

Retraction of articles by H. Zhong *et al.*

H. Zhong,^{a*} S.-H. Duan,^a Y.-P. Hong,^a M.-L. Li,^a Y.-Q. Liu,^a C.-J. Luo,^a Q.-Y. Luo,^a S.-Z. Xiao,^a H.-L. Xie,^a Y.-P. Xu,^a X.-M. Yang,^{b,a} X.-R. Zeng^a and Q. Y. Zhong^c

^aCollege of Chemistry and Chemical Engineering, Provincial Key Laboratory of Coordination Chemistry, Jinggangshan University, Jian 343009, People's Republic of China, ^bInstitute of Applied Materials, Jiangxi University of Finance and Economics, Nanchang 330032, People's Republic of China, and ^cJian Training School, Jian 343000, People's Republic of China
Correspondence e-mail: huazhong06@126.com

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A series of 41 papers by H. Zhong *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 41 papers by H. Zhong *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>Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate</i>	Zhong, Zeng, Liu & Luo (2006a)	10.1107/S1600536806041122	KERQEE
<i>cis-Dichlorobis(1,10-phenanthroline)cobalt(II)</i>	Zhong, Zeng & Luo (2006)	10.1107/S1600536806047295	MEQFOE
<i>Tris(quinolin-8-olato-κ²N,O)cobalt(III) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Liu & Luo (2006b)	10.1107/S1600536806050240	MEQHEW
<i>(8-Quinololinol-κ²N,O)bis(8-quinolinolato-κ²N,O)nickel(II) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Liu & Luo (2007)	10.1107/S1600536806053232	METVUD
<i>Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate</i>	Zhong, Zeng & Luo (2007)	10.1107/S1600536806053530	METQIM
<i>(8-Quinololinol-κ²N,O)-bis(8-quinolinolato-κ²N,O)zinc(II) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Luo, Li & Xiao (2007)	10.1107/S1600536807001171	DEXTEG
<i>(Dimethylglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')nickel(II) dinitrate dihydrate</i>	Zhong, Zeng, Yang, Luo & Li (2007a)	10.1107/S1600536807004102	YEYGOZ
<i>(Dimethylglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')zinc(II) dinitrate dihydrate</i>	Zhong, Zeng, Yang, Luo & Li (2007b)	10.1107/S1600536807004096	YEYGUF
<i>Chloridobis(1,10-phenanthroline-κN,N')copper(I) hexahydrate</i>	Zhong, Zeng, Yang, Luo & Xiao (2007)	10.1107/S160053680700791X	HEGKOU1
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)cobalt(II)</i>	Zhong, Zeng, Yang & Luo (2007a)	10.1107/S1600536807017461	ITCPCO1
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)copper(II)</i>	Zhong, Zeng, Yang & Luo (2007b)	10.1107/S160053680701879X	AVUJEG02
<i>Tetrakis(nitrato-κ²O,O')bis(4-phenylpyridine-κN)cerium(IV)</i>	Zhong, Zeng, Yang & Luo (2007c)	10.1107/S1600536807018831	CICDOI
<i>Bis(4,4'-bipyridine-κ²N,N')tetrakis(nitrato-κ²O,O')cerium(IV)</i>	Zhong, Zeng, Yang & Luo (2007d)	10.1107/S1600536807021502	YIDNEF
<i>(1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)</i>	Zhong, Zeng, Yang, Luo & Xu (2007)	10.1107/S1600536807027171	EDUROL
<i>(1,10-Phenanthroline)tris(phenoxyacetato)cerium(III)</i>	Zhong, Yang, Luo & Xu (2007a)	10.1107/S1600536807028061	EDUTUT
<i>(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)</i>	Zhong, Yang, Luo & Xu (2007b)	10.1107/S1600536807028693	RIGQEE
<i>(1,10-Phenanthroline-κ²N,N')tris(phenoxyacetato)-κO;κO;κO,O'-neodymium(III)</i>	Zhong, Yang, Luo & Xu (2007c)	10.1107/S1600536807030371	UDUMEM
<i>Bis(2,2'-bipyridyl-κ²N,N')bis(thiocyanato-κN)nickel(II)</i>	Zhong, Yang, Luo & Xu (2007d)	10.1107/S1600536807031613	YEJGOJ01
<i>Bis(2,2'-bipyridyl-κ²N,N')bis(isothiocyanato-κN)copper(II)</i>	Zhong, Yang, Luo & Xu (2007e)	10.1107/S1600536807033181	UFAPOH
<i>Bis(2,2'-bipyridyl-κ²N,N')bis(thiocyanato-κN)zinc(II)</i>	Zhong, Yang, Luo & Xu (2007f)	10.1107/S1600536807035337	TIGFAR
<i>(1,10-Phenanthroline-κ²N,N')tris(3-phenylpropanoato-κO)neodymium(III)</i>	Zhong, Yang, Luo & Xu (2007g)	10.1107/S1600536807035350	TIGFEV
<i>2-Fluoro-3,5-dinitrobenzamide monohydrate</i>	Zhong, Yang, Xie & Luo (2007j)	10.1107/S1600536807038676	VIKRAY
<i>2-Fluoro-3,5-dinitrobenzoic acid-ammonia (1/1)</i>	Zhong, Yang, Xie & Luo (2007k)	10.1107/S1600536807039724	KILKIA
<i>1-Hydroxy-4,6-dinitropyridine-2-carboxamide monohydrate</i>	Zhong, Yang, Xie & Luo (2007l)	10.1107/S1600536807040779	AFETAH
<i>N-(2-Hydroxyphenyl)carbamic acid-ammonia (1/1)</i>	Zhong, Yang, Xie & Luo (2007m)	10.1107/S160053680704086X	AFINAF
<i>catena-Poly[[bis(μ-anilinoacetato-κ²O:O')bis(μ-anilinoacetato-κ²O:O')bis(1,10-phenanthroline-κ²N,N')samarium(III)]-μ-anilinoacetato-κ²O:O']</i>	Zhong, Yang, Xie & Luo (2007a)	10.1107/S1600536807043528	PILDAQ
<i>2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate</i>	Zhong, Yang, Xie & Luo (2007n)	10.1107/S1600536807045199	XILWIZ
<i>catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dineodymium(III)]-di-μ-anilinoacetato]</i>	Zhong, Yang, Xie & Luo (2007b)	10.1107/S1600536807048489	WIMWEV
<i>Hexaaquacopper(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007c)	10.1107/S1600536807049525	TOLSCV01

Table 1 (continued)

Title	Reference	DOI	Refcode
<i>catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dilanthanum(III)]-di-μ-anilinoacetato]</i>	Zhong, Yang, Xie & Luo (2007d)	10.1107/S1600536807051240	GIMZEI
<i>Hexaaquachromium(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007e)	10.1107/S1600536807051227	GIMZIM
<i>Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007f)	10.1107/S1600536807052051	QUKQES01
<i>catena-Poly[(acetato-κO)(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-acetato-κ^2O:O']</i>	Zhong, Yang, Xie & Luo (2007g)	10.1107/S1600536807053494	NIQLAB
<i>Hexaaquanickel(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Zhong, Xie & Luo (2007a)	10.1107/S1600536807054372	HIPZOW
<i>catena-Poly[(acetato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)]-μ-acetato-κ^2O:O']</i>	Zhong, Yang, Xie & Luo (2007h)	10.1107/S160053680705622X	XIRGOV
<i>Hexaaquazinc(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Zhong, Xie & Luo (2007b)	10.1107/S1600536807056498	XIRJEO
<i>catena-Poly[(acetato-κO)(1,10-phenanthroline-κ^2N,N')nickel(II)]-μ-acetato-κ^2O:O']</i>	Zhong, Yang, Xie & Luo (2007i)	10.1107/S1600536807058540	HIQJOH
<i>Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Xie & Luo (2007)	10.1107/S1600536807058527	HIQJUN
<i>catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dieuropium(III)]-di-μ-anilinoacetato]</i>	Zhong, Yang, Duan & Hong (2007)	10.1107/S1600536807060643	YIQMAN
<i>(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinirate dihydrate</i>	Zhong, Yang, Luo & Li (2007)	10.1107/S1600536807061193	YIQNUI
<i>catena-Poly[(1,10-phenanthroline-κ^2N,N')praseodymium(III)]-di-μ-phenoxyacetato-κ^4O:O'-[(1,10-phenanthroline-κ^2N,N')praseodymium(III)]-di-μ-phenoxyacetato-κ^4O:O'-di-μ-phenoxyacetato-κ^3O,O':κ^3O:O,O']</i>	Zhong, Yang, Luo & Xu (2008)	10.1107/S1600536807068614	GISJIC

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Hexaaquachromium(II) bis(4-methylbenzenesulfonate)

 H. Zhong,^{a*} X.-M. Yang,^b H.-L. Xie^a and C.-J. Luo^a

^aCollege of Chemistry & Chemical Engineering, Provincial Key Laboratory of Coordination Chemistry, Jinggangshan University, Jian 343009, People's Republic of China, and ^bInstitute of Applied Materials, Jiangxi University of Finance & Economics, Nanchang 330032, People's Republic of China
Correspondence e-mail: huazhong06@126.com

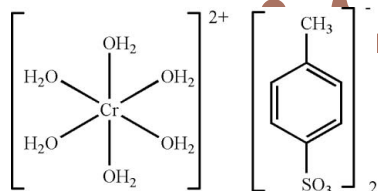
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Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.049; wR factor = 0.142; data-to-parameter ratio = 13.3.

The asymmetric unit of the title compound, $[\text{Cr}(\text{H}_2\text{O})_6](\text{C}_7\text{H}_7\text{O}_3\text{S})_2$, contains one half-cation and one anion; the Cr atom lies on an inversion centre. In the crystal structure, intermolecular $\text{O}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{S}$ hydrogen bonds result in the formation of a supramolecular network; an intramolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bond is also present.

Related literature

For a related structure, see: Zhong *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[\text{Cr}(\text{H}_2\text{O})_6](\text{C}_7\text{H}_7\text{O}_3\text{S})_2$
 $M_r = 502.47$
 Monoclinic, $P2_1/n$
 $a = 7.0181$ (11) Å
 $b = 6.3017$ (12) Å
 $c = 24.9978$ (15) Å
 $\beta = 91.607$ (3)°
 $V = 1105.1$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.76$ mm⁻¹
 $T = 273$ (2) K
 $0.49 \times 0.37 \times 0.19$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.709$, $T_{\max} = 0.866$
 6659 measured reflections
 2117 independent reflections
 1842 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.142$
 $S = 0.98$
 2117 reflections
 159 parameters
 9 restraints
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.63$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.46$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cr1—O4	2.050 (3)	Cr1—O6	2.048 (3)
Cr1—O5	2.020 (3)		
O4—Cr1—O4 ⁱ	180	O5—Cr1—O5 ⁱ	180
O4—Cr1—O5	91.19 (13)	O5—Cr1—O6	91.19 (13)
O4 ⁱ —Cr1—O5	88.81 (13)	O5 ⁱ —Cr1—O6	88.81 (13)
O4—Cr1—O6	92.21 (17)	O6—Cr1—O6 ⁱ	180
O4 ⁱ —Cr1—O6	87.79 (17)		

 Symmetry code: (i) $-x + 1, -y, -z$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H4A ⁱ ···O1 ⁱⁱ	0.832 (18)	1.953 (19)	2.784 (4)	176 (4)
O4—H4B ⁱ ···O2 ⁱⁱⁱ	0.84 (4)	2.02 (3)	2.825 (4)	160 (6)
O5—H5A ⁱ ···S1 ⁱⁱⁱ	0.89 (4)	2.99 (2)	3.871 (3)	171 (5)
O5—H5A ⁱ ···O1 ⁱⁱⁱ	0.89 (4)	1.93 (2)	2.793 (4)	166 (5)
O5—H5B ⁱ ···O3 ^{iv}	0.87 (5)	2.14 (6)	2.766 (4)	128 (7)
O6—H6B ⁱ ···O2 ^{iv}	0.87 (4)	1.95 (2)	2.813 (4)	175 (6)
O6—H6A ⁱ ···O3 ^v	0.858 (19)	1.96 (2)	2.785 (4)	162 (6)
C2—H2 ⁱ ···O2	0.93	2.56	2.916 (6)	103

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

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.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2344).

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supplementary materials

Article retracted

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Hexaaquachromium(II) bis(4-methylbenzenesulfonate)

H. Zhong, X.-M. Yang, H.-L. Xie and C.-J. Luo

Comment

The crystal structure of hexaaquacopper(II) bis(4-methylbenzenesulfonate), (II), has previously been reported (Zhong *et al.*, 2007). The crystal structure determination of the title compound, (I), has been carried out in order to elucidate the molecular conformation and to compare it with that of (II). We report herein the crystal structure of (I).

The asymmetric unit of the title compound, (I), (Fig. 1) contains one half -cation and one anion; the Cr atom lies on an inversion centre, as in (II). The bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987).

In the crystal structure, intermolecular O—H \cdots O and O—H \cdots S hydrogen bonds (Fig. 2 and Table 2) result in the formation of a supramolecular network structure; an intramolecular C—H \cdots O hydrogen bond is also present, as in (II).

The both compounds, (I) and (II), are isostructural.

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb. Lanthanum(III) nitrate hexahydrate (216.4 mg, 0.5 mmol), chromium(II) acetate dihydrate (103.1 mg, 0.5 mmol), 4-methylbenzenesulfonic acid (344.4 mg, 2 mmol), ammonia (0.5 mol/l, 4 ml) and distilled water (10 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 443 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 (for H₂O) were located in difference syntheses and refined isotropically [O—H = 0.832 (18)–0.89 (4) Å and $U_{\text{iso}}(\text{H}) = 0.092 (11)$ – $0.12 (2)$ Å²]. The remaining H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å, for aromatic and methyl H atoms and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$, where $x = 1.2$ for aromatic H and $x = 1.5$ for methyl H atoms.

Figures

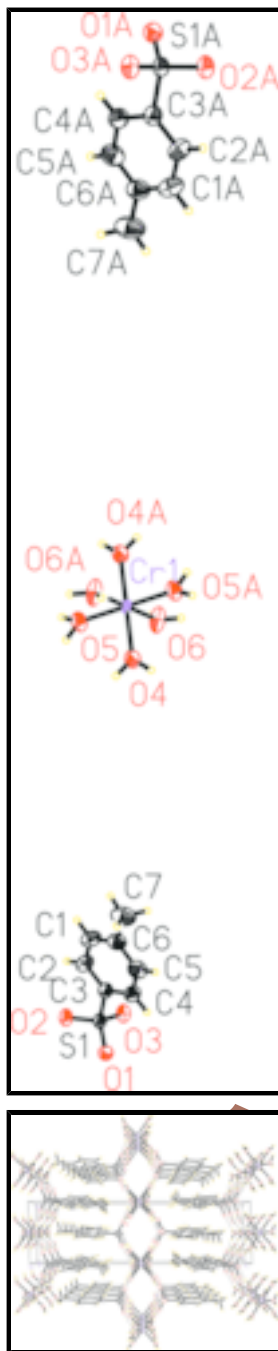


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): $3/2 - x, 1/2 - y, 1/2 - z$].

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

Hexaaquachromium(II) bis(4-methylbenzenesulfonate)

Crystal data

$[\text{Cr}(\text{H}_2\text{O})_6](\text{C}_7\text{H}_7\text{O}_3\text{S})_2$

$M_r = 502.47$

$F_{000} = 524$

$D_x = 1.510 \text{ Mg m}^{-3}$

Monoclinic, $P2_1/n$
 Hall symbol: -P 2yn
 $a = 7.0181 (11) \text{ \AA}$
 $b = 6.3017 (12) \text{ \AA}$
 $c = 24.9978 (15) \text{ \AA}$
 $\beta = 91.607 (3)^\circ$
 $V = 1105.1 (3) \text{ \AA}^3$
 $Z = 2$

Mo $K\alpha$ radiation
 $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 4992 reflections
 $\theta = 2.5\text{--}28.0^\circ$
 $\mu = 0.76 \text{ mm}^{-1}$
 $T = 273 (2) \text{ K}$
 Prism, colorless
 $0.49 \times 0.37 \times 0.19 \text{ mm}$

Data collection

Bruker SMART CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Monochromator: graphite
 $T = 273(2) \text{ K}$
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.709$, $T_{\max} = 0.866$
 6659 measured reflections

2117 independent reflections
 1842 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$
 $\theta_{\max} = 26.0^\circ$
 $\theta_{\min} = 3.0^\circ$
 $h = -8 \rightarrow 8$
 $k = -6 \rightarrow 7$
 $l = -30 \rightarrow 30$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.142$
 $S = 0.98$
 2117 reflections
 159 parameters
 9 restraints
 Primary atom site location: structure-invariant direct
 methods

Secondary atom site location: difference Fourier map
 Hydrogen site location: inferred from neighbouring
 sites
 H atoms treated by a mixture of
 independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0803P)^2 + 1.3523P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.63 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.46 \text{ e \AA}^{-3}$
 Extinction correction: SHELXL97 (Sheldrick, 1997),
 $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.018 (3)

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 calculat-

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ing 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	$U_{\text{iso}}^*/U_{\text{eq}}$
Cr1	0.5000	0.0000	0.0000	0.0351 (2)
S1	-0.01450 (13)	0.60820 (14)	0.90526 (4)	0.0533 (3)
O1	0.1535 (4)	0.5146 (4)	0.93049 (12)	0.0677 (7)
O2	-0.0146 (4)	0.8388 (4)	0.90904 (11)	0.0671 (7)
O3	-0.1907 (4)	0.5171 (4)	0.92380 (13)	0.0687 (8)
O4	0.7234 (5)	-0.1027 (5)	0.04787 (16)	0.0866 (10)
O5	0.5081 (4)	0.2891 (5)	0.03491 (13)	0.0688 (7)
O6	0.3035 (5)	-0.1042 (5)	0.05307 (16)	0.0877 (11)
C1	-0.0456 (7)	0.6319 (10)	0.7447 (2)	0.0888 (15)
H1	-0.0812	0.7296	0.7184	0.107*
C2	-0.0533 (7)	0.6920 (8)	0.79866 (18)	0.0773 (12)
H2	-0.0914	0.8279	0.8082	0.093*
C3	-0.0033 (5)	0.5456 (6)	0.83687 (16)	0.0585 (9)
C4	0.0535 (7)	0.3419 (7)	0.82200 (17)	0.0734 (11)
H4	0.0851	0.2411	0.8479	0.088*
C5	0.0621 (7)	0.2926 (9)	0.7688 (2)	0.0858 (14)
H5	0.1029	0.1579	0.7590	0.103*
C6	0.0127 (7)	0.4345 (10)	0.72959 (18)	0.0787 (12)
C7	0.0319 (9)	0.3685 (13)	0.6717 (2)	0.117 (2)
H7B	0.1644	0.3624	0.6632	0.175*
H7A	-0.0317	0.4702	0.6488	0.175*
H7C	-0.0249	0.2313	0.6663	0.175*
H4A	0.764 (5)	-0.224 (3)	0.0552 (15)	0.092 (11)*
H5A	0.621 (4)	0.330 (8)	0.048 (2)	0.094 (16)*
H6A	0.249 (7)	-0.226 (4)	0.055 (2)	0.12 (2)*
H4B	0.793 (6)	-0.024 (5)	0.0674 (19)	0.095 (18)*
H5B	0.456 (8)	0.413 (6)	0.040 (4)	0.11 (4)*
H6B	0.210 (5)	-0.025 (6)	0.063 (2)	0.10 (2)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cr1	0.0339 (4)	0.0249 (4)	0.0466 (4)	0.0007 (2)	0.0015 (2)	0.0017 (2)
S1	0.0534 (5)	0.0422 (5)	0.0642 (6)	0.0006 (4)	0.0032 (4)	-0.0004 (4)
O1	0.0729 (18)	0.0544 (16)	0.0750 (17)	0.0043 (12)	-0.0112 (14)	-0.0023 (12)
O2	0.0705 (17)	0.0440 (14)	0.0871 (19)	-0.0010 (12)	0.0058 (14)	-0.0025 (13)
O3	0.0705 (17)	0.0536 (16)	0.0828 (19)	-0.0049 (12)	0.0180 (14)	-0.0027 (13)
O4	0.087 (2)	0.0471 (17)	0.123 (3)	0.0055 (16)	-0.045 (2)	0.0009 (17)
O5	0.0590 (16)	0.0508 (16)	0.097 (2)	-0.0011 (13)	0.0030 (14)	-0.0130 (14)
O6	0.095 (2)	0.0483 (18)	0.123 (3)	-0.0001 (16)	0.052 (2)	0.0048 (17)
C1	0.084 (3)	0.112 (4)	0.071 (3)	0.009 (3)	0.000 (2)	0.024 (3)
C2	0.078 (3)	0.076 (3)	0.078 (3)	0.014 (2)	0.006 (2)	0.016 (2)

C3	0.0501 (19)	0.056 (2)	0.070 (2)	-0.0002 (16)	0.0019 (16)	0.0053 (17)
C4	0.092 (3)	0.061 (3)	0.066 (2)	0.012 (2)	-0.002 (2)	-0.003 (2)
C5	0.090 (3)	0.089 (4)	0.078 (3)	0.007 (3)	0.003 (2)	-0.019 (3)
C6	0.068 (3)	0.105 (4)	0.063 (2)	-0.009 (3)	0.002 (2)	0.002 (2)
C7	0.102 (4)	0.176 (7)	0.073 (3)	-0.008 (4)	0.008 (3)	-0.009 (4)

Geometric parameters (Å, °)

Cr1—O4	2.050 (3)	O6—H6B	0.87 (4)
Cr1—O5	2.020 (3)	C1—C6	1.366 (8)
Cr1—O6	2.048 (3)	C1—C2	1.404 (7)
Cr1—O4 ⁱ	2.050 (3)	C1—H1	0.9300
Cr1—O5 ⁱ	2.020 (3)	C2—C3	1.367 (6)
Cr1—O6 ⁱ	2.048 (3)	C2—H2	0.9300
S1—O1	1.447 (3)	C3—C4	1.397 (6)
S1—O3	1.451 (3)	C4—C5	1.370 (6)
S1—O2	1.456 (3)	C4—H4	0.9300
S1—C3	1.758 (4)	C5—C6	1.364 (7)
O4—H4A	0.832 (18)	C5—H5	0.9300
O4—H4B	0.84 (4)	C6—C7	1.516 (7)
O5—H5A	0.89 (4)	C7—H7B	0.9600
O5—H5B	0.87 (5)	C7—H7A	0.9600
O6—H6A	0.858 (19)	C7—H7C	0.9600
O4—Cr1—O4 ⁱ	180	H6A—O6—H6B	99 (3)
O4—Cr1—O5	91.19 (13)	C6—C1—C2	122.1 (5)
O4 ⁱ —Cr1—O5	88.81 (13)	C6—C1—H1	118.9
O4—Cr1—O6	92.21 (17)	C2—C1—H1	118.9
O4 ⁱ —Cr1—O6	87.79 (17)	C3—C2—C1	118.2 (5)
O5—Cr1—O5 ⁱ	180	C3—C2—H2	120.9
O5—Cr1—O6	91.19 (13)	C1—C2—H2	120.9
O5 ⁱ —Cr1—O6	88.81 (13)	C2—C3—C4	120.3 (4)
O6—Cr1—O6 ⁱ	180	C2—C3—S1	120.7 (3)
O4 ⁱ —Cr1—O5 ⁱ	91.19 (13)	C4—C3—S1	119.1 (3)
O4 ⁱ —Cr1—O6 ⁱ	92.21 (17)	C5—C4—C3	119.2 (4)
O5 ⁱ —Cr1—O6 ⁱ	91.19 (13)	C5—C4—H4	120.4
O1—S1—O3	112.99 (19)	C3—C4—H4	120.4
O1—S1—O2	112.35 (17)	C6—C5—C4	122.1 (5)
O3—S1—O2	111.85 (17)	C6—C5—H5	118.9
O1—S1—C3	105.91 (18)	C4—C5—H5	118.9
O3—S1—C3	106.48 (19)	C5—C6—C1	118.1 (4)
O2—S1—C3	106.70 (18)	C5—C6—C7	118.6 (6)
Cr1—O4—H4A	132 (2)	C1—C6—C7	123.3 (5)
Cr1—O4—H4B	125 (3)	C6—C7—H7B	109.5
H4A—O4—H4B	103 (3)	C6—C7—H7A	109.5
Cr1—O5—H5A	116 (4)	H7B—C7—H7A	109.5
Cr1—O5—H5B	149 (4)	C6—C7—H7C	109.5

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H5A—O5—H5B	94 (3)	H7B—C7—H7C	109.5
Cr1—O6—H6A	130 (3)	H7A—C7—H7C	109.5
Cr1—O6—H6B	122 (3)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H4A \cdots O1 ⁱⁱ	0.832 (18)	1.953 (19)	2.784 (4)	176 (4)
O4—H4B \cdots O2 ⁱⁱⁱ	0.84 (4)	2.02 (3)	2.825 (4)	160 (6)
O5—H5A \cdots S1 ⁱⁱⁱ	0.89 (4)	2.99 (2)	3.871 (3)	171 (5)
O5—H5A \cdots O1 ⁱⁱⁱ	0.89 (4)	1.93 (2)	2.793 (4)	166 (5)
O5—H5B \cdots O3 ^{iv}	0.87 (5)	2.14 (6)	2.766 (4)	128 (7)
O6—H6B \cdots O2 ^{iv}	0.87 (4)	1.95 (2)	2.813 (4)	175 (6)
O6—H6A \cdots O3 ^v	0.858 (19)	1.96 (2)	2.785 (4)	162 (6)
C2—H2 \cdots O2	0.93	2.56	2.916 (6)	103

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

Article retracted

Fig. 1

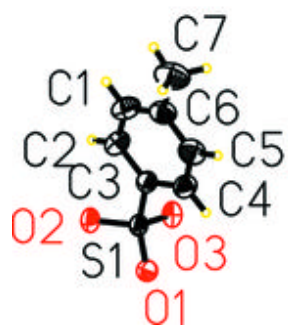
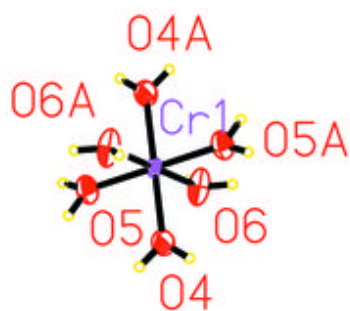
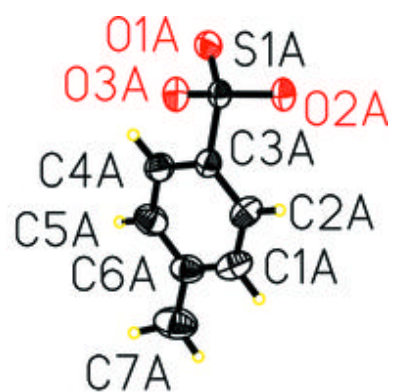
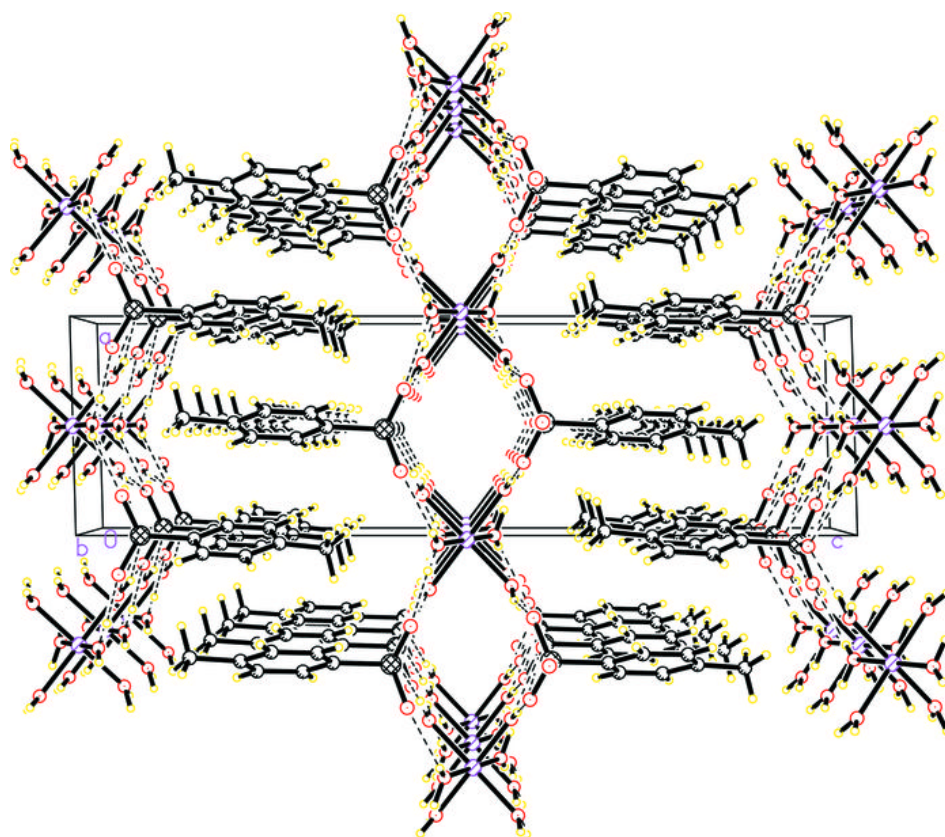


Fig. 2



Article