

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
<i>trans</i> -Bis[1-β-(cyclohexylamino)propyliminomethyl]-2-naphtholato]copper(II) dichloride dihydrate	Zhang (2004)	Journal	10.1107/S1600536804028296	BIPDUA
Bis(4-bromo-2-formylphenolato-κ ² O,O')copper(II)	Sun & Gao (2005)	Author	10.1107/S16005368050187X	FEYSUY
Bis(salicylaldehyde)zinc(II)	Xiong & Liu (2005)	Journal	10.1107/S1600536805010913	GAMDUU
Bis(4-bromo-2-formylphenolato-κ ² O,O')zinc(II)	Chen (2006)	Journal	10.1107/S1600536805040432	SAZCUS
Bis(2-formylphenolato-κ ² O,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 ² O,O')manganese(II)	Wang & Fang (2006)	Journal	10.1107/S1600536806021039	IDOVED
Tetraqua(1,10-phenanthroline-κ ² N,N')copper(II) naphthalene-1,5-disulfonate dihydrate	Liu <i>et al.</i> (2006)	Author	10.1107/S1600536806030637	GENYOO
Tetraqua(1,10-phenanthroline-κ ² N,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 <i>et al.</i> (2006)	Journal	10.1107/S160053680604565X	HESPEP
Bis(2-formylphenolato-κ ² O,O')iron(II)	Yang <i>et al.</i> (2007)	Author	10.1107/S1600536807021721	PIFCAJ
2,6-Dimethoxybenzohydrazide	Qadeer <i>et al.</i> (2007a)	Journal	10.1107/S1600536807022593	PIFHES
2-(2,4-Dichlorophenylsulfanylmethylidyne)acetohydrazide	Qadeer <i>et al.</i> (2007b)	Journal	10.1107/S1600536807022891	YIFSOW
{6,6'-Diethoxy-2,2'-ethane-1,2-diylbis(nitrilomethylidyne)}diphenolato]-trinitratoeuropium(III)zinc(II)	Hu <i>et al.</i> (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]-trinitratorpaseodymium(III)zinc(II)	Chen <i>et al.</i> (2007)	Author	10.1107/S1600536807032540	WIHRIP
{μ-6,6'-Diethoxy-2,2'-ethane-1,2-diylbis(nitrilomethylidyne)}diphenolato]-trinitratorpaseodymium(III)nickel(II)	Sui, Li <i>et al.</i> (2007)	Author	10.1107/S1600536807032618	UFACUA
{6,6'-Dimethoxy-2,2'-ethane-1,2-diylbis(nitrilomethylidyne)}diphenolato-1κ ⁴ O ^I ,O ^V ,O ⁶ :2κ ⁴ O ^I ,N,N',O ^V](methanol-1κO)-μ-nitrito-1:2κ ² O:O'-dinitrato-1κ ⁴ O,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-nitrito-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-nitrito-dinitratorpaseodymium(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-nitrito-dinitratolutetium(III)zinc(II)	Sui, Sui <i>et al.</i> (2007)	Author	10.1107/S1600536807037737	AFEFOH
catena-Poly[chloridonickel(II)-di-μ-chlorido-chloridonickel(II)]-μ-4,4'-methylenebis(3,5-dimethylpyrazole)-κ ² N ² :N ^{2'}]	Huang & Chen (2007)	Author	10.1107/S1600536807039384	VIJYOD
{2,2'-{o-Phenylenebis(nitrilomethylidyne)}}diphenolato]zinc(II)	Liu <i>et al.</i> (2007a)	Author	10.1107/S1600536807040640	DIKYUS
trans-Bis(ethylenediamine-2 ^N ,N')bis(nitrato-κO)zinc(II)	Liu, Zeng & Chen (2007)	Author	10.1107/S1600536807042390	XIKYEW
[N,N'-{o-Phenylenebis(picolinamido)}-κ ² N,N',N'',N''']cobalt(II)	Liu & Zeng (2007a)	Author	10.1107/S1600536807044571	XILFII
[N,N'-{o-Phenylenebis(picolinamide)}-κ ⁴ N]nickel(II)	Liu & Zeng (2007b)	Author	10.1107/S1600536807048386	WINWEW
{2,2'-{o-Phenylenebis(nitrilomethylidyne)}}diphenolato)manganese(II)	Liu <i>et al.</i> (2007b)	Author	10.1107/S1600536807052993	VIQPIV
N-(2-Amino-3-pyridyl)urea monohydrate	Li <i>et al.</i> (2007)	Author	10.1107/S1600536807047526	SIMFEA
N-(2-Fluorophenyl)carbamic acid monohydrate	Yang (2007)	Author	10.1107/S1600536807052464	WINMOW
Aqua(dimethylglyoxime-κ ² N,N')(3,5-dinitro-2-oxidobenzoato-κ ² O ^I ,O ²)-copper(II)	Liu & Wen (2007)	Author	10.1107/S1600536807054244	HIQCAM
μ-Acetoato-tri-μ-ferrocenecarboxylatobis[(N,N-dimethylformamide)-copper(II)]	Liu, Lin <i>et al.</i> (2007)	Journal	10.1107/S1600536807059041	HIQQEE

addenda and errata

Table 1 (continued)

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

References

- Chen, Q. (2006). *Acta Cryst.* **E62**, m56–m57.
- Chen, J.-R., Sui, Y., Luo, Q.-Y. & Jiang, R.-Q. (2007). *Acta Cryst.* **E63**, m2091–m2092.
- Chen, J.-R., Sui, Y., Wen, J.-W. & Yin, L.-Y. (2008). *Acta Cryst.* **E64**, m562–m563.
- Han, Z.-Q. (2008). *Acta Cryst.* **E64**, m592.
- Harrison, W. T. A., Simpson, J. & Weil, M. (2010). *Acta Cryst.* **E66**, e1–e2.
- Hu, R.-H., Sui, Y., Chen, L. & He, C.-M. (2008). *Acta Cryst.* **E64**, m8–m9.
- Hu, R.-H., Sui, Y., Fang, X.-N. & Chen, H.-M. (2007). *Acta Cryst.* **E63**, m2039–m2040.
- Huang, C.-F. & Chen, H.-L. (2007). *Acta Cryst.* **E63**, m2356–m2357.
- Huang, Q., Sui, Y.-H. & Zhang, G.-X. (2009). *Acta Cryst.* **E65**, m1161–m1162.
- Li, Y.-G. & Chen, H.-J. (2006). *Acta Cryst.* **E62**, m1038–m1039.
- Li, N.-G., Tao, R.-M. & Fu, B.-F. (2007). *Acta Cryst.* **E63**, o4228.
- Li, Z., Zhang, X. & Pu, X. (2008). *Acta Cryst.* **E64**, m215.
- Liu, J.-T. & Fan, S.-D. (2006). *Acta Cryst.* **E62**, m2507–m2508.
- Liu, J.-T., Fan, S.-D. & Li, D.-Q. (2006). *Acta Cryst.* **E62**, m2165–m2166.
- Liu, D., Lin, J., Xu, Y., Huang, C. & Li, X. (2007). *Acta Cryst.* **E63**, m3094.
- Liu, Y.-Q. & Wen, H.-R. (2007). *Acta Cryst.* **E63**, m2928.
- Liu, Y.-Q. & Zeng, X.-R. (2007a). *Acta Cryst.* **E63**, m2547.
- Liu, Y.-Q. & Zeng, X.-R. (2007b). *Acta Cryst.* **E63**, m2684.
- Liu, Y.-Q., Zeng, X.-R. & Chen, W.-T. (2007). *Acta Cryst.* **E63**, m2462.
- Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007a). *Acta Cryst.* **E63**, m2396.
- Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007b). *Acta Cryst.* **E63**, m2854.
- Qadeer, G., Rama, N. H. & Chen, W.-T. (2007a). *Acta Cryst.* **E63**, o2892.
- Qadeer, G., Rama, N. H. & Chen, W.-T. (2007b). *Acta Cryst.* **E63**, o2932.
- Qiu, X.-Y. (2006). *Acta Cryst.* **E62**, m1190–m1191.
- Sui, Y., Fang, X.-N., Hu, P. & Lin, J. (2007). *Acta Cryst.* **E63**, m2135–m2136.
- Sui, Y., Fang, X.-N. & Yuan, M.-W. (2007). *Acta Cryst.* **E63**, m2275–m2276.
- Sui, Y., Li, X.-F., Huang, G.-S. & Wang, G.-J. (2007). *Acta Cryst.* **E63**, m2093–m2094.
- Sui, Y., Sui, Y.-H., Luo, Q.-Y. & Wang, Y.-D. (2007). *Acta Cryst.* **E63**, m2277–m2278.
- Sui, Y., Xiao, Y.-A., Fang, X.-N., Zeng, X.-R. & Li, M.-H. (2006). *Acta Cryst.* **E62**, m3205–m3207.
- Sui, Y., Zhang, J.-H., Hu, R.-H. & Jiang, R.-Q. (2007). *Acta Cryst.* **E63**, m2256–m2257.
- Sui, Y., Zhang, J.-H., Hu, R.-H. & Yin, L.-Y. (2007). *Acta Cryst.* **E63**, m2089–m2090.
- Sun, Y.-X. & Gao, G.-Z. (2005). *Acta Cryst.* **E61**, m354–m355.
- Wang, Q. & Fang, Z.-N. (2006). *Acta Cryst.* **E62**, m1492–m1493.
- Wang, S., Yang, T., Li, Z. & Yu, X. (2009). *Acta Cryst.* **E65**, o2198.
- Xiao, Y.-A., Fu, X.-K., Sui, Y., Wu, Q. & Xiong, S.-H. (2008). *Acta Cryst.* **E64**, m806–m807.
- Xiao, Y.-A., Sui, Y., Yi, X.-G., Wu, J.-H. & Zhang, L.-P. (2008). *Acta Cryst.* **E64**, m804–m805.
- Xiong, Z.-Y. & Liu, L.-J. (2005). *Acta Cryst.* **E61**, m863–m864.
- Yang, X.-M. (2007). *Acta Cryst.* **E63**, o4453.
- Yang, Y.-M., Lu, P.-C., Zhu, T.-T. & Liu, C.-H. (2007). *Acta Cryst.* **E63**, m1613.
- Zhang, P. (2004). *Acta Cryst.* **E60**, m1808–m1810.

2-(2,4-Dichlorophenylsulfanyl)aceto-hydrazide

Ghulam Qadeer,^a Nasim Hasan Rama^{a*} and Wen-Tong Chen^b

^aDepartment of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan, and ^bCollege of Chemistry and Chemical Engineering, JiangXi Province Key

Laboratory of Coordination Chemistry, JingGangShan University, Jí'an, JiangXi 343009, People's Republic of China

Correspondence e-mail: nasimhra@yahoo.com

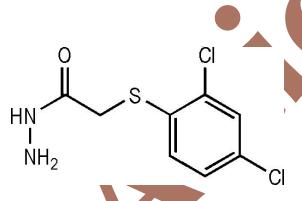
Received 4 May 2007; accepted 9 May 2007

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$; R factor = 0.044; wR factor = 0.136; data-to-parameter ratio = 12.9.

The title compound, $C_8H_8Cl_2N_2OS$, 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 $88.93(3)^\circ$.

Related literature

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



Experimental

Crystal data

$C_8H_8Cl_2N_2OS$

$M_r = 251.13$

Triclinic, $P\bar{1}$

$a = 7.350(5) \text{ \AA}$

$b = 8.133(6) \text{ \AA}$

$c = 8.545(6) \text{ \AA}$

$\alpha = 94.802(10)^\circ$

$\beta = 90.140(9)^\circ$

$\gamma = 98.492(10)^\circ$

$V = 503.4(6) \text{ \AA}^3$

$Z = 2$

Mo $K\alpha$ radiation

$\mu = 0.82 \text{ mm}^{-1}$
 $T = 293(2) \text{ K}$

$0.15 \times 0.14 \times 0.14 \text{ mm}$

Data collection

Bruker SMART CCD
diffractometer
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.882$, $T_{\max} = 0.892$

3032 measured reflections
1644 independent reflections
1160 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.136$
 $S = 1.14$
1644 reflections

127 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.22 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.12 \text{ e \AA}^{-3}$

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).

The authors gratefully acknowledge funds from the Higher Education Commission, Islamabad, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2105).

References

- Ahmad, R., Iqbal, R., Akhtar, R. H., Haq, Z. U., Duddeck, H., Stefaniak, L. & Sitkowski, J. (2001). *Nucleosides Nucleotides Nucleic Acids*, **20**, 1671–1682.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L. & Orpen, A. G. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Al-Soud, Y. A., Al-Deeri, M. N. & Al-Mosoudi, N. A. (2004). *Il Farmaco*, **59**, 775–783.
Al-Talib, M., Tastoush, H. & Odeh, N. (1990). *Synth. Commun.* **20**, 1811–1814.
Bruker (1998). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
El-Emam, A. A., Al-Deeb, O. A., Al-Omar, M. & Lehmann, J. (2004). *Bioorg. Med. Chem.* **12**, 5107–5113.
Furniss, B. S., Hannaford, A. J., Rogers, V., Smith, P. W. G. & Tatchell, A. R. (1978). *Vogel's Textbook of Practical Organic Chemistry*, 4th ed., p. 1125. London: Longman.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Yousif, M. Y., Ismail, A. M., Elman, A. A. & El-Kerdawy, M. M. (1986). *J. Chem. Soc. Pak.* **8**, 183–187.
Zheng, X., Li, Z., Wang, Y., Chen, W., Huang, Q., Liu, C. & Song, G. (2003). *J. Fluorine Chem.* **117**, 163–169.

supplementary materials

Article retracted

Acta Cryst. (2007). E63, o2932 [doi:10.1107/S1600536807022891]

2-(2,4-Dichlorophenylsulfanyl)acetohydrazide

G. Qadeer, N. H. Rama and W.-T. Chen

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 (Fig. 1). Bond distances and angles are within expected ranges (Allen *et al.*, 1987). The dihedral angle between the planar hydrazidic group ($C_8/O_1/N_1/N_2$) and benzene ring ($C_1—C_6$) is $91.07(3)^\circ$. The two centrosymmetrically related $N_1—H_1A\cdots O_1$ ($N_1\cdots O_1$, 3.078 \AA , $H_1A\cdots O_1$, 2.666 \AA , $N_1—H_1A\cdots O_1$, 110.8°) hydrogen bonds form a dimer (Fig. 3).

Experimental

A mixture of methyl-2-(2,4-dichlorophenylthio)acetate (2.51 g, 10 mmol) and hydrazine hydrate (15 ml, 80%) 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, 2.28 g; 91%, m.p. 333–335 K). Colourless single crystals of (I) were obtained by slow evaporation of an ethanol solution at room temperature.

Refinement

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

Figures

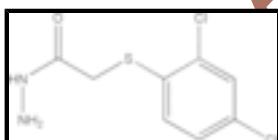


Fig. 1. Chemical diagram of (I).

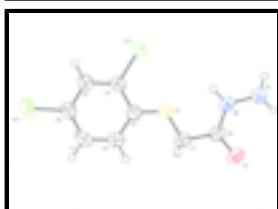
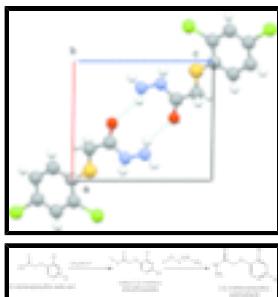


Fig. 2. The molecular structure of (I) with the 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

Fig. 3. The packing diagram of (I), viewed down the b axis.

supplementary materials



2-(2,4-Dichlorophenylsulfanyl)acetohydrazide

Crystal data

C ₈ H ₈ Cl ₂ N ₂ O ₁ S ₁	Z = 2
M _r = 251.13	F ₀₀₀ = 240
Triclinic, P <bar>1</bar>	D _x = 1.657 Mg m ⁻³
Hall symbol: -P 1	Melting point: 333(2) K
a = 7.350 (5) Å	Mo K α radiation
b = 8.133 (6) Å	λ = 0.71073 Å
c = 8.545 (6) Å	Cell parameters from 1520 reflections
α = 94.802 (10) $^\circ$	θ = 2.7–24.9 $^\circ$
β = 90.140 (9) $^\circ$	μ = 0.82 mm ⁻¹
γ = 98.492 (10) $^\circ$	T = 293 (2) K
V = 503.4 (6) Å ³	Block, colourless
	0.15 × 0.14 × 0.14 mm

Data collection

Bruker SMART CCD diffractometer	1644 independent reflections
Radiation source: rotating-anode generator	1160 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.018$
T = 293(2) K	$\theta_{\text{max}} = 25.0^\circ$
φ – ω scans	$\theta_{\text{min}} = 2.8^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8 \rightarrow 8$
$T_{\text{min}} = 0.882$, $T_{\text{max}} = 0.892$	$k = -9 \rightarrow 9$
3032 measured reflections	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.136$	$w = 1/[\sigma^2(F_o^2) + (0.0784P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$S = 1.14$	$(\Delta/\sigma)_{\max} < 0.001$
1644 reflections	$\Delta\rho_{\max} = 0.22 \text{ e \AA}^{-3}$
127 parameters	$\Delta\rho_{\min} = -0.12 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.26701 (14)	1.01419 (12)	-0.39917 (10)	0.0743 (4)
Cl2	0.29479 (11)	0.81304 (11)	0.18225 (9)	0.0635 (3)
S1	-0.0786 (2)	0.6652 (3)	0.1237 (2)	0.0532 (6)
O1	-0.4782 (3)	0.4371 (3)	0.2779 (3)	0.0636 (7)
N1	-0.2216 (3)	0.4350 (3)	0.5150 (3)	0.0590 (7)
H1A	-0.3282	0.3804	0.5317	0.071*
H1B	-0.1347	0.4414	0.5838	0.071*
N2	-0.1897 (3)	0.5134 (3)	0.3760 (3)	0.0493 (6)
H2A	-0.0822	0.5674	0.3615	0.059*
C1	-0.0239 (4)	0.8374 (4)	-0.2621 (4)	0.0553 (8)
H1C	-0.0901	0.8442	-0.3536	0.066*
C2	-0.1059 (4)	0.7541 (4)	-0.1410 (4)	0.0530 (8)
H2B	-0.2280	0.7042	-0.1521	0.064*
C3	-0.0111 (4)	0.7427 (3)	-0.0025 (3)	0.0420 (7)
C4	0.1726 (4)	0.8207 (4)	0.0105 (3)	0.0440 (7)
C5	0.2569 (4)	0.9021 (4)	-0.1106 (3)	0.0500 (8)
H5A	0.3796	0.9509	-0.1015	0.060*
C6	0.1565 (4)	0.9103 (4)	-0.2466 (4)	0.0489 (7)
C7	-0.2690 (3)	0.5928 (4)	0.1181 (4)	0.0480 (8)
H7A	-0.2920	0.5122	0.0274	0.058*
H7B	-0.3450	0.6792	0.1076	0.058*
C8	-0.3188 (4)	0.5081 (4)	0.2650 (4)	0.0465 (7)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0896 (7)	0.0862 (7)	0.0453 (5)	-0.0039 (5)	0.0005 (4)	0.0252 (5)

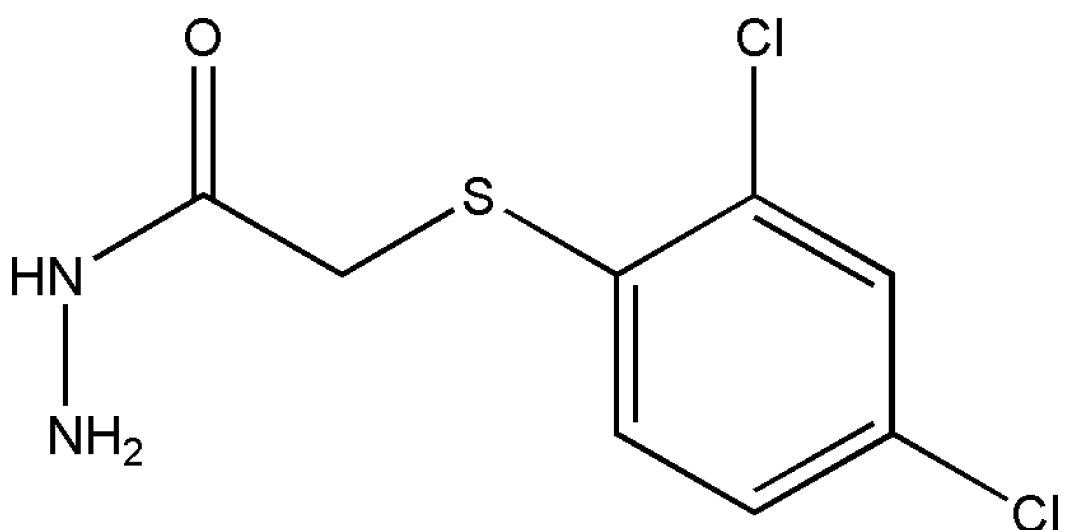
supplementary materials

Cl2	0.0477 (5)	0.0938 (7)	0.0471 (5)	-0.0065 (4)	-0.0114 (3)	0.0262 (4)
S1	0.0355 (11)	0.0735 (14)	0.0494 (13)	-0.0026 (9)	-0.0025 (9)	0.0172 (11)
O1	0.0348 (11)	0.0873 (17)	0.0636 (15)	-0.0072 (11)	0.0015 (10)	0.0057 (12)
N1	0.0428 (14)	0.085 (2)	0.0482 (16)	-0.0029 (13)	-0.0014 (11)	0.0211 (14)
N2	0.0376 (13)	0.0612 (16)	0.0485 (15)	-0.0014 (11)	0.0028 (11)	0.0158 (12)
C1	0.061 (2)	0.067 (2)	0.0393 (18)	0.0140 (16)	-0.0130 (15)	0.0063 (16)
C2	0.0393 (16)	0.069 (2)	0.050 (2)	0.0043 (14)	-0.0081 (14)	0.0072 (16)
C3	0.0410 (15)	0.0484 (17)	0.0376 (16)	0.0080 (13)	0.0005 (12)	0.0075 (13)
C4	0.0432 (15)	0.0502 (17)	0.0382 (16)	0.0057 (13)	-0.0063 (12)	0.0033 (14)
C5	0.0521 (17)	0.0557 (19)	0.0398 (17)	-0.0019 (14)	-0.0020 (14)	0.0080 (14)
C6	0.0595 (18)	0.0514 (18)	0.0356 (16)	0.0073 (14)	-0.0010 (13)	0.0043 (13)
C7	0.0322 (14)	0.0607 (19)	0.0501 (19)	0.0027 (13)	-0.0025 (13)	0.0057 (15)
C8	0.0359 (15)	0.0531 (18)	0.0493 (18)	0.0052 (13)	0.0026 (13)	-0.0006 (14)

Geometric parameters (\AA , $^\circ$)

Cl1—C6	1.749 (3)	C1—C2	1.376 (4)
Cl2—C4	1.729 (3)	C1—H1C	0.9300
S1—C3	1.353 (3)	C2—C3	1.388 (4)
S1—C7	1.435 (3)	C2—H2B	0.9300
O1—C8	1.237 (3)	C3—C4	1.405 (4)
N1—N2	1.399 (4)	C4—C5	1.375 (4)
N1—H1A	0.8600	C5—C6	1.387 (4)
N1—H1B	0.8600	C5—H5A	0.9300
N2—C8	1.334 (4)	C7—C8	1.502 (4)
N2—H2A	0.8600	C7—H7A	0.9700
C1—C6	1.371 (4)	C7—H7B	0.9700
C3—S1—C7	117.5 (2)	C5—C4—Cl2	119.6 (2)
N2—N1—H1A	120.0	C3—C4—Cl2	119.1 (2)
N2—N1—H1B	120.0	C4—C5—C6	119.0 (3)
H1A—N1—H1B	120.0	C4—C5—H5A	120.5
C8—N2—N1	122.8 (2)	C6—C5—H5A	120.5
C8—N2—H2A	118.6	C1—C6—C5	121.0 (3)
N1—N2—H2A	118.6	C1—C6—Cl1	120.8 (2)
C6—C1—C2	119.4 (3)	C5—C6—Cl1	118.2 (2)
C6—C1—H1C	120.3	S1—C7—C8	110.3 (2)
C2—C1—H1C	120.3	S1—C7—H7A	109.6
C1—C2—C3	121.7 (3)	C8—C7—H7A	109.6
C1—C2—H2B	119.2	S1—C7—H7B	109.6
C3—C2—H2B	119.2	C8—C7—H7B	109.6
S1—C3—C2	126.5 (3)	H7A—C7—H7B	108.1
S1—C3—C4	116.0 (2)	O1—C8—N2	122.9 (3)
C2—C3—C4	117.5 (3)	O1—C8—C7	118.5 (3)
C5—C4—C3	121.3 (3)	N2—C8—C7	118.6 (2)

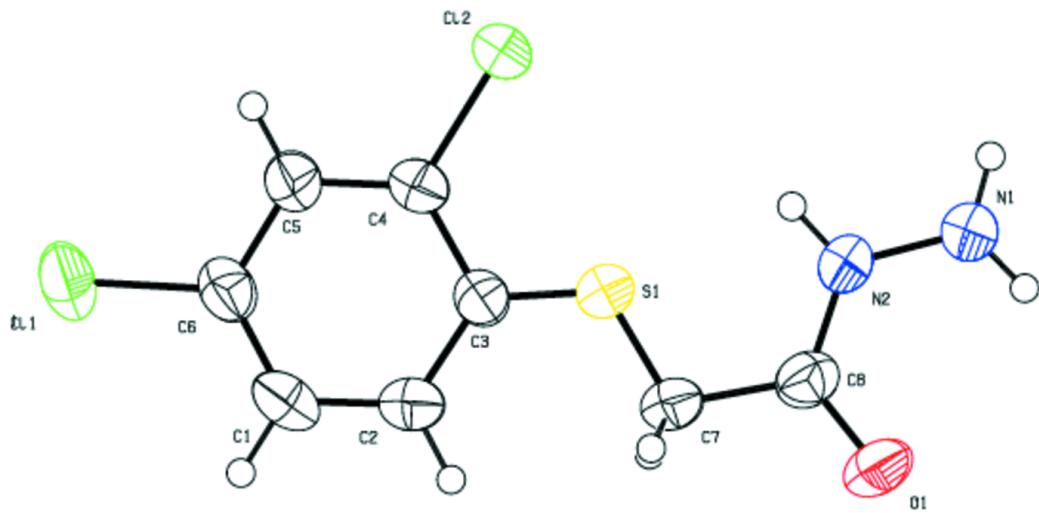
Fig. 1



Article retraction

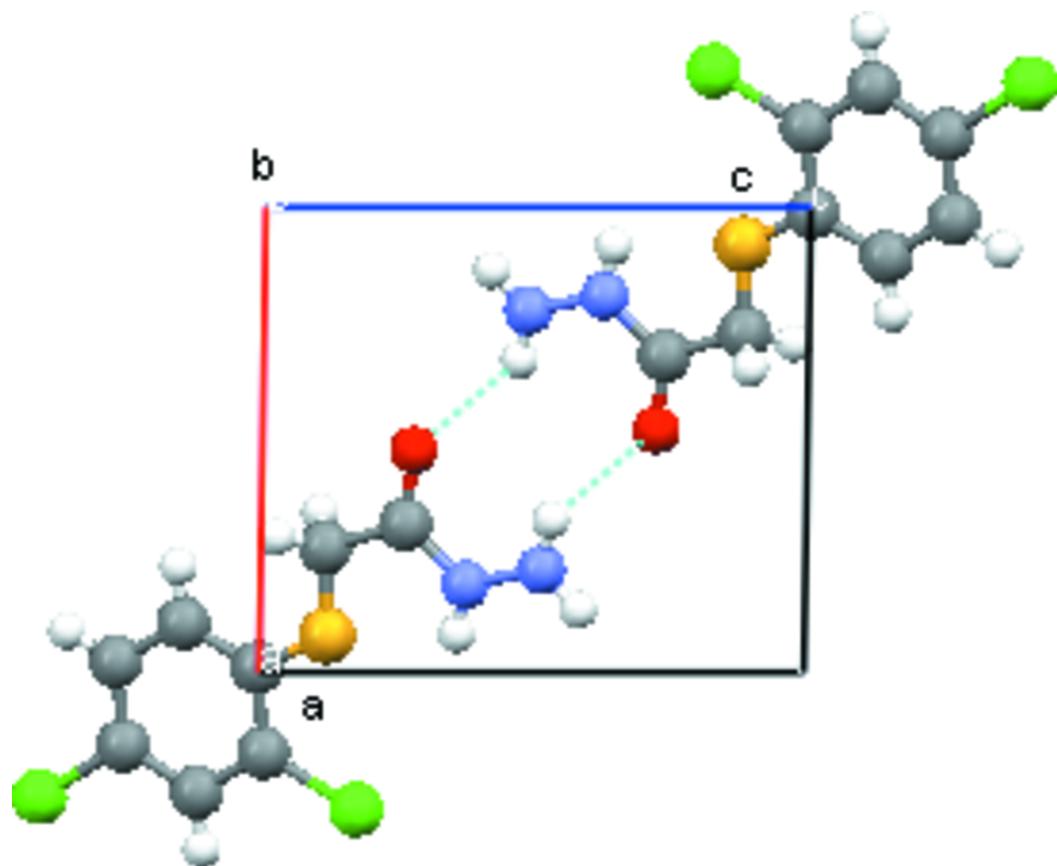
supplementary materials

Fig. 2



Article r^c

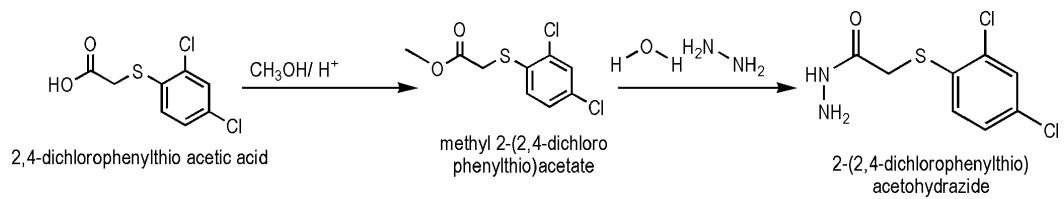
Fig. 3



Article

supplementary materials

Fig. 4



Article retracted