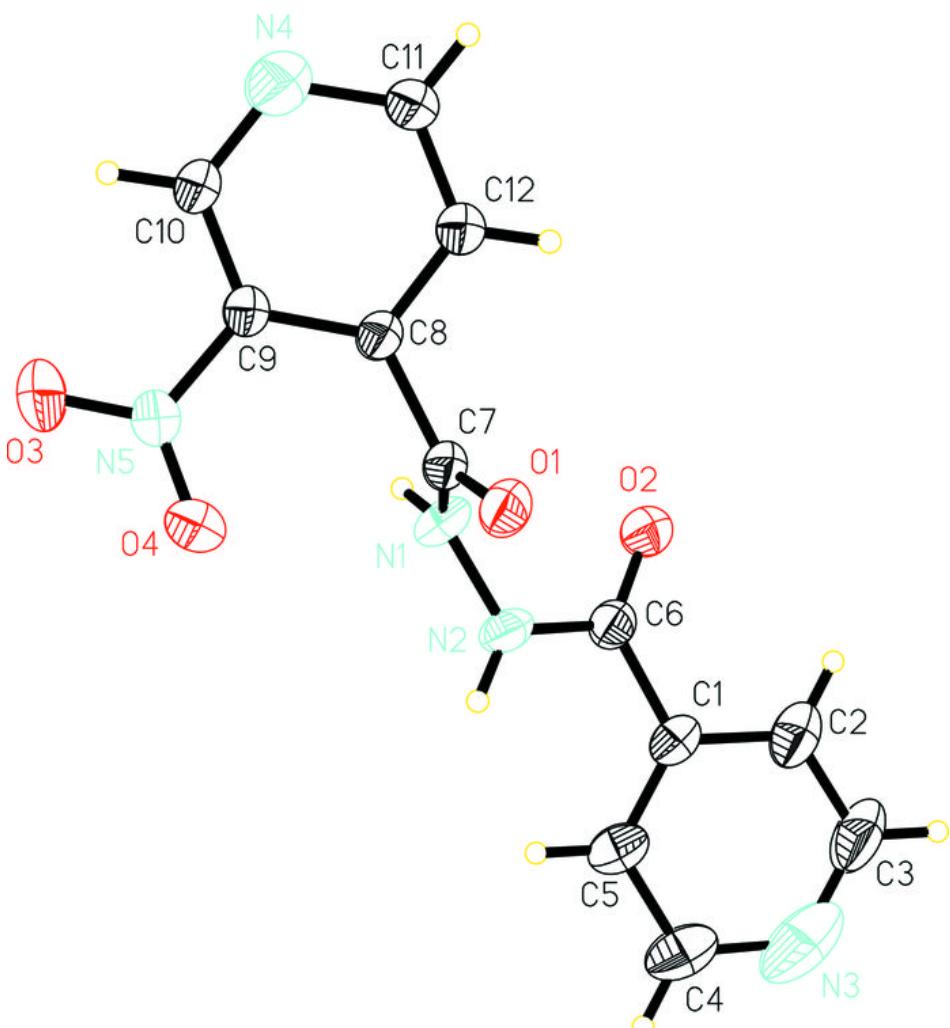
<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N1—H1A···O2 <sup>i</sup>	0.86	1.97	2.823 (3)	170
N2—H2A···O1 <sup>ii</sup>	0.86	2.07	2.862 (3)	152

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

## supplementary materials

---

Fig. 1



Art

Fig. 2

