

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, Jingtangshan University, Jian 343009, People's Republic of China, <sup>b</sup>College of Mathematics and Physics, Jingtangshan 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>	Liu & Xie (2007a)	10.1107/S1600536807026852	EDUMAS
<i>(Dihydroxyglyoxime-κ<sup>2</sup>N,N')bis(1,10-phenanthroline-κ<sup>2</sup>N,N')copper(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007b)	10.1107/S1600536807028255	EDUVAB
<i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)</i>	Liu & Xie (2007b)	10.1107/S1600536807028735	RIGQAA
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]</i>	Liu, Wang, Wang & Xie (2007c)	10.1107/S1600536807030917	UDUMIQ
<i>Polymeric KNOF<sub>2</sub></i>	Liu Wang, Wang & Xie (2007a)	10.1107/S1600536807027195	ICSD 240891
<i>(Dihydroxyglyoxime-κ<sup>2</sup>N,N')bis(1,10-phenanthroline-κ<sup>2</sup>N,N')cobalt(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007d)	10.1107/S1600536807031224	WIHJED
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]</i>	Liu, Wang, Wang & Xie (2007e)	10.1107/S1600536807032679	WIHQEK
<i>Tetrakis[μ-(2-pyridyloxy)acetato-κ<sup>2</sup>O:O']bis[(1,10-phenanthroline-κ<sup>2</sup>N,N')-(2-pyridyloxy)acetato-κO]neodymium(III)]</i>	Liu, Wang, Wang & Xie (2007f)	10.1107/S1600536807035349	TIGDAP
<i>(Dihydroxyglyoxime-κ<sup>2</sup>N,N')bis(1,10-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-ammonia (1/1)</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(1,10-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(1,10-phenanthroline)-dipraseodymium(III)]</i>	Liu & Zhu (2007c)	10.1107/S1600536807047733	SILZET
<i>catena-Poly[[tetra-μ-anilinoacetamidato-bis(1,10-phenanthroline)dicerium(III)]-di-μ-anilinoacetamidato]</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[[nitrate-κO](1,10-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[[nitrate-κO](1,10-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[[nitrate-κO](1,10-phenanthroline-κ<sup>2</sup>N,N')cobalt(II)]-μ-acetamidato-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

**Table 1 (continued)**

Title	Reference	DOI	Refcode
<i>Ethylenediammonium sulfate</i>	Liu & Zhu (2007r)	10.1107/S1600536807056280	ETDAMS03
<i>Ethylenediammonium perchlorate</i>	Liu & Zhu (2007s)	10.1107/S1600536807059909	HIRYEN
<i>catena-Poly[[[nitrate-κO](1,10-phenanthroline-κ<sup>2</sup>N,N')manganese(II)]-μ-nitrate-κ<sup>2</sup>O:O']</i>	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.

## Tetrakis(pyridine- $\kappa$ N)bis(thiocyanato- $\kappa$ N)chromium(II)

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

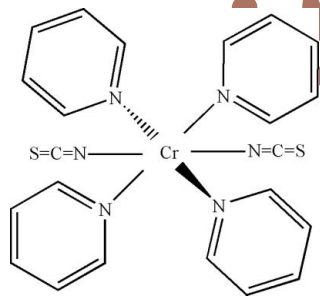
Received 13 October 2007; accepted 19 October 2007

Key indicators: single-crystal X-ray study;  $T = 273$  K; mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å;  $R$  factor = 0.047;  $wR$  factor = 0.161; data-to-parameter ratio = 15.3.

In the molecule of the title complex,  $[\text{Cr}(\text{NCS})_2(\text{C}_5\text{H}_5\text{N})_4]$ , the  $\text{Cr}^{\text{II}}$  atom is bonded in a distorted octahedral arrangement to two N atoms of two  $\text{SCN}^-$  ligands and four N atoms of four pyridine ligands. The Cr atom is located on a centre of inversion. In the crystal structure,  $\text{C}-\text{H} \cdots \text{N}$  hydrogen bonds result in the formation of a supramolecular network structure.

### Related literature

For related literature, see: Allen *et al.* (1987); Li *et al.* (2005); Liu *et al.* (2004); Pan & Xu (2004); Pope & Müller (2001); Wu *et al.* (2003); Zhong *et al.* (2007a,b).



### Experimental

#### Crystal data

$[\text{Cr}(\text{NCS})_2(\text{C}_5\text{H}_5\text{N})_4]$   
 $M_r = 484.56$   
 Monoclinic,  $C2/c$   
 $a = 12.4232$  (11) Å  
 $b = 12.9354$  (12) Å  
 $c = 15.1331$  (14) Å  
 $\beta = 107.313$  (1)°

$V = 2321.7$  (4) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.69$  mm<sup>-1</sup>  
 $T = 273$  (2) K  
 $0.31 \times 0.30 \times 0.16$  mm

#### Data collection

Bruker APEXII area-detector diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\text{min}} = 0.814$ ,  $T_{\text{max}} = 0.897$

7288 measured reflections  
 2187 independent reflections

1843 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.019$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$   
 $wR(F^2) = 0.161$   
 $S = 1.03$   
 2187 reflections

143 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.93$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.51$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Cr1—N1	2.172 (2)	Cr1—N2	2.161 (2)
		Cr1—N3	2.057 (2)
N1—Cr1—N1 <sup>i</sup>	180	N2 <sup>i</sup> —Cr1—N2	180
N1 <sup>i</sup> —Cr1—N2	87.17 (9)	N2—Cr1—N3 <sup>i</sup>	89.03 (10)
N1—Cr1—N2	92.83 (9)	N2—Cr1—N3	90.97 (10)
N1 <sup>i</sup> —Cr1—N3	89.43 (10)	N3 <sup>i</sup> —Cr1—N3	180
N1—Cr1—N3	90.57 (10)		

Symmetry code: (i)  $-x + \frac{3}{2}, -y + \frac{3}{2}, -z + 1$ .

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{C5}-\text{H5} \cdots \text{N3}^i$	0.93	2.54	3.063 (5)	116
$\text{C1}-\text{H1} \cdots \text{N3}$	0.93	2.59	3.120 (4)	117

Symmetry code: (i)  $-x + \frac{3}{2}, -y + \frac{3}{2}, -z + 1$ .

Data collection: APEX2 (Bruker, 2005); 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: AT2432).

### 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.
- Bruker (2005). APEX2. Bruker AXS Inc., Madison, Wisconsin, USA.
- Liu, B.-X., Su, J.-R. & Xu, D.-J. (2004). *Acta Cryst. C60*, m183–m185.
- Li, H., Yin, K.-L. & Xu, D.-J. (2005). *Acta Cryst. C61*, m19–m21.
- Pan, T.-T. & Xu, D.-J. (2004). *Acta Cryst. E60*, m56–m58.
- Pope, M. T. & Müller, A. (2001). *Polyoxometalate Chemistry: From Topology via Self-Assembly to Applications*, p. 319. Dordrecht, Boston, London: Kluwer Academic Publishers.
- Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
- Siemens (1996). SAINT and SHELXTL. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Wu, Z.-Y., Xue, Y.-H. & Xu, D.-J. (2003). *Acta Cryst. E59*, m809–m811.
- Zhong, H., Zeng, X.-R., Yang, X.-M. & Luo, Q.-Y. (2007a). *Acta Cryst. E63*, m1379.
- Zhong, H., Zeng, X.-R., Yang, X.-M. & Luo, Q.-Y. (2007b). *Acta Cryst. E63*, m1445.

**supplementary materials**

**Article retracted**

*Acta Cryst.* (2007). E63, m2809 [ doi:10.1107/S1600536807051756 ]

## Tetrakis(pyridine- $\kappa$ N)bis(thiocyanato- $\kappa$ N)chromium(II)

T. Liu and J. Y. Zhu

### Comment

In recent years, interest in the chemistry of metal-oxygen clusters has grown because of their applications in areas including catalysis, materials, chemistry and biochemistry (Pope & Müller, 2001). Aromatic polycyclic compounds, such as pyridine, phenanthroline, quinoline and benzimidazole, have commonly shown  $\pi$ - $\pi$  stacking in metal complexes (Wu *et al.*, 2003; Pan & Xu, 2004; Liu *et al.*, 2004; Li *et al.*, 2005; Zhong *et al.*, 2007a,b). We herein report the crystal structure of the title compound, (I).

In the molecule of (I), (Fig. 1) the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The two N atoms of two  $\text{SCN}^-$  and four N atoms of four pyridine ligands are coordinated to the Cr atom, in a distorted octahedral arrangement (Table 1). The Cr—N distances for the  $\text{SCN}^-$  and pyridine ligand are 2.057 (2) Å and in the range of [2.161 (2)–2.172 (2) Å], respectively (Table 1).

In the crystal structure, the C—H $\cdots$ N hydrogen bonds result in the formation of a supramolecular network structure (Fig. 2).

### Experimental

Crystals of the title compound were synthesized using hydrothermal method in a Teflon-lined Parr bomb (23 ml), which was then sealed. Lanthanum (III) nitrate hexahydrate (216.4 mg, 0.5 mmol), chromium(II) acetate dihydrate (103.1 mg, 0.5 mmol), potassium thiocyanate (97.1 mg, 1 mmol), pyridine (4 ml), and distilled water (6 g) were placed into the bomb and sealed. The bomb was heated under autogenous pressure for 7 d at 453 K and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colourless solution was decanted from small brown 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 C—H = 0.93 Å for aromatic H and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Figures

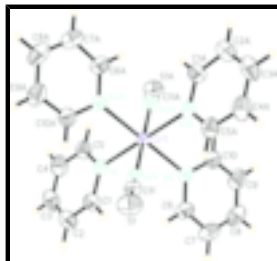


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A):  $3/2 - x, 3/2 - y, 1 - z$ ].

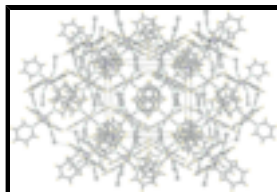


Fig. 2. A packing diagram for (I).

**Tetrakis(pyridine- $\kappa$ N)bis(thiocyanato- $\kappa$ N)chromium(II)**

*Crystal data*

$[\text{Cr}(\text{NCS})_2(\text{C}_5\text{H}_5\text{N})_4]$

$M_r = 484.56$

Monoclinic,  $C2/c$

Hall symbol:  $-C\ 2yc$

$a = 12.4232$  (11) Å

$b = 12.9354$  (12) Å

$c = 15.1331$  (14) Å

$\beta = 107.3130$  (10)°

$V = 2321.7$  (4) Å<sup>3</sup>

$Z = 4$

$F_{000} = 1000$

$D_x = 1.386$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 4510 reflections

$\theta = 2.3$ – $28.2^\circ$

$\mu = 0.69$  mm<sup>-1</sup>

$T = 273$  (2) K

Block, colourless

$0.31 \times 0.30 \times 0.16$  mm

*Data collection*

Bruker APEXII area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 273$ (2) K

$\varphi$  and  $\omega$  scans

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

$T_{\min} = 0.814$ ,  $T_{\max} = 0.897$

7288 measured reflections

2187 independent reflections

1843 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.019$

$\theta_{\text{max}} = 26.0^\circ$

$\theta_{\text{min}} = 2.3^\circ$

$h = -15 \rightarrow 15$

$k = -15 \rightarrow 15$

$l = -18 \rightarrow 18$

Refinement

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.047$	$w = 1/[\sigma^2(F_o^2) + (0.1244P)^2 + 0.7474P]$
$wR(F^2) = 0.161$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\max} < 0.001$
2187 reflections	$\Delta\rho_{\max} = 0.93 \text{ e } \text{\AA}^{-3}$
143 parameters	$\Delta\rho_{\min} = -0.50 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 1997), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.0134 (19)

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

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Cr1	0.7500	0.7500	0.5000	0.0358 (3)
S1	1.07279 (8)	0.64366 (7)	0.41890 (7)	0.0776 (4)
N1	0.7869 (2)	0.68986 (19)	0.63983 (16)	0.0552 (6)
N2	0.6398 (2)	0.62220 (19)	0.44152 (16)	0.0560 (6)
N3	0.8863 (2)	0.6721 (2)	0.48200 (18)	0.0608 (6)
C1	0.8410 (3)	0.6007 (3)	0.6647 (2)	0.0666 (8)
H1	0.8658	0.5655	0.6207	0.080*
C2	0.8626 (3)	0.5571 (3)	0.7514 (3)	0.0792 (10)
H2	0.8993	0.4938	0.7648	0.095*
C3	0.8289 (3)	0.6094 (4)	0.8169 (3)	0.0857 (11)
H3	0.8432	0.5830	0.8764	0.103*
C4	0.7737 (4)	0.7014 (4)	0.7931 (3)	0.0848 (11)
H4	0.7504	0.7386	0.8368	0.102*
C5	0.7525 (4)	0.7389 (3)	0.7047 (3)	0.0697 (9)
H5	0.7129	0.8005	0.6892	0.084*
C6	0.6747 (3)	0.5247 (3)	0.4543 (2)	0.0703 (9)

## supplementary materials

H6	0.7499	0.5122	0.4866	0.084*
C7	0.6049 (4)	0.4405 (3)	0.4222 (3)	0.0861 (11)
H7	0.6319	0.3733	0.4342	0.103*
C8	0.4946 (4)	0.4591 (3)	0.3720 (3)	0.0916 (13)
H8	0.4457	0.4046	0.3483	0.110*
C9	0.4583 (4)	0.5597 (3)	0.3577 (3)	0.0896 (12)
H9	0.3840	0.5744	0.3245	0.108*
C10	0.5323 (3)	0.6375 (3)	0.3926 (3)	0.0708 (9)
H10	0.5066	0.7052	0.3818	0.085*
C11	0.9642 (2)	0.65943 (19)	0.45611 (19)	0.0519 (6)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cr1	0.0318 (4)	0.0365 (4)	0.0401 (4)	0.00192 (18)	0.0124 (2)	-0.00210 (18)
S1	0.0726 (6)	0.0752 (6)	0.1001 (7)	0.0086 (4)	0.0488 (5)	-0.0010 (5)
N1	0.0513 (12)	0.0607 (14)	0.0531 (13)	-0.0014 (11)	0.0149 (10)	-0.0013 (10)
N2	0.0524 (13)	0.0544 (13)	0.0624 (14)	-0.0017 (10)	0.0191 (11)	-0.0037 (10)
N3	0.0533 (13)	0.0643 (14)	0.0680 (15)	0.0041 (11)	0.0229 (12)	-0.0020 (12)
C1	0.0653 (18)	0.0713 (19)	0.0633 (18)	0.0078 (16)	0.0193 (15)	0.0058 (15)
C2	0.070 (2)	0.091 (2)	0.075 (2)	0.0073 (18)	0.0195 (17)	0.0213 (19)
C3	0.073 (2)	0.119 (3)	0.062 (2)	-0.006 (2)	0.0160 (17)	0.023 (2)
C4	0.084 (3)	0.111 (3)	0.064 (2)	-0.005 (2)	0.0297 (19)	-0.009 (2)
C5	0.070 (2)	0.080 (2)	0.061 (2)	-0.0007 (16)	0.0203 (17)	-0.0114 (15)
C6	0.072 (2)	0.0583 (18)	0.083 (2)	-0.0016 (15)	0.0270 (17)	-0.0089 (15)
C7	0.096 (3)	0.061 (2)	0.109 (3)	-0.0131 (19)	0.042 (3)	-0.0133 (19)
C8	0.096 (3)	0.081 (3)	0.104 (3)	-0.038 (2)	0.040 (2)	-0.026 (2)
C9	0.071 (2)	0.094 (3)	0.097 (3)	-0.019 (2)	0.014 (2)	-0.020 (2)
C10	0.0581 (17)	0.071 (2)	0.080 (2)	-0.0016 (15)	0.0146 (16)	-0.0034 (16)
C11	0.0547 (15)	0.0450 (14)	0.0553 (15)	0.0041 (11)	0.0150 (13)	-0.0006 (11)

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

Cr1—N1	2.172 (2)	C2—H2	0.9300
Cr1—N1 <sup>i</sup>	2.172 (2)	C3—C4	1.368 (7)
Cr1—N2 <sup>i</sup>	2.161 (2)	C3—H3	0.9300
Cr1—N2	2.161 (2)	C4—C5	1.373 (5)
Cr1—N3 <sup>i</sup>	2.057 (2)	C4—H4	0.9300
Cr1—N3	2.057 (2)	C5—H5	0.9300
S1—C11	1.622 (3)	C6—C7	1.387 (5)
N1—C1	1.332 (4)	C6—H6	0.9300
N1—C5	1.341 (4)	C7—C8	1.375 (7)
N2—C6	1.330 (4)	C7—H7	0.9300
N2—C10	1.335 (4)	C8—C9	1.373 (6)
N3—C11	1.159 (4)	C8—H8	0.9300
C1—C2	1.379 (5)	C9—C10	1.359 (5)
C1—H1	0.9300	C9—H9	0.9300
C2—C3	1.365 (6)	C10—H10	0.9300



N1—Cr1—N1 <sup>i</sup>	180	C2—C3—C4	118.6 (3)
N1 <sup>i</sup> —Cr1—N2	87.17 (9)	C2—C3—H3	120.7
N1—Cr1—N2	92.83 (9)	C4—C3—H3	120.7
N1 <sup>i</sup> —Cr1—N2 <sup>i</sup>	92.83 (9)	C3—C4—C5	119.9 (4)
N1 <sup>i</sup> —Cr1—N3	89.43 (10)	C3—C4—H4	120.0
N1—Cr1—N3	90.57 (10)	C5—C4—H4	120.0
N1 <sup>i</sup> —Cr1—N3 <sup>i</sup>	90.57 (10)	N1—C5—C4	122.5 (4)
N2 <sup>i</sup> —Cr1—N2	180	N1—C5—H5	118.8
N2 <sup>i</sup> —Cr1—N3 <sup>i</sup>	90.97 (10)	C4—C5—H5	118.8
N2—Cr1—N3 <sup>i</sup>	89.03 (10)	N2—C6—C7	123.4 (4)
N2—Cr1—N3	90.97 (10)	N2—C6—H6	118.3
N3 <sup>i</sup> —Cr1—N3	180	C7—C6—H6	118.3
C1—N1—C5	116.6 (3)	C8—C7—C6	118.3 (4)
C1—N1—Cr1	121.8 (2)	C8—C7—H7	120.9
C5—N1—Cr1	121.5 (2)	C6—C7—H7	120.9
C6—N2—C10	116.8 (3)	C9—C8—C7	118.6 (4)
C6—N2—Cr1	121.8 (2)	C9—C8—H8	120.7
C10—N2—Cr1	121.4 (2)	C7—C8—H8	120.7
C11—N3—Cr1	156.5 (2)	C10—C9—C8	119.2 (4)
N1—C1—C2	124.1 (3)	C10—C9—H9	120.4
N1—C1—H1	117.9	C8—C9—H9	120.4
C2—C1—H1	117.9	N2—C10—C9	123.7 (4)
C3—C2—C1	118.3 (4)	N2—C10—H10	118.1
C3—C2—H2	120.8	C9—C10—H10	118.1
C1—C2—H2	120.8	N3—C11—S1	179.0 (3)

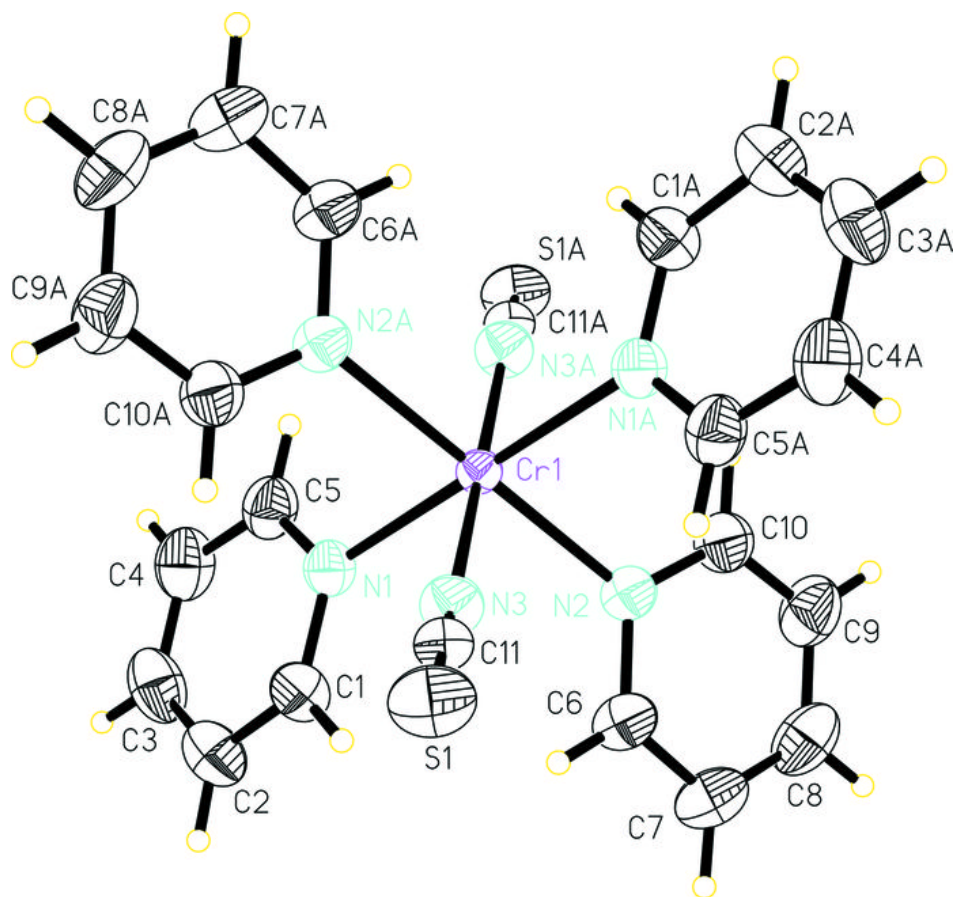
Symmetry codes: (i)  $-x+3/2, -y+3/2, -z+1$ .

*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>
C5—H5...N3 <sup>i</sup>	0.93	2.54	3.063 (5)	116
C1—H1...N3	0.93	2.59	3.120 (4)	117

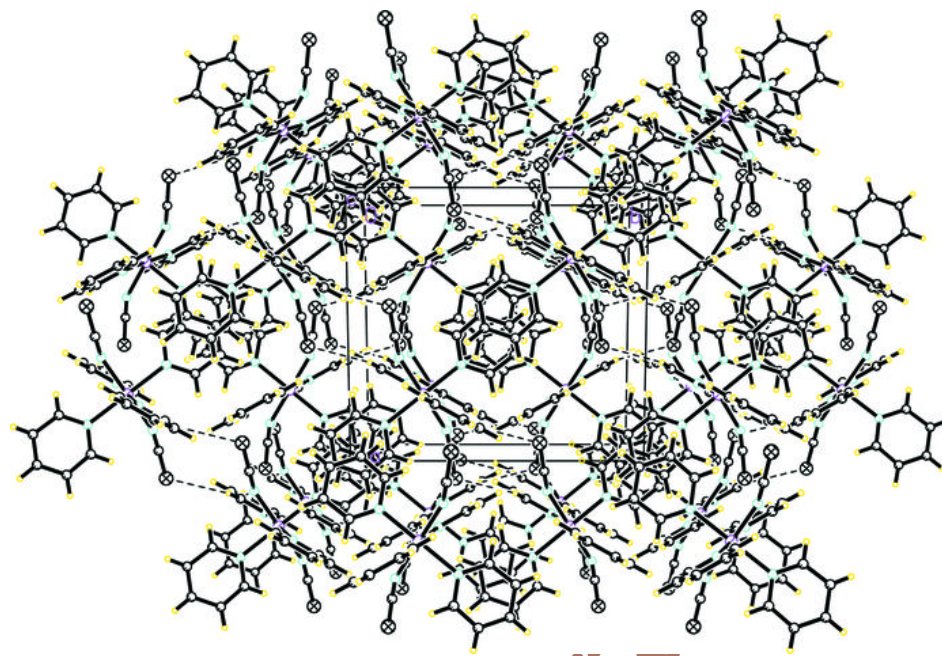
Symmetry codes: (i)  $-x+3/2, -y+3/2, -z+1$ .

Fig. 1



Article

Fig. 2



Article retr