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Dicaesium tetrachloridodioxido-plutonate(VI)

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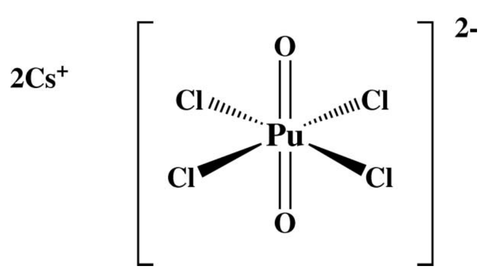
Key indicators: single-crystal X-ray study; T = 141 K; mean σ(Pu–O) = 0.004 Å; R factor = 0.015; wR factor = 0.037; data-to-parameter ratio = 26.3.

The anion of the title complex, $Cs_2[PuCl_4O_2]$, adopts a pseudo-octahedral geometry ($2/m$ crystallographic site symmetry) with two plutonyl oxide ligands in axial sites and four chloride ligands occupying the equatorial plane. Charge balance is maintained by two caesium cations per tetrachloridodioxidoplutonate(VI) anion. Principal bond lengths include Pu—O = 1.752 (3) Å and Pu—Cl = 2.6648 (8) Å.

Related literature

For related literature, see: Hall *et al.* (1966); Watkin *et al.* (1991); Wilkerson *et al.* (2004); Wilkerson *et al.* (2007); Bean *et al.* (2004, 2005); Grenthe *et al.* (2006); Grigoriev *et al.* (2004); Runde *et al.* (2003); Sessler *et al.* (2002).



Experimental

Crystal data

$Cs_2[PuCl_4O_2]$
M_r = 678.67
Monoclinic, $C2/m$
a = 11.9489 (7) Å
b = 7.7286 (5) Å
c = 5.7855 (4) Å
β = 96.439 (1)°
V = 530.91 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 13.92 mm^{-1}
T = 141 (2) K
0.22 × 0.18 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.150, T_{max} = 0.286 (expected range = 0.099–0.188)
3212 measured reflections
711 independent reflections
659 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.015
$wR(F^2)$ = 0.037
S = 1.26
711 reflections
27 parameters
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); 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: FI2048).

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supplementary materials

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Dicaesium tetrachloridodioxidoplutonate(VI)

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Comment

The title compound, (1), is isostructural with the uranium analogue Cs2U(VI)O2Cl4 and the neptunium analogue Cs2Np(VI)O2Cl4, which crystallize in the space group C2/m (Hall *et al.*, 1966; Watkin *et al.*, 1991; Wilkerson *et al.*, 2007). The Pu atom sits on a site of 2/m crystallographic symmetry; the twofold rotation axis bisects the Cl—U—Cl angle, and the plutonyl axis lies in the mirror plane. The plutonium metal is coordinated in a pseudo-octahedral fashion by two oxo groups and four chloride ligands. The oxo groups of the plutonyl ion lie *trans* to one another with a bond angle of 180.0 (3). This angle is equivalent within 3 σ to those reported for the limited number of plutonyl structures published (range 178.0 (4)–179.4 (2)) (Bean *et al.*, 2004; Bean *et al.*, 2005; Grigoriev *et al.*, 2004; Runde *et al.*, 2003). This value is within the range reported for the majority of actinyl compounds (Grenthe *et al.*, 2006). The Pu—O(oxo) distances are 1.752 (3) Å. Although there are no reported six coordinate plutonyl structures with which to compare, this value is within range of Pu—O(oxo) bond lengths reported for seven coordinate plutonyl structures (1.727 (4)–1.771 (11) Å) (Bean *et al.*, 2004; Bean *et al.*, 2005; Grigoriev *et al.*, 2004; Runde *et al.*, 2003). The chloride ligands lie in the equatorial plane of the plutonyl ion, and the Pu—Cl bond distances are 2.6648 (8) Å. Although there are no plutonyl chloride structures reported, these values are longer than Np—Cl bond lengths reported for six-coordinate $Cs_2NpO_2Cl_4$ (2.653 (3) Å) (Wilkerson *et al.*, 2004).

Experimental

Caesium chloride (0.021 g, 0.12 mmol; Aldrich, 99.999%) was dissolved in 2*M* HCl (0.5 ml; Aldrich, ACS reagent, 37%), and this solution was added to a stock solution of 0.063 *M* $Pu(VI)O_2^{2+}$ in 2*M* HCl (1 ml, 0.063 mmol; Fisher, Certified ACS Plus) (Sessler *et al.*, 2002). The vial containing the solution was covered loosely with parafilm and allowed to stand for 2 weeks at room temperature. Following evaporation of the solvent, dark golden-brown blocks formed. A dark golden-brown block of 0.22 *x* 0.18 *x* 0.12 mm was cut from a larger crystal, and then thinly coated with epoxy and placed in a capillary. The capillary was coated with a thin film of acrylic dissolved in ethyl acetate. (Note: this triple containment was necessitated by the health hazards of transuranic materials.)

Figures

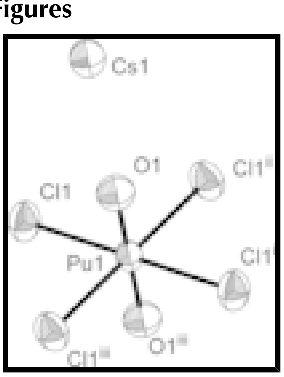

Fig. 1. Molecular structure (70% probability displacement ellipsoids) of $Cs_2PuO_2Cl_4$ and the atom-numbering scheme used in Table 1. Symmetry codes as in Table 1.

Dicaesium tetrachloridodioxidoplutonium(VI)

Crystal data

$Cs_2[PuCl_4O_2]$	$Z = 2$
$M_r = 678.67$	$F_{000} = 576$
Monoclinic, $C2/m$	$D_x = 4.245$ Mg m^{-3}
Hall symbol: -C 2y	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 11.9489$ (7) Å	$\theta = 3.2–28.7°$
$b = 7.7286$ (5) Å	$\mu = 13.92$ mm^{-1}
$c = 5.7855$ (4) Å	$T = 141$ (2) K
$\beta = 96.4390$ (10)°	Irregular, golden brown
$V = 530.91$ (6) Å^3	0.22 × 0.18 × 0.12 mm

Data collection

Bruker D8 with APEXII CCD diffractometer	711 independent reflections
Radiation source: fine-focus sealed tube	659 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.025$
$T = 141(2)$ K	$\theta_{max} = 28.7°$
ω scans	$\theta_{min} = 3.2°$
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	$h = -15 \rightarrow 15$
$T_{min} = 0.150$, $T_{max} = 0.286$	$k = -10 \rightarrow 10$
3212 measured reflections	$l = -7 \rightarrow 7$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0151P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.015$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.037$	$\Delta\rho_{max} = 0.78$ e Å^{-3}
$S = 1.26$	$\Delta\rho_{min} = -0.64$ e Å^{-3}
711 reflections	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
27 parameters	Extinction coefficient: 0.0050 (2)
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2sigma(F^2)$ 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}
Pu1	0.0000	0.0000	0.0000	0.02605 (11)
Cs1	0.34147 (2)	0.0000	0.69601 (6)	0.03801 (11)
Cl1	−0.10351 (7)	−0.24889 (10)	0.21367 (16)	0.0390 (2)
O1	0.1124 (3)	0.0000	0.2222 (6)	0.0395 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pu1	0.02849 (15)	0.02078 (14)	0.02946 (15)	0.000	0.00583 (9)	0.000
Cs1	0.03790 (19)	0.03608 (19)	0.0419 (2)	0.000	0.01250 (15)	0.000
Cl1	0.0436 (4)	0.0305 (4)	0.0454 (5)	−0.0015 (3)	0.0162 (4)	0.0058 (3)
O1	0.0381 (19)	0.0424 (19)	0.0371 (19)	0.000	0.0002 (16)	0.000

Geometric parameters (Å, °)

Pu1—O1^{i}	1.752 (3)	Cs1—Cl1^{xii}	3.5201 (8)
Pu1—O1	1.752 (3)	Cs1—Cl1^{viii}	3.5201 (8)
Pu1—Cl1^{ii}	2.6648 (8)	Cs1—Cl1^{xiii}	3.5674 (10)
Pu1—Cl1	2.6648 (8)	Cs1—Cl1^{xiv}	3.5674 (10)
Pu1—Cl1^{iii}	2.6648 (8)	Cs1—O1	3.650 (4)
Pu1—Cl1^{i}	2.6648 (8)	Cs1—Cl1^{xv}	3.6710 (9)
Pu1—Cs1^{iv}	4.5680 (3)	Cs1—Cl1^{vi}	3.6710 (9)
Pu1—Cs1^{v}	4.5680 (3)	Cs1—Pu1^{xiii}	4.5680 (3)
Pu1—Cs1^{vi}	4.5680 (3)	Cs1—Pu1^{xvi}	4.5680 (3)
Pu1—Cs1^{vii}	4.5680 (3)	Cs1—Pu1^{xvii}	4.6207 (3)
Pu1—Cs1^{viii}	4.6207 (3)	Cl1—Cs1^{xviii}	3.5209 (9)
Pu1—Cs1^{ix}	4.6207 (3)	Cl1—Cs1^{viii}	3.5201 (8)
Cs1—Cl1^{x}	3.5209 (9)	Cl1—Cs1^{iv}	3.5674 (10)
Cs1—Cl1^{xi}	3.5209 (9)	Cl1—Cs1^{vi}	3.6710 (9)
O1^{i}—Pu1—O1	180.0 (3)	Cl1^{x}—Cs1—Cl1^{xiii}	158.75 (3)
O1^{i}—Pu1—Cl1^{ii}	90.98 (8)	Cl1^{xi}—Cs1—Cl1^{xiii}	109.41 (2)
O1—Pu1—Cl1^{ii}	89.02 (8)	Cl1^{xii}—Cs1—Cl1^{xiii}	104.390 (15)
O1^{i}—Pu1—Cl1	89.02 (8)	Cl1^{viii}—Cs1—Cl1^{xiii}	69.76 (2)
O1—Pu1—Cl1	90.98 (8)	Cl1^{x}—Cs1—Cl1^{xiv}	109.41 (2)

$Cl1^{ii}$—Pu1—Cl1	87.58 (3)	$Cl1^{xi}$—Cs1—$Cl1^{xiv}$	158.75 (3)
$O1^{i}$—Pu1—$Cl1^{iii}$	89.02 (8)	$Cl1^{xii}$—Cs1—$Cl1^{xiv}$	69.76 (2)
O1—Pu1—$Cl1^{iii}$	90.98 (8)	$Cl1^{viii}$—Cs1—$Cl1^{xiv}$	104.390 (15)
$Cl1^{ii}$—Pu1—$Cl1^{iii}$	180.00 (5)	$Cl1^{xiii}$—Cs1—$Cl1^{xiv}$	65.91 (3)
Cl1—Pu1—$Cl1^{iii}$	92.42 (3)	$Cl1^{x}$—Cs1—O1	66.15 (5)
$O1^{i}$—Pu1—$Cl1^{i}$	90.98 (8)	$Cl1^{xi}$—Cs1—O1	66.15 (5)
O1—Pu1—$Cl1^{i}$	89.02 (8)	$Cl1^{xii}$—Cs1—O1	63.98 (5)
$Cl1^{ii}$—Pu1—$Cl1^{i}$	92.42 (3)	$Cl1^{viii}$—Cs1—O1	63.98 (5)
Cl1—Pu1—$Cl1^{i}$	180.00 (4)	$Cl1^{xiii}$—Cs1—O1	133.04 (4)
$Cl1^{iii}$—Pu1—$Cl1^{i}$	87.58 (3)	$Cl1^{xiv}$—Cs1—O1	133.04 (4)
$O1^{i}$—Pu1—$Cs1^{iv}$	57.778 (4)	$Cl1^{x}$—Cs1—$Cl1^{xv}$	99.912 (18)
O1—Pu1—$Cs1^{iv}$	122.222 (4)	$Cl1^{xi}$—Cs1—$Cl1^{xv}$	65.75 (3)
$Cl1^{ii}$—Pu1—$Cs1^{iv}$	53.469 (18)	$Cl1^{xii}$—Cs1—$Cl1^{xv}$	163.34 (3)
Cl1—Pu1—$Cs1^{iv}$	51.24 (2)	$Cl1^{viii}$—Cs1—$Cl1^{xv}$	112.348 (8)
$Cl1^{iii}$—Pu1—$Cs1^{iv}$	126.531 (18)	$Cl1^{xiii}$—Cs1—$Cl1^{xv}$	61.25 (2)
$Cl1^{i}$—Pu1—$Cs1^{iv}$	128.76 (2)	$Cl1^{xiv}$—Cs1—$Cl1^{xv}$	95.403 (19)
$O1^{i}$—Pu1—$Cs1^{v}$	122.222 (4)	O1—Cs1—$Cl1^{xv}$	131.50 (4)
O1—Pu1—$Cs1^{v}$	57.778 (4)	$Cl1^{x}$—Cs1—$Cl1^{vi}$	65.75 (3)
$Cl1^{ii}$—Pu1—$Cs1^{v}$	126.531 (18)	$Cl1^{xi}$—Cs1—$Cl1^{vi}$	99.912 (18)
Cl1—Pu1—$Cs1^{v}$	128.76 (2)	$Cl1^{xii}$—Cs1—$Cl1^{vi}$	112.348 (8)
$Cl1^{iii}$—Pu1—$Cs1^{v}$	53.469 (18)	$Cl1^{viii}$—Cs1—$Cl1^{vi}$	163.34 (3)
$Cl1^{i}$—Pu1—$Cs1^{v}$	51.24 (2)	$Cl1^{xiii}$—Cs1—$Cl1^{vi}$	95.403 (19)
$Cs1^{iv}$—Pu1—$Cs1^{v}$	180.000 (8)	$Cl1^{xiv}$—Cs1—$Cl1^{vi}$	61.25 (2)
$O1^{i}$—Pu1—$Cs1^{vi}$	122.222 (4)	O1—Cs1—$Cl1^{vi}$	131.50 (4)
O1—Pu1—$Cs1^{vi}$	57.778 (4)	$Cl1^{xv}$—Cs1—$Cl1^{vi}$	63.83 (3)
$Cl1^{ii}$—Pu1—$Cs1^{vi}$	51.24 (2)	$Cl1^{x}$—Cs1—$Pu1^{xiii}$	131.698 (14)
Cl1—Pu1—$Cs1^{vi}$	53.469 (18)	$Cl1^{xi}$—Cs1—$Pu1^{xiii}$	74.494 (15)
$Cl1^{iii}$—Pu1—$Cs1^{vi}$	128.76 (2)	$Cl1^{xii}$—Cs1—$Pu1^{xiii}$	135.406 (14)
$Cl1^{i}$—Pu1—$Cs1^{vi}$	126.531 (18)	$Cl1^{viii}$—Cs1—$Pu1^{xiii}$	77.734 (14)
$Cs1^{iv}$—Pu1—$Cs1^{vi}$	64.454 (8)	$Cl1^{xiii}$—Cs1—$Pu1^{xiii}$	35.626 (12)
$Cs1^{v}$—Pu1—$Cs1^{vi}$	115.546 (8)	$Cl1^{xiv}$—Cs1—$Pu1^{xiii}$	96.174 (16)
$O1^{i}$—Pu1—$Cs1^{vii}$	57.778 (4)	O1—Cs1—$Pu1^{xiii}$	122.194 (5)
O1—Pu1—$Cs1^{vii}$	122.222 (4)	$Cl1^{xv}$—Cs1—$Pu1^{xiii}$	35.683 (12)
$Cl1^{ii}$—Pu1—$Cs1^{vii}$	128.76 (2)	$Cl1^{vi}$—Cs1—$Pu1^{xiii}$	94.713 (15)
Cl1—Pu1—$Cs1^{vii}$	126.531 (18)	$Cl1^{x}$—Cs1—$Pu1^{xvi}$	74.494 (15)
$Cl1^{iii}$—Pu1—$Cs1^{vii}$	51.24 (2)	$Cl1^{xi}$—Cs1—$Pu1^{xvi}$	131.698 (14)
$Cl1^{i}$—Pu1—$Cs1^{vii}$	53.469 (18)	$Cl1^{xii}$—Cs1—$Pu1^{xvi}$	77.734 (14)
$Cs1^{iv}$—Pu1—$Cs1^{vii}$	115.546 (8)	$Cl1^{viii}$—Cs1—$Pu1^{xvi}$	135.406 (14)
$Cs1^{v}$—Pu1—$Cs1^{vii}$	64.454 (8)	$Cl1^{xiii}$—Cs1—$Pu1^{xvi}$	96.174 (16)
$Cs1^{vi}$—Pu1—$Cs1^{vii}$	180.000 (7)	$Cl1^{xiv}$—Cs1—$Pu1^{xvi}$	35.626 (12)
$O1^{i}$—Pu1—$Cs1^{viii}$	69.04 (11)	O1—Cs1—$Pu1^{xvi}$	122.194 (5)

O1—Pu1—Cs1^{viii}	110.96 (11)	Cl1^{xv}—Cs1—Pu1^{xvi}	94.713 (15)
Cl1^{ii}—Pu1—Cs1^{viii}	130.706 (17)	Cl1^{vi}—Cs1—Pu1^{xvi}	35.683 (12)
Cl1—Pu1—Cs1^{viii}	49.294 (17)	Pu1^{xiii}—Cs1—Pu1^{xvi}	115.546 (8)
Cl1^{iii}—Pu1—Cs1^{viii}	49.294 (17)	Cl1^{x}—Cs1—Pu1^{xvii}	123.572 (15)
Cl1^{i}—Pu1—Cs1^{viii}	130.706 (17)	Cl1^{xi}—Cs1—Pu1^{xvii}	123.572 (15)
Cs1^{iv}—Pu1—Cs1^{viii}	78.510 (5)	Cl1^{xii}—Cs1—Pu1^{xvii}	35.021 (13)
Cs1^{v}—Pu1—Cs1^{viii}	101.490 (5)	Cl1^{viii}—Cs1—Pu1^{xvii}	35.021 (13)
Cs1^{vi}—Pu1—Cs1^{viii}	101.490 (5)	Cl1^{xiii}—Cs1—Pu1^{xvii}	76.579 (13)
Cs1^{vii}—Pu1—Cs1^{viii}	78.510 (5)	Cl1^{xiv}—Cs1—Pu1^{xvii}	76.579 (13)
O1^{i}—Pu1—Cs1^{ix}	110.96 (11)	O1—Cs1—Pu1^{xvii}	70.49 (5)
O1—Pu1—Cs1^{ix}	69.04 (11)	Cl1^{xv}—Cs1—Pu1^{xvii}	136.161 (13)
Cl1^{ii}—Pu1—Cs1^{ix}	49.294 (17)	Cl1^{vi}—Cs1—Pu1^{xvii}	136.161 (13)
Cl1—Pu1—Cs1^{ix}	130.706 (17)	Pu1^{xiii}—Cs1—Pu1^{xvii}	101.490 (5)
Cl1^{iii}—Pu1—Cs1^{ix}	130.706 (17)	Pu1^{xvi}—Cs1—Pu1^{xvii}	101.490 (5)
Cl1^{i}—Pu1—Cs1^{ix}	49.294 (17)	Pu1—Cl1—Cs1^{xviii}	154.58 (3)
Cs1^{iv}—Pu1—Cs1^{ix}	101.490 (5)	Pu1—Cl1—Cs1^{viii}	95.68 (2)
Cs1^{v}—Pu1—Cs1^{ix}	78.510 (5)	Cs1^{xviii}—Cl1—Cs1^{viii}	87.583 (18)
Cs1^{vi}—Pu1—Cs1^{ix}	78.510 (5)	Pu1—Cl1—Cs1^{iv}	93.13 (2)
Cs1^{vii}—Pu1—Cs1^{ix}	101.490 (5)	Cs1^{xviii}—Cl1—Cs1^{iv}	109.41 (2)
Cs1^{viii}—Pu1—Cs1^{ix}	180.000 (3)	Cs1^{viii}—Cl1—Cs1^{iv}	110.24 (2)
Cl1^{x}—Cs1—Cl1^{xi}	66.90 (3)	Pu1—Cl1—Cs1^{vi}	90.85 (2)
Cl1^{x}—Cs1—Cl1^{xii}	92.417 (18)	Cs1^{xviii}—Cl1—Cs1^{vi}	80.088 (18)
Cl1^{xi}—Cs1—Cl1^{xii}	130.133 (13)	Cs1^{viii}—Cl1—Cs1^{vi}	163.34 (3)
Cl1^{x}—Cs1—Cl1^{viii}	130.133 (13)	Cs1^{iv}—Cl1—Cs1^{vi}	84.597 (19)
Cl1^{xi}—Cs1—Cl1^{viii}	92.417 (18)	Pu1—O1—Cs1	178.55 (16)
Cl1^{xii}—Cs1—Cl1^{viii}	66.25 (3)		

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) −*x*, *y*, −*z*; (iii) *x*, −*y*, *z*; (iv) *x*−1/2, *y*−1/2, *z*−1; (v) −*x*+1/2, −*y*+1/2, −*z*+1; (vi) −*x*+1/2, −*y*−1/2, −*z*+1; (vii) *x*−1/2, *y*+1/2, *z*−1; (viii) −*x*, −*y*, −*z*+1; (ix) *x*, *y*, *z*−1; (x) *x*+1/2, −*y*−1/2, *z*; (xi) *x*+1/2, *y*+1/2, *z*; (xii) −*x*, *y*, −*z*+1; (xiii) *x*+1/2, *y*+1/2, *z*+1; (xiv) *x*+1/2, −*y*−1/2, *z*+1; (xv) −*x*+1/2, *y*+1/2, −*z*+1; (xvi) *x*+1/2, *y*−1/2, *z*+1; (xvii) *x*, *y*, *z*+1; (xviii) *x*−1/2, *y*−1/2, *z*.

Fig. 1