Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Hemi(piperazinediium) hexaaquaaluminium(III) bis(sulfate) tetrahydrate: a redetermination at 100 K

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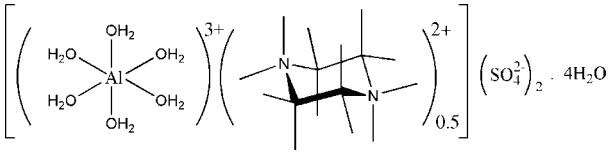
Received 29 May 2007; accepted 7 June 2007

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.001 Å; R factor = 0.024; wR factor = 0.064; data-to-parameter ratio = 22.3.

The reaction of aluminium(III) sulfate with piperazinediium pyridine-2,6-dicarboxylate, $(pipzH_2)(pydc)$, where pipz is piperazine and $pydcH_2$ is pyridine-2,6-dicarboxylic acid, in aqueous solution leads to the formation of the title complex, $(C_4H_{12}N_2)_{1/2}[Al(H_2O)_6](SO_4)_2{\cdot}4H_2O$. The crystal structure of this compound has been published previously [Bataille (2003), *Acta Cryst.* C**59**, m459–m461], and our report is a redetermination of the structure at 100 K. As previously observed, intermolecular O—H···O and N—H···O hydrogen bonds result in the formation of a three-dimensional network and a supramolecular structure.

Related literature

For the crystal structure of the title compound at 293 K, see: Bataille (2003). For related literature, see: Aghabozorg *et al.* (2006).



Experimental

Crystal data

$(C_4H_{12}N_2)_{0.5}[Al(H_2O)_6](SO_4)_2{\cdot}4H_2O$
M_r = 443.34
Monoclinic, $P2_1/n$
a = 6.5438 (3) Å
b = 11.9938 (5) Å
c = 21.4916 (9) Å
β = 90.164 (1)°
V = 1686.76 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.46 mm^{-1}
T = 100 (2) K
0.55 × 0.50 × 0.45 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: none
21192 measured reflections
4847 independent reflections
4639 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.065
S = 1.12
4847 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O91—H11···O22^{i}	0.93	1.69	2.6205 (10)	171
O91—H12···O99^{i}	0.95	1.70	2.6546 (10)	174
O92—H21···O910^{ii}	0.94	1.70	2.6411 (10)	175
O92—H22···O21^{iii}	0.92	1.71	2.6302 (10)	175
O93—H31···O14^{iv}	0.93	1.68	2.6046 (10)	176
O93—H32···O99	0.92	1.72	2.6313 (10)	169
O94—H41···O11	0.91	1.71	2.6232 (10)	174
O94—H42···O21^{v}	0.94	1.71	2.6547 (10)	177
O95—H51···O97	0.94	1.74	2.6677 (10)	169
O95—H52···O12^{i}	0.95	1.77	2.7161 (10)	177
O96—H61···O24	0.93	1.71	2.6345 (10)	173
O96—H62···O22^{v}	0.92	1.79	2.6997 (10)	173
N2—H21N···O23^{vi}	0.97	1.82	2.7864 (11)	174
N2—H22N···O14	0.98	1.91	2.8769 (11)	167
O97—H71···O12^{iv}	0.95	1.89	2.8149 (10)	166
O97—H72···O23^{vi}	0.94	1.89	2.8203 (10)	172
O98—H81···O11	0.94	1.84	2.7663 (10)	169
O98—H82···O13^{i}	0.92	1.95	2.8594 (11)	168
O99—H91···O98^{iv}	0.93	1.80	2.7042 (11)	164
O99—H92···O910	0.96	1.88	2.8091 (11)	161
O910—H101···O97	0.95	1.90	2.8468 (11)	177
O910—H102···O13	0.94	1.76	2.6974 (10)	173

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to Islamic Azad University, Shahr-e Rey Branch, for financial support of this work. The Teacher Training University is also gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2188).

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supplementary materials

Acta Cryst. (2007). E**63**, m1919 [**doi:10.1107/S1600536807028152**]

Hemi(piperazinediium) hexaaquaaluminium(III) bis(sulfate) tetrahydrate: a redetermination at 100 K

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Comment

In this work, our goal was the generation of the self-assembling coordination compound using a self-assembling ligand. The structure of the Al(III) complex was reported recently (Bataille, 2003), but the goal and method of synthesis were completely different from ours. The data collection temperature in our work was 100 K, whereas, the previous work was conducted at room temperature. For our complex, the final *R* value was 0.0237, whereas in the reported structure it was 0.0384. In the present study the measured reflections was 4639, while in the earlier work it was 2991.

As previously observed (Bataille, 2003), the structure of (I) consists of Al^{3+} ions octahedrally coordinated to six water molecules, together with sulfate tetrahedra, piperazinium cations (lying about inversion centres) and non-bonded water molecules, linked by hydrogen bonds only (Fig. 1, Table 1). All the O—H···O and N—H···O hydrogen bonds build up a three dimensionnal network as previously reported (Table 1).

Experimental

A solution of $Al_2(SO_4)_3.18H_2O$ (333 mg, 0.5 mmol) in water (10 ml) was added to an aqueous solution of the proton-transfer compound $(pipzH_2)(pydc)$ (Aghabozorg *et al.*, 2006) (506 mg, 2 mmol) in water (20 ml). Colorless crystals of (I) were obtained after allowing the mixture to stand for seven weeks at room temperature.

Refinement

All H atoms were located in difference Fourier maps but they were treated in the refinement as riding on their parent atoms with $U_{iso}(H) = 1.2U_{eq}$(C or N). H or $U_{iso}(H) = 1.5U_{eq}(O)$.

Figures

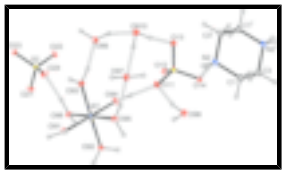


Fig. 1. / The asymmetric unit of (I), showing the atom-labelling scheme. Ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines. H atoms are represented as small spheres of arbitrary radii.

Hemi(piperazinediium) hexaaquaaluminium(III) bis(sulfate) tetrahydrate

Crystal data

$(C_4H_{12}N_2)_{0.5}[Al(H_2O)_6](SO_4)_2{\cdot}4H_2O$ $F_{000} = 936$

M_r = 443.34	D_x = 1.746 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 9176 reflections
a = 6.5438 (3) Å	θ = 3.1–33.5º
b = 11.9938 (5) Å	μ = 0.46 mm^{-1}
c = 21.4916 (9) Å	T = 100 (2) K
β = 90.164 (1)º	Needle, colourless
V = 1686.76 (13) Å^3	0.55 × 0.50 × 0.45 mm
Z = 4	

Data collection

Bruker APEXII CCD area-detector diffractometer	4639 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.017
Monochromator: graphite	θ_{max} = 30.0º
T = 100(2) K	θ_{min} = 1.9º
ω scans	h = −9→9
Absorption correction: none	k = −16→16
21192 measured reflections	l = −30→30
4847 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.024	H-atom parameters constrained
$wR(F^2)$ = 0.065	$w = 1/[\sigma^2(F_o^2) + (0.0314P)^2 + 0.8179P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.12	$(\Delta/\sigma)_{max}$ = 0.002
4847 reflections	$\Delta\rho_{max}$ = 0.45 e Å^{-3}
217 parameters	$\Delta\rho_{min}$ = −0.43 e Å^{-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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Al1	0.46318 (4)	0.06332 (2)	0.367174 (13)	0.00638 (6)
S1	−0.04729 (3)	−0.026950 (19)	0.191802 (10)	0.00698 (6)
S2	−0.03384 (3)	0.191544 (19)	0.543172 (10)	0.00664 (6)
O11	0.15644 (11)	0.00561 (7)	0.21597 (3)	0.01263 (14)
O12	−0.16492 (11)	−0.08210 (6)	0.24163 (3)	0.01111 (13)
O13	−0.15781 (11)	0.07318 (6)	0.16977 (3)	0.01059 (13)
O14	−0.02011 (11)	−0.10239 (6)	0.13764 (3)	0.01058 (13)
O21	0.03790 (11)	0.10582 (6)	0.58850 (3)	0.01070 (13)
O22	−0.23346 (11)	0.15446 (6)	0.51731 (3)	0.01083 (13)
O23	−0.06166 (12)	0.29846 (6)	0.57654 (3)	0.01124 (14)
O24	0.11598 (12)	0.20524 (6)	0.49313 (4)	0.01263 (14)
O91	0.70177 (11)	0.13100 (6)	0.39764 (3)	0.00987 (13)
H11	0.7381	0.1366	0.4396	0.015*
H12	0.7911	0.1736	0.3719	0.015*
O92	0.58088 (11)	−0.07843 (6)	0.37551 (3)	0.00921 (13)
H21	0.5367	−0.1358	0.3490	0.014*
H22	0.7117	−0.0898	0.3904	0.014*
O93	0.34321 (11)	0.20329 (6)	0.35718 (3)	0.00985 (13)
H31	0.4107	0.2713	0.3579	0.015*
H32	0.2067	0.2122	0.3475	0.015*
O94	0.22216 (11)	−0.00281 (6)	0.33634 (3)	0.00985 (13)
H41	0.1923	−0.0035	0.2948	0.015*
H42	0.1263	−0.0395	0.3618	0.015*
O95	0.56726 (11)	0.07184 (6)	0.28547 (3)	0.00972 (13)
H51	0.5402	0.1244	0.2538	0.015*
H52	0.6632	0.0199	0.2693	0.015*
O96	0.36145 (11)	0.05062 (6)	0.44869 (3)	0.00899 (13)
H61	0.2661	0.1014	0.4637	0.013*
H62	0.3291	−0.0208	0.4604	0.013*
C1	0.21352 (15)	−0.03328 (9)	−0.00316 (5)	0.01139 (17)
H1A	0.3297	−0.0764	0.0140	0.014*
H1B	0.2622	0.0082	−0.0401	0.014*
N2	0.13773 (13)	0.04702 (7)	0.04474 (4)	0.01019 (15)
H21N	0.2469	0.0966	0.0571	0.012*
H22N	0.0929	0.0036	0.0808	0.012*
C3	0.04290 (15)	−0.11226 (8)	−0.02208 (5)	0.01135 (17)
H3A	0.0914	−0.1625	−0.0555	0.014*
H3B	0.0028	−0.1586	0.0140	0.014*
O97	0.46083 (11)	0.23332 (6)	0.20641 (3)	0.01154 (14)
H71	0.5473	0.2917	0.2201	0.017*
H72	0.4663	0.2247	0.1630	0.017*
O98	0.46950 (11)	−0.03204 (6)	0.13234 (3)	0.01213 (14)
H81	0.3761	−0.0178	0.1645	0.018*
H82	0.5871	0.0082	0.1394	0.018*
O99	−0.03940 (11)	0.25482 (6)	0.33251 (3)	0.01119 (13)

H91	−0.0342	0.3254	0.3500	0.017*
H92	−0.0442	0.2657	0.2883	0.017*
O910	0.02956 (12)	0.26417 (6)	0.20367 (4)	0.01238 (14)
H101	0.1734	0.2544	0.2030	0.019*
H102	−0.0246	0.1950	0.1915	0.019*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.00647 (12)	0.00660 (13)	0.00607 (12)	−0.00009 (9)	0.00003 (9)	0.00003 (9)
S1	0.00685 (10)	0.00767 (10)	0.00641 (10)	0.00039 (7)	0.00017 (7)	0.00016 (7)
S2	0.00686 (10)	0.00652 (10)	0.00655 (10)	0.00020 (7)	0.00028 (7)	0.00008 (7)
O11	0.0081 (3)	0.0195 (4)	0.0103 (3)	−0.0020 (3)	−0.0016 (2)	−0.0005 (3)
O12	0.0118 (3)	0.0117 (3)	0.0099 (3)	0.0006 (3)	0.0035 (2)	0.0028 (2)
O13	0.0119 (3)	0.0073 (3)	0.0126 (3)	0.0018 (2)	−0.0009 (2)	0.0012 (2)
O14	0.0139 (3)	0.0095 (3)	0.0083 (3)	0.0017 (3)	0.0005 (2)	−0.0017 (2)
O21	0.0089 (3)	0.0105 (3)	0.0127 (3)	0.0008 (2)	−0.0013 (2)	0.0045 (2)
O22	0.0099 (3)	0.0129 (3)	0.0097 (3)	−0.0026 (3)	−0.0030 (2)	0.0013 (3)
O23	0.0142 (3)	0.0085 (3)	0.0110 (3)	0.0025 (3)	−0.0014 (3)	−0.0031 (2)
O24	0.0135 (3)	0.0111 (3)	0.0133 (3)	−0.0001 (3)	0.0069 (3)	0.0009 (3)
O91	0.0095 (3)	0.0125 (3)	0.0076 (3)	−0.0034 (2)	−0.0011 (2)	0.0007 (2)
O92	0.0087 (3)	0.0080 (3)	0.0109 (3)	0.0013 (2)	−0.0018 (2)	−0.0008 (2)
O93	0.0083 (3)	0.0070 (3)	0.0142 (3)	0.0001 (2)	−0.0004 (2)	0.0008 (2)
O94	0.0089 (3)	0.0126 (3)	0.0081 (3)	−0.0030 (2)	−0.0014 (2)	0.0008 (2)
O95	0.0110 (3)	0.0110 (3)	0.0071 (3)	0.0025 (2)	0.0016 (2)	0.0014 (2)
O96	0.0107 (3)	0.0081 (3)	0.0082 (3)	0.0000 (2)	0.0017 (2)	0.0005 (2)
C1	0.0094 (4)	0.0137 (4)	0.0110 (4)	0.0004 (3)	0.0003 (3)	−0.0022 (3)
N2	0.0103 (4)	0.0112 (4)	0.0091 (4)	−0.0012 (3)	−0.0011 (3)	−0.0004 (3)
C3	0.0122 (4)	0.0102 (4)	0.0117 (4)	0.0008 (3)	−0.0021 (3)	−0.0008 (3)
O97	0.0146 (3)	0.0111 (3)	0.0089 (3)	−0.0003 (3)	−0.0001 (2)	0.0011 (2)
O98	0.0106 (3)	0.0126 (3)	0.0131 (3)	−0.0005 (3)	0.0006 (3)	0.0000 (3)
O99	0.0110 (3)	0.0104 (3)	0.0122 (3)	0.0001 (3)	0.0002 (2)	0.0014 (3)
O910	0.0129 (3)	0.0086 (3)	0.0156 (3)	−0.0001 (3)	−0.0009 (3)	0.0006 (3)

Geometric parameters (Å, °)

Al1—O93	1.8654 (8)	O95—H51	0.9440
Al1—O92	1.8748 (8)	O95—H52	0.9504
Al1—O91	1.8760 (8)	O96—H61	0.9304
Al1—O96	1.8820 (8)	O96—H62	0.9177
Al1—O94	1.8841 (8)	C1—N2	1.4954 (13)
Al1—O95	1.8880 (8)	C1—C3	1.5187 (14)
S1—O12	1.4770 (7)	C1—H1A	0.9900
S1—O13	1.4791 (7)	C1—H1B	0.9900
S1—O11	1.4818 (7)	N2—C3^{i}	1.4977 (13)
S1—O14	1.4854 (7)	N2—H21N	0.9666
S2—O24	1.4666 (7)	N2—H22N	0.9802
S2—O23	1.4808 (7)	C3—N2^{i}	1.4977 (13)

S2—O22	1.4862 (7)	C3—H3A	0.9900
S2—O21	1.4913 (7)	C3—H3B	0.9900
O91—H11	0.9343	O97—H71	0.9466
O91—H12	0.9543	O97—H72	0.9395
O92—H21	0.9386	O98—H81	0.9403
O92—H22	0.9229	O98—H82	0.9208
O93—H31	0.9273	O99—H91	0.9268
O93—H32	0.9227	O99—H92	0.9595
O94—H41	0.9126	O910—H101	0.9484
O94—H42	0.9433	O910—H102	0.9390
O93—Al1—O92	178.68 (4)	Al1—O93—H32	122.5
O93—Al1—O91	90.02 (3)	H31—O93—H32	111.3
O92—Al1—O91	91.02 (3)	Al1—O94—H41	121.6
O93—Al1—O96	91.73 (3)	Al1—O94—H42	123.3
O92—Al1—O96	89.08 (3)	H41—O94—H42	115.0
O91—Al1—O96	90.36 (3)	Al1—O95—H51	129.7
O93—Al1—O94	89.24 (3)	Al1—O95—H52	123.0
O92—Al1—O94	89.72 (3)	H51—O95—H52	107.3
O91—Al1—O94	179.26 (4)	Al1—O96—H61	120.6
O96—Al1—O94	89.73 (3)	Al1—O96—H62	114.4
O93—Al1—O95	89.83 (3)	H61—O96—H62	111.1
O92—Al1—O95	89.36 (3)	N2—C1—C3	109.93 (8)
O91—Al1—O95	89.95 (3)	N2—C1—H1A	109.7
O96—Al1—O95	178.41 (4)	C3—C1—H1A	109.7
O94—Al1—O95	89.97 (3)	N2—C1—H1B	109.7
O12—S1—O13	109.90 (4)	C3—C1—H1B	109.7
O12—S1—O11	109.52 (4)	H1A—C1—H1B	108.2
O13—S1—O11	109.68 (5)	C1—N2—C3^{i}	112.06 (7)
O12—S1—O14	111.05 (4)	C1—N2—H21N	109.9
O13—S1—O14	107.65 (4)	C3^{i}—N2—H21N	110.5
O11—S1—O14	109.00 (4)	C1—N2—H22N	107.7
O24—S2—O23	109.97 (5)	C3^{i}—N2—H22N	107.3
O24—S2—O22	110.36 (4)	H21N—N2—H22N	109.3
O23—S2—O22	109.34 (4)	N2^{i}—C3—C1	109.88 (8)
O24—S2—O21	110.27 (4)	N2^{i}—C3—H3A	109.7
O23—S2—O21	108.64 (4)	C1—C3—H3A	109.7
O22—S2—O21	108.22 (4)	N2^{i}—C3—H3B	109.7
Al1—O91—H11	125.3	C1—C3—H3B	109.7
Al1—O91—H12	122.7	H3A—C3—H3B	108.2
H11—O91—H12	111.5	H71—O97—H72	111.4
Al1—O92—H21	118.7	H81—O98—H82	109.1
Al1—O92—H22	123.2	H91—O99—H92	106.2
H21—O92—H22	112.7	H101—O910—H102	105.1
Al1—O93—H31	126.1		

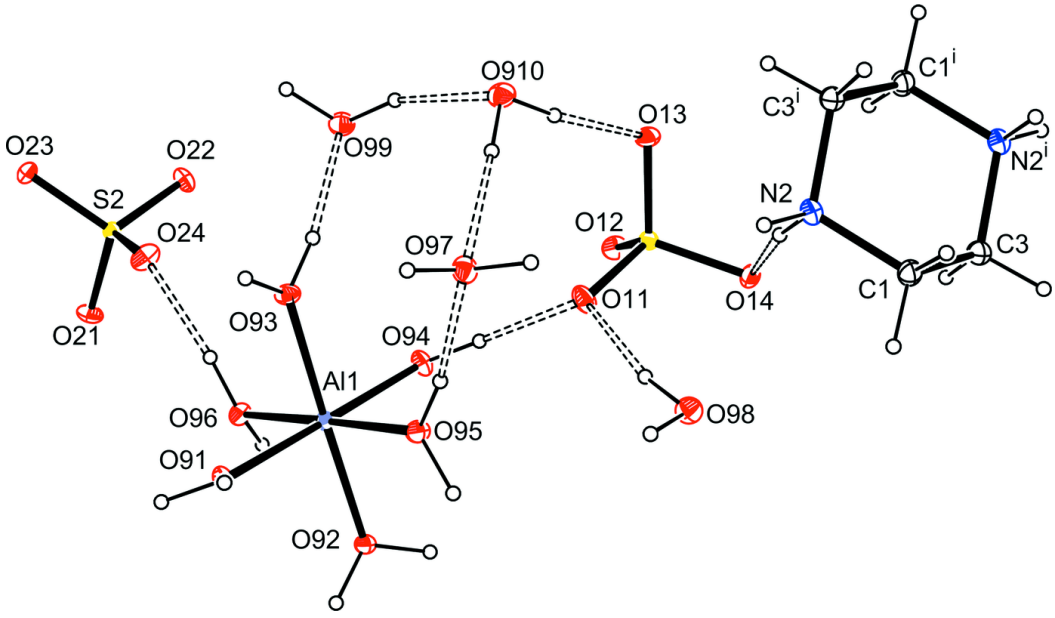
Symmetry codes: (i) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O91—H11···O22^{ii}	0.93	1.69	2.6205 (10)	171
O91—H12···O99^{ii}	0.95	1.70	2.6546 (10)	174
O92—H21···O910^{iii}	0.94	1.70	2.6411 (10)	175
O92—H22···O21^{iv}	0.92	1.71	2.6302 (10)	175
O93—H31···O14^{v}	0.93	1.68	2.6046 (10)	176
O93—H32···O99	0.92	1.72	2.6313 (10)	169
O94—H41···O11	0.91	1.71	2.6232 (10)	174
O94—H42···O21^{vi}	0.94	1.71	2.6547 (10)	177
O95—H51···O97	0.94	1.74	2.6677 (10)	169
O95—H52···O12^{ii}	0.95	1.77	2.7161 (10)	177
O96—H61···O24	0.93	1.71	2.6345 (10)	173
O96—H62···O22^{vi}	0.92	1.79	2.6997 (10)	173
N2—H21N···O23^{vii}	0.97	1.82	2.7864 (11)	174
N2—H22N···O14	0.98	1.91	2.8769 (11)	167
O97—H71···O12^{v}	0.95	1.89	2.8149 (10)	166
O97—H72···O23^{vii}	0.94	1.89	2.8203 (10)	172
O98—H81···O11	0.94	1.84	2.7663 (10)	169
O98—H82···O13^{ii}	0.92	1.95	2.8594 (11)	168
O99—H91···O98^{v}	0.93	1.80	2.7042 (11)	164
O99—H92···O910	0.96	1.88	2.8091 (11)	161
O910—H101···O97	0.95	1.90	2.8468 (11)	177
O910—H102···O13	0.94	1.76	2.6974 (10)	173

Symmetry codes: (ii) *x*+1, *y*, *z*; (iii) −*x*+1/2, *y*−1/2, −*z*+1/2; (iv) −*x*+1, −*y*, −*z*+1; (v) −*x*+1/2, *y*+1/2, −*z*+1/2; (vi) −*x*, −*y*, −*z*+1; (vii) *x*+1/2, −*y*+1/2, *z*−1/2.

Fig. 1


O910
O13
C1i
C3i
N2i
O99
O23
O22
S2
O24
N2
O12
C3
O97
O14
C1
O11
O21
O93
O94
Al1
O98
O96
O95
O91
O92