

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

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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	ITPCOO1
<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	VIKGAY
<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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2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate

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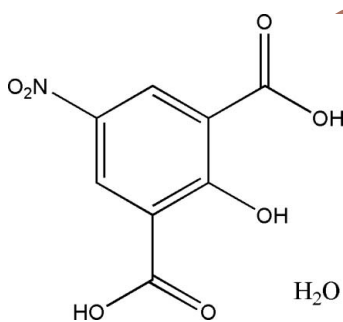
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Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.052; wR factor = 0.148; data-to-parameter ratio = 11.4.

In the crystal structure of the title complex, $\text{C}_8\text{H}_5\text{NO}_7 \cdot \text{H}_2\text{O}$, intra- and intermolecular $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds result in the formation of a supramolecular network structure.

Related literature

For general background, see: Desiraju (1995, 1997); Braga *et al.* (1998); McCann *et al.* (1995, 1996); Wai *et al.* (1990); Yaghi *et al.* (1996); Min & Lee (2002); Maira *et al.* (2001). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_8\text{H}_5\text{NO}_7 \cdot \text{H}_2\text{O}$
 $M_r = 245.15$
Monoclinic, $C2/c$
 $a = 25.21$ (2) Å
 $b = 6.5072$ (16) Å
 $c = 12.331$ (2) Å
 $\beta = 112.019$ (4)°

$V = 1875.3$ (17) Å³
 $Z = 8$
Mo $K\alpha$ radiation
 $\mu = 0.16$ mm⁻¹
 $T = 273$ (2) K
 $0.24 \times 0.15 \times 0.15$ mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.963$, $T_{\max} = 0.977$

6094 measured reflections
1885 independent reflections
972 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.148$
 $S = 1.02$
1885 reflections
166 parameters
4 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.35$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.21$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O7}-\text{H7} \cdots \text{O2}^i$	0.82	2.25	2.876 (3)	134
$\text{O1}-\text{H1} \cdots \text{O6}^{ii}$	0.82	2.73	2.816 (3)	88
$\text{O8}-\text{H8A} \cdots \text{O2}$	0.84 (4)	2.31 (5)	3.043 (3)	145 (7)
$\text{O7}-\text{H7} \cdots \text{O2}$	0.82	1.81	2.541 (3)	148

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

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: HK2323).

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supplementary materials

Article retracted

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2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate

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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 carboxyl groups are one of the most important classes of biological ligands, the coordination of metal-carboxyl groups complexes are of critical importance in biological systems, organic materials and coordination chemistry. Recently, carboxyl groups with variable coordination modes have been used to construct metal-organic supramolecular structures (McCann *et al.*, 1996; McCann *et al.*, 1995; Wai *et al.*, 1990; Yaghi *et al.*, 1996; Min & Lee 2002; Maira *et al.*, 2001). We originally attempted to synthesize complexes featuring La metal chains by reaction of the lanthanum(III) ion with 2-hydroxy-5-nitro-1,3-benzenedicarboxylic acid 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). It contains one (C₈H₅NO₇) molecule and one water molecule.

In the crystal structure, intramolecular and intermolecular O—H...O hydrogen bonds (Table 1, Fig. 2) 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, which was then sealed. Lanthanum (III) nitrate hexahydrate (216.4 mg, 0.5 mmol), 2-hydroxy-5-nitro-1,3-benzenedicarboxylic acid (226.2 mg, 1 mmol), ammonia (0.5 mol/l, 4 ml) and distilled water (2 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. Found: C 39.08, H 2.84, N 5.67%; analysis calculated for C₈H₇NO₈: C 39.20, H 2.88, N 5.71%.

Refinement

H8A and H8B (for H₂O) were located in difference syntheses and refined isotropically [O—H = 0.84 (4) and 0.841 (19) Å, $U_{\text{iso}}(\text{H}) = 0.11$ (5) and 0.114 (18) Å²]. The remaining H atoms were positioned geometrically, with O—H = 0.82 Å (for OH) and C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C}, \text{O})$, where $x = 1.2$ for aromatic H atoms and $x = 1.5$ for all other H atoms.

Figures

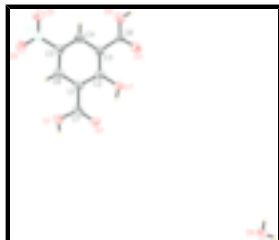


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

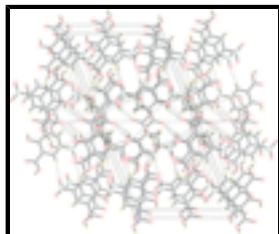


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate

Crystal data

$C_8H_5NO_7 \cdot H_2O$

$M_r = 245.15$

Monoclinic, $C2/c$

Hall symbol: $-C 2yc$

$a = 25.21 (2) \text{ \AA}$

$b = 6.5072 (16) \text{ \AA}$

$c = 12.331 (2) \text{ \AA}$

$\beta = 112.019 (4)^\circ$

$V = 1875.3 (17) \text{ \AA}^3$

$Z = 8$

$F_{000} = 1008$

$D_x = 1.737 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 1481 reflections

$\theta = 2.8\text{--}26.6^\circ$

$\mu = 0.16 \text{ mm}^{-1}$

$T = 273 (2) \text{ K}$

Prism, colourless

$0.24 \times 0.15 \times 0.15 \text{ mm}$

Data collection

Bruker APEXII 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)

$T_{\min} = 0.963$, $T_{\max} = 0.977$

6094 measured reflections

1885 independent reflections

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

$R_{\text{int}} = 0.032$

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

$\theta_{\min} = 3.3^\circ$

$h = -31 \rightarrow 31$

$k = -7 \rightarrow 8$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.052$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.148$	$w = 1/[\sigma^2(F_o^2) + (0.078P)^2 + 0.002P]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
1885 reflections	$(\Delta/\sigma)_{\max} < 0.001$
166 parameters	$\Delta\rho_{\max} = 0.35 \text{ e } \text{\AA}^{-3}$
4 restraints	$\Delta\rho_{\min} = -0.21 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 1997), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.0090 (18)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.53249 (7)	0.2530 (3)	1.04704 (15)	0.0707 (6)
H1	0.5645	0.2442	1.0450	0.106*
O2	0.50754 (9)	0.2174 (4)	0.86014 (17)	0.0995 (8)
O3	0.29255 (7)	0.1309 (3)	0.63171 (16)	0.0799 (7)
O4	0.24253 (8)	0.3055 (3)	0.70484 (16)	0.0794 (6)
H4	0.2176	0.2804	0.6409	0.119*
O5	0.30610 (8)	0.3717 (3)	1.11233 (16)	0.0838 (7)
O6	0.39253 (10)	0.3002 (4)	1.21843 (18)	0.0951 (8)
O7	0.40213 (7)	0.2101 (3)	0.72900 (15)	0.0714 (6)
H7	0.4369	0.2112	0.7461	0.107*
O8	0.63201 (8)	0.2289 (3)	1.02771 (18)	0.0718 (6)
N1	0.35410 (10)	0.3194 (4)	1.1251 (2)	0.0646 (6)
C1	0.43547 (9)	0.2452 (4)	0.9353 (2)	0.0525 (6)
C2	0.39111 (11)	0.2307 (4)	0.8239 (2)	0.0548 (6)
C3	0.33520 (10)	0.2446 (4)	0.8197 (2)	0.0515 (6)

supplementary materials

C4	0.32271 (10)	0.2745 (3)	0.9165 (2)	0.0542 (6)
H4A	0.2850	0.2882	0.9108	0.105*
C5	0.36655 (10)	0.2839 (4)	1.0212 (2)	0.0523 (6)
C6	0.42274 (10)	0.2691 (4)	1.0321 (2)	0.0544 (6)
H6	0.4519	0.2754	1.1057	0.105*
C7	0.49519 (10)	0.2385 (4)	0.9441 (2)	0.0605 (7)
C8	0.28731 (9)	0.2262 (3)	0.71083 (18)	0.0424 (6)
H8B	0.630 (2)	0.215 (7)	0.959 (2)	0.114 (18)*
H8A	0.5964 (12)	0.22 (3)	1.010 (6)	0.11 (5)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0384 (11)	0.1043 (15)	0.0618 (12)	-0.0009 (10)	0.0099 (9)	-0.0009 (9)
O2	0.0435 (11)	0.198 (3)	0.0589 (13)	0.0025 (12)	0.0217 (10)	0.0002 (12)
O3	0.0514 (11)	0.1153 (17)	0.0653 (12)	-0.0086 (11)	0.0131 (9)	-0.0093 (11)
O4	0.0411 (11)	0.1231 (17)	0.0646 (12)	0.0067 (11)	0.0092 (9)	0.0062 (11)
O5	0.0599 (13)	0.1226 (17)	0.0794 (13)	0.0043 (11)	0.0382 (11)	-0.0094 (12)
O6	0.0739 (15)	0.157 (2)	0.0506 (12)	0.0154 (13)	0.0186 (11)	-0.0037 (12)
O7	0.0377 (10)	0.1242 (16)	0.0524 (11)	0.0002 (10)	0.0171 (8)	-0.0026 (9)
O8	0.0440 (11)	0.0945 (15)	0.0713 (14)	0.0003 (9)	0.0152 (9)	0.0031 (10)
N1	0.0570 (15)	0.0803 (16)	0.0606 (14)	0.0003 (11)	0.0269 (13)	-0.0038 (11)
C1	0.0351 (13)	0.0693 (16)	0.0517 (15)	0.0004 (11)	0.0146 (12)	0.0017 (11)
C2	0.0440 (14)	0.0723 (16)	0.0478 (14)	0.0008 (12)	0.0170 (12)	-0.0006 (11)
C3	0.0385 (13)	0.0645 (16)	0.0490 (13)	-0.0005 (10)	0.0136 (11)	0.0046 (11)
C4	0.0423 (14)	0.0608 (16)	0.0605 (16)	0.0002 (10)	0.0205 (13)	0.0033 (11)
C5	0.0480 (15)	0.0633 (15)	0.0471 (13)	0.0036 (11)	0.0197 (11)	0.0008 (11)
C6	0.0397 (13)	0.0674 (16)	0.0517 (14)	-0.0008 (11)	0.0119 (11)	-0.0003 (11)
C7	0.0388 (14)	0.0849 (19)	0.0535 (15)	0.0001 (12)	0.0123 (13)	0.0042 (12)
C8	0.0260 (12)	0.0659 (15)	0.0347 (12)	-0.0002 (10)	0.0106 (9)	0.0025 (10)

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

O1—C7	1.268 (3)	N1—C5	1.448 (3)
O1—H1	0.8200	C1—C6	1.356 (3)
O2—C7	1.196 (3)	C1—C2	1.412 (3)
O3—C8	1.204 (3)	C1—C7	1.469 (4)
O4—C8	1.218 (3)	C2—C3	1.393 (4)
O4—H4	0.8200	C3—C4	1.358 (3)
O5—N1	1.209 (3)	C3—C8	1.435 (3)
O6—N1	1.201 (3)	C4—C5	1.350 (3)
O7—C2	1.308 (3)	C4—H4A	0.9300
O7—H7	0.8200	C5—C6	1.375 (4)
O8—H8B	0.841 (19)	C6—H6	0.9300
O8—H8A	0.84 (4)		
C7—O1—H1	109.5	C5—C4—C3	118.1 (2)
C8—O4—H4	109.5	C5—C4—H4A	121.0
C2—O7—H7	109.5	C3—C4—H4A	121.0

H8B—O8—H8A	95 (3)	C4—C5—C6	122.3 (2)
O6—N1—O5	124.2 (2)	C4—C5—N1	118.8 (2)
O6—N1—C5	117.8 (2)	C6—C5—N1	118.8 (2)
O5—N1—C5	117.9 (2)	C1—C6—C5	119.8 (2)
C6—C1—C2	120.1 (2)	C1—C6—H6	120.1
C6—C1—C7	120.8 (2)	C5—C6—H6	120.1
C2—C1—C7	119.1 (2)	O2—C7—O1	122.6 (2)
O7—C2—C3	121.6 (2)	O2—C7—C1	122.1 (2)
O7—C2—C1	121.4 (2)	O1—C7—C1	115.3 (2)
C3—C2—C1	117.0 (2)	O3—C8—O4	123.3 (2)
C4—C3—C2	122.7 (2)	O3—C8—C3	119.4 (2)
C4—C3—C8	116.3 (2)	O4—C8—C3	117.2 (2)
C2—C3—C8	121.0 (2)		

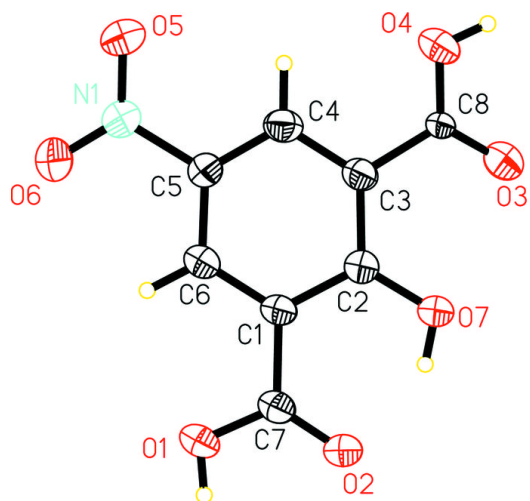
Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O7—H7 \cdots O2 ⁱ	0.82	2.25	2.876 (3)	134
O1—H1 \cdots O6 ⁱⁱ	0.82	2.73	2.816 (3)	88
O8—H8A \cdots O2	0.84 (4)	2.31 (5)	3.043 (3)	145 (7)
O7—H7 \cdots O2	0.82	1.81	2.541 (3)	148

Symmetry codes: (i) $-x+1, y, -z+3/2$; (ii) $-x+1, y, -z+5/2$.

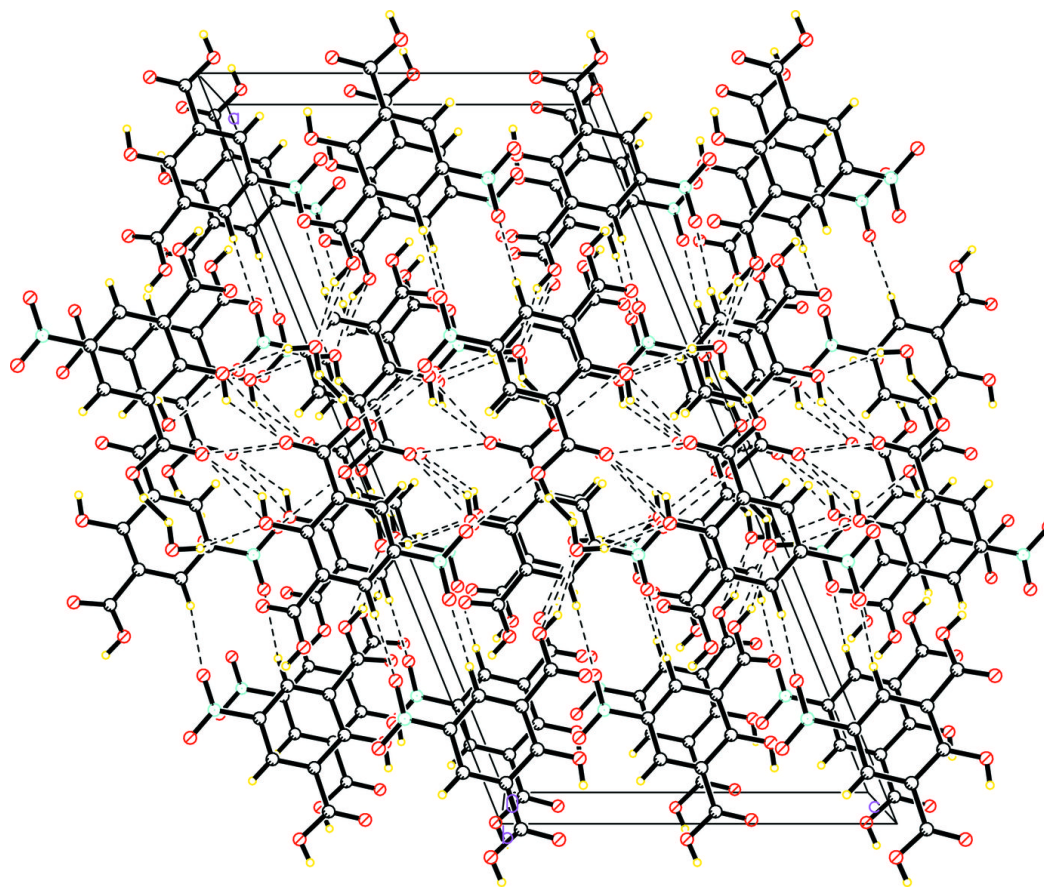
Article retracted

Fig. 1



Article

Fig. 2



Article