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Dipotassium zinc tetraiodate(V) dihydrate

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Key indicators: single-crystal X-ray study; T = 295 K; mean σ(Zn–O) = 0.005 Å; R factor = 0.019; wR factor = 0.055; data-to-parameter ratio = 15.6.

The title compound, $K_2Zn(IO_3)_4 \cdot 2H_2O$, contains two symmetry-independent K and I atoms. These atoms, as well as the Zn atom, are coordinated by shared O atoms and, moreover, the Zn atom is coordinated by two water molecules in *trans* positions. The K, Zn and water O atoms atoms are situated in special positions on twofold symmetry axes. The hydrogen atoms are involved in strong O—H⋯O hydrogen bonds and O—H⋯I interactions also occur. The crystals of the title compound are, in general, twinned, but the sample used for this experiment was free of twinning.

Related literature

Single crystals of KIO_3 grown from aqueous solution develop as domained crystals of poor quality but the quality of the crystals obtained can be affected by additional reagents such as HIO_3, see: Hamid (1974); Lü & Zhang (1987). For related structures, see Vinogradov *et al.* (1979); Maneva & Rabadjieva (1994); Juncheng *et al.* (2000); Lepeshkov *et al.* (1977); Lucas (1984). For hydrogen bonding, see: Desiraju & Steiner (1999). For a description of the Cambridge Structural Database, see: Allen (2002). For the PDF-2 Powder Diffraction Database, see: ICDD (2000) and for the Inorganic Crystal Structure Database, see: ICSD (2009). For the extinction correction, see: Becker & Coppens (1974).

Experimental

Crystal data

$K_2Zn(IO_3)_4 \cdot 2H_2O$
M_r = 879.2
Monoclinic, $C2$
a = 13.8044 (3) Å
b = 7.7285 (2) Å
c = 8.2860 (2) Å
β = 126.5726 (13)°

V = 709.95 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 11.08 mm^{-1}
T = 295 K
0.17 × 0.12 × 0.05 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: gaussian (Coppens, 1970)
T_{min} = 0.241, T_{max} = 0.581

11909 measured reflections
1639 independent reflections
1595 reflections with $I > 3\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.055
S = 1.72
1639 reflections
105 parameters
4 restraints

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}
Absolute structure: Flack (1983), 761 Friedel pairs
Flack parameter: −0.01 (3)

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O7—H1*O*7⋯O4^{i}	0.85 (9)	1.88 (10)	2.672 (6)	155 (5)
O7—H1*O*7^{ii}⋯O4^{iii}	0.85 (9)	1.88 (10)	2.672 (6)	155 (5)
O8—H1*O*8⋯O3^{ii}	0.845 (16)	1.837 (16)	2.610 (4)	151 (4)
O8—H1*O*8⋯I1^{ii}	0.845 (16)	2.96 (3)	3.4119 (10)	116 (3)

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

Data collection: *COLLECT* (Nonius, 2000) and *HKL DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); cell refinement: *COLLECT* and *HKL DENZO* and *SCALEPACK*; data reduction: *COLLECT* and *HKL DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *JANA2006* (Petříček *et al.*, 2006); molecular graphics: Spek (2009); software used to prepare material for publication: *JANA2006*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2279).

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supplementary materials

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Dipotassium zinc tetraiodate(V) dihydrate

J. Fábry, **R. Krupková** and **I. Císarová**

Comment

Motivation for the present structure determination was growth of single crystals of KIO_3 that develop as domained crystals of poor quality from the water solution only (Hamid, 1974; Lü & Zhang, 1987). However, quality of the obtained crystals can be affected by additional reagents, such as HIO_3 (Hamid, 1974; Lü & Zhang, 1987). The matter of interest was to find a suitable solution with other additives from which good-quality crystals of KIO_3 can be obtained.

In this case, the title structure has been grown as it is given in the preparative section.

The compound of the same chemical composition has already been synthesized (Maneva & Rabadjieva, 1994; Juncheng *et al.*, 2000; Vinogradov *et al.*, 1979) along with similar compounds with different central atoms instead of Zn: According to the powder diffraction experiments, Ni and Co analogoues are isostructural to Zn (Maneva & Rabadjieva, 1994). (However, the powder diffractograms have been given only for the Ni and Co compounds in the latter reference.) Juncheng *et al.* (2000) investigated thermodynamic properties of $K_2ME(IO_3)_4.2H_2O$ where ME=Mg, Ni and Zn. Lepeshkov *et al.* (1977) studied the systems $Zn(IO_3)_2$ - KIO_3 - H_2O as well as $Co(IO_3)_2$ - KIO_3 - H_2O at 50°C. The *d* values of $K_2Zn(IO_3)_4.2H_2O$ obtained from the powder diffraction experiment by Lepeshkov *et al.* (1977) - see also ICDD Card 31-1135, PDF-2 database, ICDD (2000) - fairly correspond to the intensive peaks, that have been calculated from the title structure (Spek, 2009). However, Lepeshkov *et al.* (1977) did not give any details about the conditions of the powder diffraction experiment. Lepeshkov *et al.* (1977) have shown that infrared spectra as well as thermal and differential thermal gravimetric analyses (TGA and DTA) of $K_2Zn(IO_3)_4.2H_2O$ and $K_2Co(IO_3)_4.2H_2O$ are similar. The latter authors concluded from the infrared spectra that water molecules as well as four iodates are involved in the coordination sphere of the respective central atoms Zn and Co. Vinogradov *et al.* (1979) further studied systems of $ME(IO_3)_2$ - KIO_3 - H_2O, where ME=Co, Mn and Zn. The latter authors confirmed and extended the former findings (Lepeshkov *et al.*, 1977) that the central metal atoms (Co, Mn and Zn) are situated in an octahedron formed by the oxygens stemming from four $[IO_3]^-$ and two H_2O molecules.

However, the Inorganic Crystal Structure Database (ICSD, 2009) does not contain any structure of the composition given above. Nevertheless, the findings by Lepeshkov *et al.* (1977) as well as by Vinogradov *et al.* (1979) have been confirmed and precised in the present article: The environment of Zn in the title structure is formed by two pairs of symmetry independent iodate groups as well as two independent coordinated water molecules in *trans* positions.

There are several points of interest regarding the title structure. The primitive unit cell (p index) of the title structure can be obtained by the transformation from the centred C cell (C index) $[a_p,b_p,c_p]$=[//0 -1 0//1/2 -1/2 0//1/2 -1/2 1//]$[a_C,b_C,c_C]$. ($[a_p,b_p,c_p]$ and $[a_C,b_C,c_C]$ are the column matrices while //0 -1 0//1/2 -1/2 0//1/2 -1/2 1// are the first, the second and the third row, respectively, of the 3×3 matrix.) The transformed unit cell parameters are equal to 7.7285 (2), 7.9103 (1), 7.9421 (3) Å, 63.0265 (25), 60.8856 (9), 60.7574 (13)°; V=354.978 (18) $Å^3$.

Taking the metric of the unit cell into consideration there is no wonder that twinning has been observed in the title structure, either in the polarization microscope and by preliminary diffraction measurements of several samples that have shown rather broad peaks. However, it seems that the twinning is less severe in the title structure than in KIO_3. The single-domained crystals can be easily obtained mechanically. Observation of the crystals in the microscope did not show ferroelastic switching of the domains.

The volume of the primitive unit cell as well as lengths of the primitive unit cell axes of the title structure are comparable to those of KIO_3 that easily forms twins: 7.7436 (4), 7.7183 (4), 7.7328 (5) Å, 108.986 (4), 109.449 (4), 109.209 (5)°; $V=359.11 Å^3$ - Lucas (1984).

In the title structure, the I atoms are surrounded by a highly distorted oxygen environment, each I is bonded to three oxygens that are substantially closer. In the case of I1 the other three oxygens including the former ones form a distorted octahedron around I1 (Fig. 4) while in the case of I2 there are four more distant oxygens completing the coordination of the latter atom (Fig. 5). The environments of the iodines (Figs. 4 and 5) are rather similar to that in KIO_3 where are also 3 oxygens substantially closer to the central I atom with respect to the remaining three. Especially the coordination of I1 resembles that of I in KIO_3 where I is coordinated in a distorted octahedron (Lucas, 1984).

There are two strong hydrogen O—H···O bonds in the structure (Desiraju & Steiner, 1999) - see Tab. 1, Fig. 1. Moreover, there is also O-H···I interaction present in the structure (Tab. 1). Lepeshkov *et al.* (1977) report that dehydration takes place at 210°C, *i.e.* at quite a high temperature. Various sections from the title structure are depicted in Figs 1-5.

Experimental

The title structure has been prepared by adding to 0.93 g of dissolved KIO_3 in 20 ml of water of 0.4 g of KCl and 0.364 g of $ZnCl_2$. The solution was heated up to 60 °C while adding water to 300 ml. A very fine precipitate has developed that did not dissolve completely. Fragile prism-like colourless crystals with length of several tenths of mm have developed in the course of three months. The crystals were twinned by a domain boundary perpendicular to the longer axis of the prism. The crystals that served for the measurement could be easily separated mechanically. However, these parts in some cases were not single-domained crystals. There seem to be other domain states as indicated measurement of several samples.

Refinement

The water hydrogens have been detected in the difference electron density maps. It should be noted that they were observed with difficulties since close to O7 and O8 there have been other higher maxima situated precisely on the two-fold axis. The restraints were taken from the search in the Cambridge Structural Database (Allen, 2002). The search in the Database referred to the O—H distances and the angle H—O—H of the coordinated water molecules on Zn. The Database provided 1000 hits. The restrained values were: Zn—O—H = 125.50 (1)° and O—H = 0.845 (1) Å. The used constraints: $U_{iso}(H)=1.5U_{eq}O$. Moreover, because of the space group C2 the *y*-coordinate of I1 has been fixed.

Figures

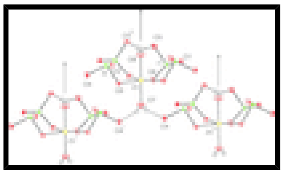

Fig. 1. View of the environment of Zn atoms (Spek, 2009) with omission of the K atoms. The displacement ellipsoids are shown at the 50% probability level. The hydrogen bonds are indicated by the dashed lines. The arrows depict two-fold axes. Symmetry code: (i) -*x* + 1/2, *y* + 1/2, -*z* + 1; (ii) -*x* + 1, *y*, -*z* + 1; (iii) -*x* + 3/2, *y* + 1/2, -*z* + 1.

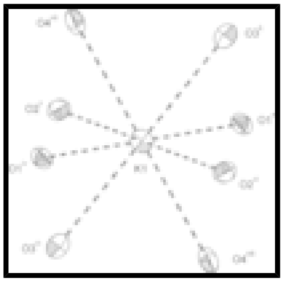

Fig. 2. View of of the environment of K1 atom (Spek, 2009). The displacement ellipsoids are shown at the 50% probability level. Symmetry code: as above and (iv) -*x* + 3/2, *y* - 1/2, -*z* + 1; (v) *x* - 1/2, *y* - 1/2, *z* - 1; (vi) *x*, *y*, *z* - 1; (vii) *x* + 1/2, *y* - 1/2, *z*; (viii) -*x* + 1/2, *y* - 1/2, -*z*.

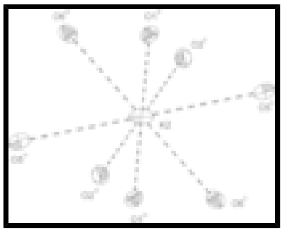

Fig. 3. View of of the environment of K2 atom (Spek, 2009). The displacement ellipsoids are shown at the 50% probability level. Symmetry code: as above and (ix) *x* - 1/2, *y* + 1/2, *z* - 1.

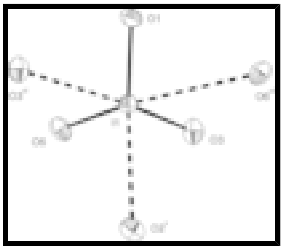

Fig. 4. View of of the environment of I1 atom (Spek, 2009). The displacement ellipsoids are shown at the 50% probability level. Symmetry code: as above and (x) -*x* + 1, *y*, -*z* + 2; (xi) -*x* + 3/2, *y* + 1/2, -*z* + 2; (xii) -*x* + 3/2, *y* - 1/2, -*z* + 2.

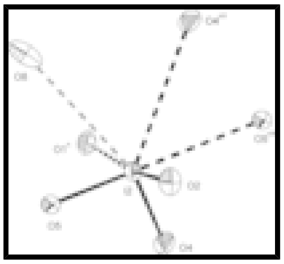

Fig. 5. View of of the environment of I2 atom (Spek, 2009). The displacement ellipsoids are shown at the 50% probability level. Symmetry code: as above and (xiii) -*x* + 1/2, *y* - 1/2, -*z* + 1.

dipotassium zinc tetraiodate(V) dihydrate

Crystal data

$K_2Zn(IO_3)_4 \cdot 2H_2O$

M_r = 879.2

Monoclinic, *C*2

Hall symbol: C 2y

a = 13.8044 (3) Å

F(000) = 792

D_x = 4.112 (1) Mg m^{-3}

Mo *K*α radiation, λ = 0.71069 Å

Cell parameters from 8075 reflections

θ = 2.9–27.5°

b = 7.7285 (2) Å
c = 8.2860 (2) Å
β = 126.5726 (13)°
V = 709.95 (3) Å^3
Z = 2

μ = 11.08 mm^{-1}
T = 295 K
Prism, colourless
0.17 × 0.12 × 0.05 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Radiation source: X-ray tube
graphite
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: gaussian (Coppens, 1970)
$T_{\min}$ = 0.241, $T_{\max}$ = 0.581
11909 measured reflections

1639 independent reflections
1595 reflections with $I > 3\sigma(I)$
R_{int} = 0.045
$\theta_{\max}$ = 27.5°, $\theta_{\min}$ = 3.1°
$h = -17\rightarrow17$
$k = -10\rightarrow10$
$l = -10\rightarrow10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.055
S = 1.72
1639 reflections
105 parameters
4 restraints
3 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
Weighting scheme based on measured s.u.'s $w = 1/(\sigma^2(I) + 0.0004I^2)$
$(\Delta/\sigma)_{\max}$ = 0.040
$\Delta\rho_{\max}$ = 0.60 e Å^{-3}
$\Delta\rho_{\min}$ = −0.61 e Å^{-3}
Extinction correction: B-C type 1 Lorentzian isotropic (Becker & Coppens, 1974)
Extinction coefficient: 1040 (40)
Absolute structure: Flack (1983), 761 Friedel pairs
Flack parameter: −0.01 (3)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
K1	0.5	0.0000 (3)	0	0.0217 (9)
K2	0.5	0.5290 (3)	0	0.0239 (10)
I1	0.73832 (3)	0.270215	0.98624 (4)	0.01481 (16)
I2	0.27889 (3)	0.28124 (7)	0.51786 (4)	0.01419 (16)
Zn	0.5	0.45608 (17)	0.5	0.0173 (4)
O1	0.8188 (3)	0.2594 (6)	0.8770 (5)	0.0199 (17)
O2	0.3446 (3)	0.2678 (6)	0.7822 (5)	0.0230 (16)
O3	0.6415 (4)	0.0814 (5)	0.8708 (5)	0.0220 (19)
O4	0.1355 (4)	0.3798 (5)	0.4160 (6)	0.023 (2)

O5	0.3581 (3)	0.4756 (5)	0.5308 (5)	0.0201 (18)
O6	0.6246 (4)	0.4346 (5)	0.8313 (5)	0.0207 (18)
O7	0.5	0.7158 (7)	0.5	0.039 (4)
O8	0.5	0.1904 (7)	0.5	0.033 (3)
H1O8	0.471 (6)	0.1269 (7)	0.3979 (19)	0.05*
H1O7	0.478 (7)	0.7793 (7)	0.556 (10)	0.0591*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.0231 (11)	0.0199 (9)	0.0240 (8)	0	0.0151 (8)	0
K2	0.0164 (10)	0.0199 (9)	0.0345 (10)	0	0.0148 (9)	0
I1	0.01408 (17)	0.0169 (2)	0.01324 (16)	0.0000 (2)	0.00804 (13)	0.00000 (15)
I2	0.01437 (18)	0.01408 (19)	0.01467 (16)	0.00005 (19)	0.00895 (13)	0.00057 (14)
Zn	0.0182 (5)	0.0151 (4)	0.0223 (4)	0	0.0142 (4)	0
O1	0.0197 (17)	0.0216 (19)	0.0229 (17)	0.0030 (18)	0.0152 (15)	0.0003 (16)
O2	0.0221 (18)	0.0275 (19)	0.0177 (16)	−0.005 (2)	0.0111 (14)	−0.0010 (18)
O3	0.022 (2)	0.0181 (18)	0.0195 (18)	0.0001 (17)	0.0090 (18)	0.0001 (15)
O4	0.017 (2)	0.024 (2)	0.031 (2)	0.0035 (15)	0.0160 (18)	0.0061 (15)
O5	0.0208 (19)	0.0138 (18)	0.0319 (19)	−0.0002 (15)	0.0191 (17)	−0.0002 (15)
O6	0.017 (2)	0.0214 (19)	0.0191 (17)	0.0056 (17)	0.0080 (16)	0.0004 (15)
O7	0.052 (4)	0.017 (3)	0.082 (5)	0	0.058 (4)	0
O8	0.041 (4)	0.016 (3)	0.024 (3)	0	0.009 (3)	0

Geometric parameters (Å, °)

K1—O1^{i}	2.778 (4)	I1—O6	1.823 (4)
K1—O1^{ii}	2.778 (4)	I1—O6^{xi}	3.031 (4)
K1—O2^{iii}	2.744 (4)	I2—O1^{iv}	2.701 (4)
K1—O2^{iv}	2.744 (4)	I2—O2	1.807 (4)
K1—O3^{iii}	2.802 (6)	I2—O4	1.795 (5)
K1—O3^{iv}	2.802 (6)	I2—O4^{xii}	3.248 (4)
K1—O4^{v}	2.925 (4)	I2—O5	1.823 (4)
K1—O4^{vi}	2.925 (4)	I2—O5^{xii}	2.900 (4)
K2—O1^{vii}	2.726 (4)	I2—O8	3.2202 (13)
K2—O1^{viii}	2.726 (4)	Zn—O5	2.126 (6)
K2—O2^{iii}	2.706 (4)	Zn—O5^{iv}	2.126 (6)
K2—O2^{iv}	2.706 (4)	Zn—O6	2.212 (3)
K2—O5^{iii}	3.170 (4)	Zn—O6^{iv}	2.212 (3)
K2—O5^{iv}	3.170 (4)	Zn—O7	2.007 (6)
K2—O6^{iii}	2.883 (6)	Zn—O8	2.053 (6)
K2—O6^{iv}	2.883 (6)	O7—H1o7	0.85 (9)
I1—O1	1.805 (5)	O7—H1o7^{iv}	0.85 (9)
I1—O2^{ix}	2.758 (5)	O8—H1o8	0.845 (16)
I1—O3	1.818 (4)	O8—H1o8^{iv}	0.845 (16)

I1—O3^{x}	2.756 (4)		

H1o7—O7—H1o7^{iv}	109 (6)	O5—Zn—O5^{iv}	171.86 (15)
H1o8—O8—H1o8^{iv}	109.0 (13)	O5—Zn—O6	86.97 (18)
O1^{i}—K1—O1^{ii}	95.96 (14)	O5—Zn—O6^{iv}	93.64 (18)
O1^{i}—K1—O2^{iii}	94.78 (12)	O5—Zn—O7	85.93 (10)
O1^{i}—K1—O2^{iv}	157.90 (15)	O5—Zn—O8	94.07 (10)
O1^{i}—K1—O3^{iii}	133.68 (13)	O5^{iv}—Zn—O6	93.64 (18)
O1^{i}—K1—O3^{iv}	67.05 (13)	O5^{iv}—Zn—O6^{iv}	86.97 (18)
O1^{i}—K1—O4^{v}	91.35 (12)	O5^{iv}—Zn—O7	85.93 (10)
O1^{i}—K1—O4^{vi}	63.35 (14)	O5^{iv}—Zn—O8	94.07 (10)
O1^{ii}—K1—O2^{iii}	157.90 (15)	O6—Zn—O6^{iv}	171.39 (16)
O1^{ii}—K1—O2^{iv}	94.78 (12)	O6—Zn—O7	94.30 (11)
O1^{ii}—K1—O3^{iii}	67.05 (13)	O6—Zn—O8	85.70 (11)
O1^{ii}—K1—O3^{iv}	133.68 (13)	O6^{iv}—Zn—O7	94.30 (11)
O1^{ii}—K1—O4^{v}	63.35 (14)	O6^{iv}—Zn—O8	85.70 (11)
O1^{ii}—K1—O4^{vi}	91.35 (12)	O7—Zn—O8	180
O2^{iii}—K1—O2^{iv}	82.07 (13)	O1—I1—O2^{ix}	169.37 (11)
O2^{iii}—K1—O3^{iii}	91.68 (14)	O1—I1—O3	100.2 (2)
O2^{iii}—K1—O3^{iv}	68.40 (13)	O1—I1—O3^{x}	82.15 (18)
O2^{iii}—K1—O4^{v}	135.62 (14)	O1—I1—O6	102.0 (2)
O2^{iii}—K1—O4^{vi}	76.36 (11)	O1—I1—O6^{xi}	79.79 (17)
O2^{iv}—K1—O3^{iii}	68.40 (13)	O1—I1—O8	81.25 (8)
O2^{iv}—K1—O3^{iv}	91.68 (14)	O2^{ix}—I1—O3	83.2 (2)
O2^{iv}—K1—O4^{v}	76.36 (11)	O2^{ix}—I1—O3^{x}	95.72 (15)
O2^{iv}—K1—O4^{vi}	135.62 (14)	O2^{ix}—I1—O6	87.4 (2)
O3^{iii}—K1—O3^{iv}	154.04 (14)	O2^{ix}—I1—O6^{xi}	92.39 (14)
O3^{iii}—K1—O4^{v}	114.81 (13)	O2^{ix}—I1—O8	108.21 (6)
O3^{iii}—K1—O4^{vi}	73.91 (13)	O3—I1—O3^{x}	172.60 (14)
O3^{iv}—K1—O4^{v}	73.91 (13)	O3—I1—O6	97.71 (16)
O3^{iv}—K1—O4^{vi}	114.81 (13)	O3—I1—O6^{xi}	67.69 (14)
O4^{v}—K1—O4^{vi}	142.99 (13)	O3—I1—O8	49.04 (14)
O1^{vii}—K2—O1^{viii}	98.42 (15)	O3^{x}—I1—O6	74.92 (14)
O1^{vii}—K2—O2^{iii}	92.96 (12)	O3^{x}—I1—O6^{xi}	119.70 (10)
O1^{vii}—K2—O2^{iv}	157.39 (15)	O3^{x}—I1—O8	125.11 (11)
O1^{vii}—K2—O5^{iii}	82.40 (11)	O6—I1—O6^{xi}	165.29 (13)
O1^{vii}—K2—O5^{iv}	107.60 (12)	O6—I1—O8	58.30 (14)
O1^{vii}—K2—O6^{iii}	131.60 (13)	O6^{xi}—I1—O8	108.09 (11)
O1^{vii}—K2—O6^{iv}	70.54 (13)	O1^{iv}—I2—O2	173.13 (18)
O1^{viii}—K2—O2^{iii}	157.39 (15)	O1^{iv}—I2—O4	80.92 (18)
O1^{viii}—K2—O2^{iv}	92.96 (12)	O1^{iv}—I2—O4^{xii}	90.78 (12)

$O1^{viii}$—K2—$O5^{iii}$	107.60 (12)	$O1^{iv}$—I2—O5	88.38 (16)
$O1^{viii}$—K2—$O5^{iv}$	82.40 (11)	$O1^{iv}$—I2—$O5^{xii}$	88.12 (13)
$O1^{viii}$—K2—$O6^{iii}$	70.54 (13)	$O1^{iv}$—I2—O8	74.54 (9)
$O1^{viii}$—K2—$O6^{iv}$	131.60 (13)	O2—I2—O4	102.2 (2)
$O2^{iii}$—K2—$O2^{iv}$	83.50 (13)	O2—I2—$O4^{xii}$	82.61 (17)
$O2^{iii}$—K2—$O5^{iii}$	54.54 (12)	O2—I2—O5	97.22 (19)
$O2^{iii}$—K2—$O5^{iv}$	112.69 (13)	O2—I2—$O5^{xii}$	86.36 (17)
$O2^{iii}$—K2—$O6^{iii}$	87.30 (14)	O2—I2—O8	103.80 (15)
$O2^{iii}$—K2—$O6^{iv}$	70.70 (13)	O4—I2—$O4^{xii}$	132.34 (15)
$O2^{iv}$—K2—$O5^{iii}$	112.69 (13)	O4—I2—O5	97.63 (19)
$O2^{iv}$—K2—$O5^{iv}$	54.54 (12)	O4—I2—$O5^{xii}$	80.51 (16)
$O2^{iv}$—K2—$O6^{iii}$	70.70 (13)	O4—I2—O8	151.77 (18)
$O2^{iv}$—K2—$O6^{iv}$	87.30 (14)	$O4^{xii}$—I2—O5	129.17 (17)
$O5^{iii}$—K2—$O5^{iv}$	165.03 (13)	$O4^{xii}$—I2—$O5^{xii}$	52.21 (12)
$O5^{iii}$—K2—$O6^{iii}$	58.89 (11)	$O4^{xii}$—I2—O8	62.61 (14)
$O5^{iii}$—K2—$O6^{iv}$	116.79 (11)	O5—I2—$O5^{xii}$	176.26 (13)
$O5^{iv}$—K2—$O6^{iii}$	116.79 (11)	O5—I2—O8	68.31 (19)
$O5^{iv}$—K2—$O6^{iv}$	58.89 (11)	$O5^{xii}$—I2—O8	111.94 (14)
$O6^{iii}$—K2—$O6^{iv}$	150.67 (15)		
?—?—?—?	?		

Symmetry codes: (i) $x-1/2, y-1/2, z-1$; (ii) $-x+3/2, y-1/2, -z+1$; (iii) $x, y, z-1$; (iv) $-x+1, y, -z+1$; (v) $x+1/2, y-1/2, z$; (vi) $-x+1/2, y-1/2, -z$; (vii) $x-1/2, y+1/2, z-1$; (viii) $-x+3/2, y+1/2, -z+1$; (ix) $-x+1, y, -z+2$; (x) $-x+3/2, y+1/2, -z+2$; (xi) $-x+3/2, y-1/2, -z+2$; (xii) $-x+1/2, y-1/2, -z+1$.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H1O7···$O4^{xiii}$	0.85 (9)	1.88 (10)	2.672 (6)	155 (5)
O7—$H1O7^{iv}$···$O4^{xiv}$	0.85 (9)	1.88 (10)	2.672 (6)	155 (5)
O8—H1O8···$O3^{iv}$	0.845 (16)	1.837 (16)	2.610 (4)	151 (4)
O8—H1O8···$I1^{iv}$	0.845 (16)	2.96 (3)	3.4119 (10)	116 (3)

Symmetry codes: (xiii) $-x+1/2, y+1/2, -z+1$; (iv) $-x+1, y, -z+1$; (xiv) $x+1/2, y+1/2, z$.

Fig. 1

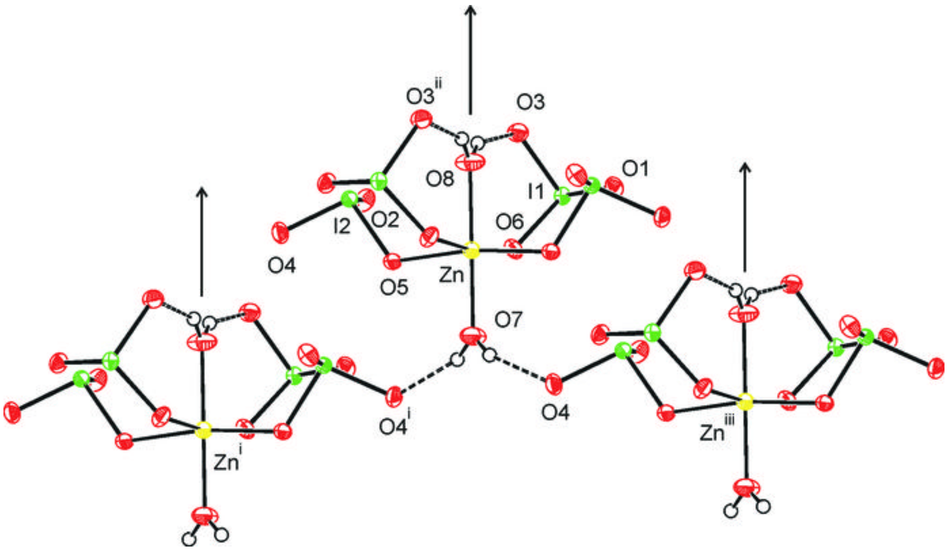

Fig. 2

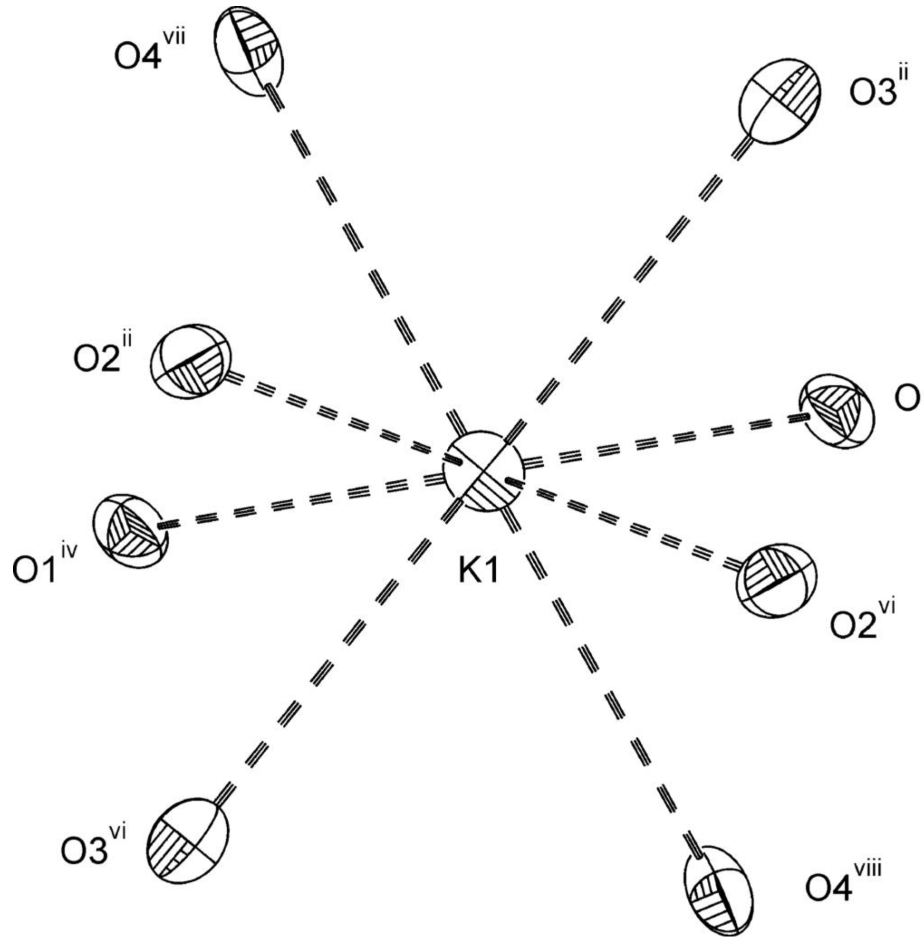

Fig. 3

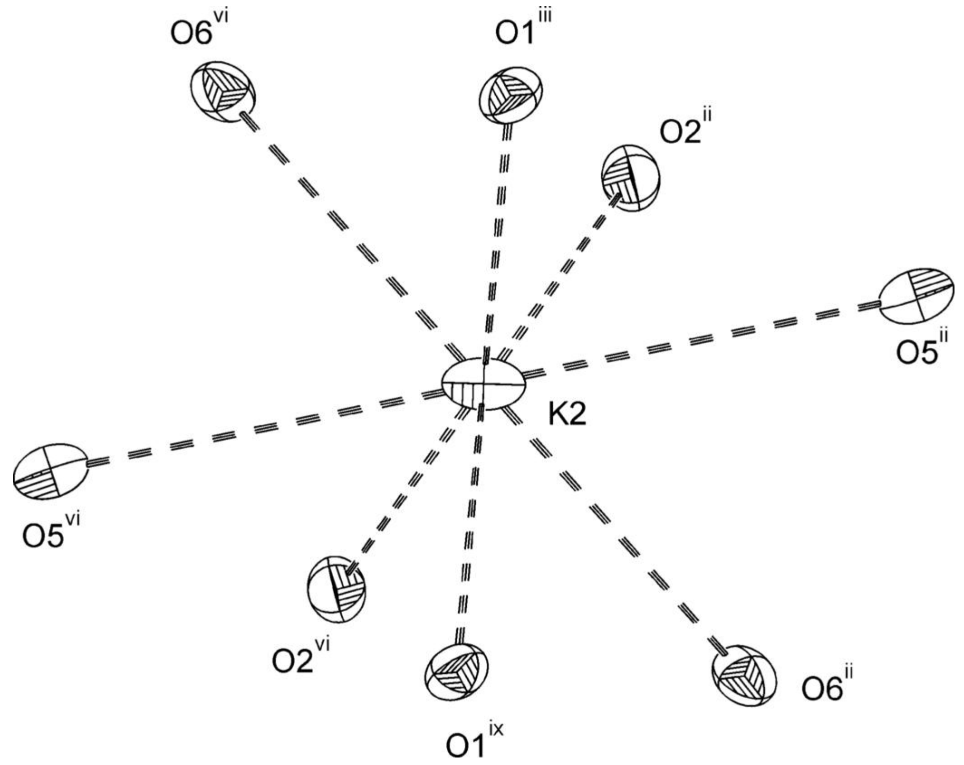

Fig. 4

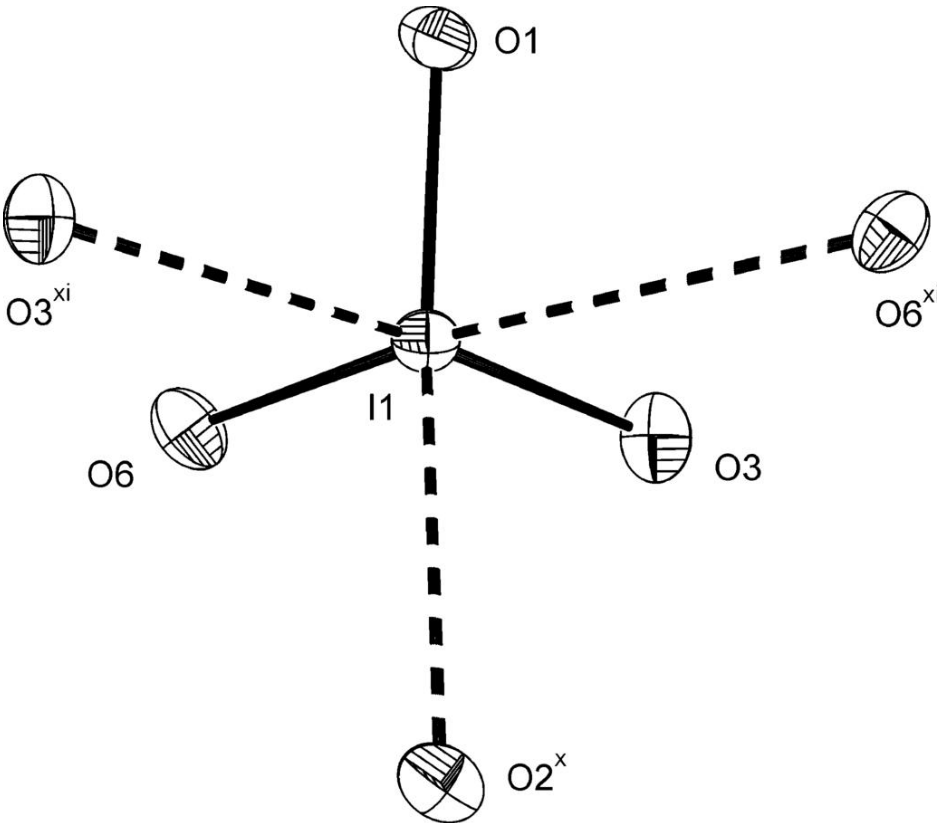

Fig. 5