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The solid solution $Ba_{5.78}Pb_{1.22}F_{12}Cl_2$

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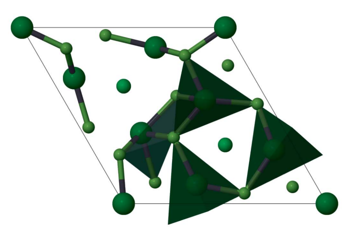
The title compound, hexabarium lead(II) decafluoride dichloride, is a solid solution in the system $Pb_7F_{12}Cl_2$–$Ba_7F_{12}Cl_2$ and crystallizes isotypically with the ordered modification of the parent compounds in the space group $P\overline{6}$. The coordination polyhedra of the three different metal sites are distorted tricapped trigonal prisms with F_7Cl_2 coordination sets for two of these sites (Wyckoff positions 3*k* and 3*j*, each with site symmetry *m*..), and the remaining site being exclusively coordinated by fluoride ions (1*a*, $\overline{6}$..). By sharing faces, a three-dimensional structure is accomplished. The three metal sites have remarkably different occupancies by the two types of metal ions. Whereas the site on the 3*k* position shows only a minor incorporation of Pb^{2+} [occupancy ratio Ba:Pb = 0.93 (4):0.07 (4)], the 3*j* site shows the highest amount of incorporated Pb^{2+} [Ba:Pb = 0.71 (5):29 (5)]. The occupancy ratio with respect to the 1*a* site is Ba:Pb = 0.86 (5):0.14 (5).

3D view



Structure description

The current study provides indications as to which of the three metal sites of the $Ba_7F_{12}Cl_2$ structure is preferentially substituted in solid solutions of the type $Ba_{7-x}M_xF_{12}Cl_2$ (*M* = divalent metal with ionic radius comparable to Ba^{2+}) and hence could help to better understand spectroscopic data of europium-doped $Ba_7F_{12}Cl_2$ phosphors (Hagemann *et al.*, 2015). The isotypic ordered parent phases $Pb_7F_{12}Cl_2$ and $Ba_7F_{12}Cl_2$ were first reported by Aurivillius (1976) and Es-Sakhi *et al.* (1998), respectively. For a review of crystal–chemical peculiarities in the system $BaF_2/BaCl_2$, including the ordered (space group $P\overline{6}$) and disordered modifications (space group $P6_3$) of $Ba_7F_{12}Cl_2$, see: Hagemann *et al.* (2012). The crystal structure of the title compound is shown in Fig. 1. Selected bond lengths are given in Table 1.

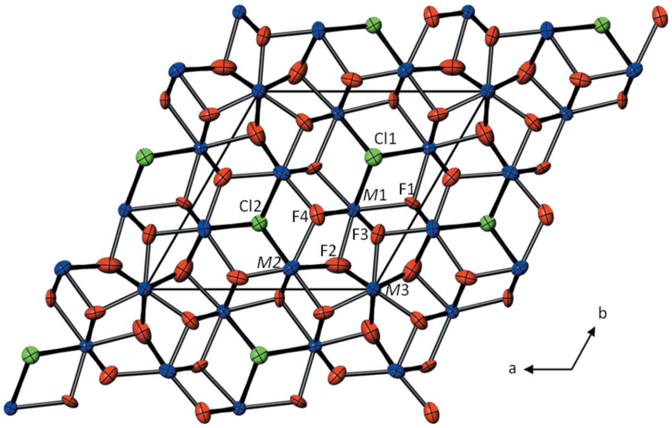


Figure 1
The crystal structure of the title compound in a projection along [00$\bar{1}$]. Displacement ellipsoids are drawn at the 97% probability level.

Table 1
Selected bond lengths (Å).

(Ba,Pb)1—F3	2.618 (8)	(Ba,Pb)2—F3^{ii}	2.560 (13)
(Ba,Pb)1—F2	2.659 (16)	(Ba,Pb)2—F4	2.746 (14)
(Ba,Pb)1—F4	2.683 (8)	(Ba,Pb)2—F2	3.001 (11)
(Ba,Pb)1—F1	2.760 (14)	(Ba,Pb)2—Cl2	3.2922 (9)
(Ba,Pb)1—Cl1	3.3375 (10)	(Ba,Pb)3—F3	2.549 (15)
(Ba,Pb)2—F4^{i}	2.531 (15)	(Ba,Pb)3—F2	2.870 (11)
(Ba,Pb)2—F1^{ii}	2.559 (7)		

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$Ba_{5.78}Pb_{1.22}F_{12}Cl_2$
M_r	1345.45
Crystal system, space group	Hexagonal, $P\bar{6}$
Temperature (K)	293
a, c (Å)	10.5878 (15), 4.1528 (8)
V (Å^3)	403.17 (16)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	27.00
Crystal size (mm)	0.50 × 0.02 × 0.02
Data collection	
Diffractometer	Philips PW100 diffractometer
Absorption correction	Numerical (*HABITUS*; Herrendorf, 1997)
T_{min}, T_{max}	0.204, 0.888
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	2616, 877, 766
R_{int}	0.145
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.704
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.057, 0.127, 1.05
No. of reflections	877
No. of parameters	48
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	4.03, −4.13
Absolute structure	Flack (1983), 466 Friedel pairs
Absolute structure parameter	0.55 (5)

Computer programs: *PW1100 Operation Software* (Philips, 1980), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008), *ATOMS* (Dowty, 2006), *publCIF* (Westrip, 2010).

Synthesis and crystallization

BaF_2, $BaCl_2$, PbF_2 and $PbCl_2$ were mixed in stoichiometric amounts according to a nominal composition of $Ba_6PbF_{12}Cl_2$. The mixture was placed in a teflon container (capacity 10 ml) which was two-thirds filled with water. The container was closed with a teflon lid and placed in a steel autoclave at 493 K for one week. Colourless crystals with a needle-like form were obtained from the mother liquor by filtration. Unit-cell determination of several selected crystals with subsequent least-squares refinements of the lattice parameters revealed nearly identical unit cells, indicating that the composition of the grown crystals was consistent and very similar to that of the title compound.

Refinement

The three M^{2+} sites are occupied by both Ba and Pb. For the final model, the three metal sites were constrained to be fully occupied. Each of the sites was refined with common coordinates and displacement parameters for the two types of metals. The highest and lowest remaining electron density peaks are found 2.08 and 0.16 Å, respectively, from the $M1$ site. The crystal measured was twinned by inversion with an approximate ratio of the twin domains of 1:1 [Flack parameter 0.55 (5)]. Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x152427 [doi:10.1107/S241431461502427X]

The solid solution $Ba_{5.78}Pb_{1.22}F_{12}Cl_2$

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Hexabarium lead(II) dodecafluoride dichloride

Crystal data

$Ba_{5.78}Pb_{1.22}F_{12}Cl_2$
M_r = 1345.45
Hexagonal, $P\overline{6}$
Hall symbol: P -6
a = 10.5878 (15) Å
c = 4.1528 (8) Å
V = 403.17 (16) Å^3
Z = 1
F(000) = 566
D_x = 5.542 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 5.4–10.9°
μ = 27.00 mm^{-1}
T = 293 K
Needle, colourless
0.50 × 0.02 × 0.02 mm

Data collection

Philips PW100 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\theta/2\theta$ scans
Absorption correction: numerical (*HABITUS*; Herrendorf, 1997)
T_{min} = 0.204, T_{max} = 0.888
2616 measured reflections
877 independent reflections
766 reflections with $I > 2\sigma(I)$
R_{int} = 0.145
θ_{max} = 30.0°, θ_{min} = 3.9°
h = −14→14
k = −14→14
l = 0→5
3 standard reflections every 120 min
intensity decay: 0.3%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.127
S = 1.05
877 reflections
48 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 4.03 e Å^{-3}
$\Delta\rho_{min}$ = −4.13 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0019 (6)
Absolute structure: Flack (1983), 466 Friedel pairs
Absolute structure parameter: 0.55 (5)

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ba1	0.28701 (11)	0.40001 (12)	0.5000	0.0144 (4)	0.93 (4)
Pb1	0.28701 (11)	0.40001 (12)	0.5000	0.0144 (4)	0.07 (4)
Ba2	0.41287 (11)	0.10688 (12)	0.0000	0.0192 (4)	0.71 (5)
Pb2	0.41287 (11)	0.10688 (12)	0.0000	0.0192 (4)	0.29 (5)
Ba3	0.0000	0.0000	0.0000	0.0269 (8)	0.86 (5)
Pb3	0.0000	0.0000	0.0000	0.0269 (8)	0.14 (5)
Cl1	0.3333	0.6667	0.0000	0.019 (2)	
Cl2	0.6667	0.3333	0.5000	0.022 (2)	
F1	0.0449 (14)	0.4338 (13)	0.5000	0.024 (4)	
F2	0.2156 (17)	0.1209 (18)	0.5000	0.038 (5)	
F3	0.1191 (14)	0.2771 (16)	0.0000	0.024 (3)	
F4	0.4344 (16)	0.3763 (16)	0.0000	0.020 (3)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.0111 (6)	0.0125 (6)	0.0194 (7)	0.0058 (5)	0.000	0.000
Pb1	0.0111 (6)	0.0125 (6)	0.0194 (7)	0.0058 (5)	0.000	0.000
Ba2	0.0131 (6)	0.0148 (6)	0.0254 (7)	0.0037 (4)	0.000	0.000
Pb2	0.0131 (6)	0.0148 (6)	0.0254 (7)	0.0037 (4)	0.000	0.000
Ba3	0.0137 (8)	0.0137 (8)	0.0533 (16)	0.0068 (4)	0.000	0.000
Pb3	0.0137 (8)	0.0137 (8)	0.0533 (16)	0.0068 (4)	0.000	0.000
Cl1	0.019 (3)	0.019 (3)	0.020 (5)	0.0094 (14)	0.000	0.000
Cl2	0.016 (2)	0.016 (2)	0.033 (7)	0.0078 (12)	0.000	0.000
F1	0.020 (6)	0.010 (6)	0.047 (10)	0.010 (5)	0.000	0.000
F2	0.036 (9)	0.016 (7)	0.055 (12)	0.009 (7)	0.000	0.000
F3	0.012 (6)	0.026 (7)	0.032 (8)	0.009 (5)	0.000	0.000
F4	0.022 (7)	0.028 (7)	0.019 (8)	0.018 (6)	0.000	0.000

Geometric parameters (Å, º)

Ba1—F3	2.618 (8)	Ba3—F2^{iii}	2.870 (11)
Ba1—F3^{i}	2.618 (8)	Ba3—F2^{vi}	2.870 (11)
Ba1—F2	2.659 (16)	Ba3—Pb2^{vi}	3.9297 (12)
Ba1—F1^{ii}	2.670 (12)	Ba3—Ba2^{vi}	3.9297 (12)
Ba1—F4^{i}	2.683 (8)	Cl1—Ba1^{ix}	3.3374 (10)

Ba1—F4	2.683 (8)	Cl1—Ba1^{x}	3.3374 (10)
Ba1—F1	2.760 (14)	Cl1—Ba1^{ii}	3.3375 (10)
Ba1—Cl1^{i}	3.3375 (10)	Cl1—Ba1^{xi}	3.3375 (10)
Ba1—Cl1	3.3375 (10)	Cl1—Ba1^{iii}	3.3375 (10)
Ba1—Ba1^{i}	4.1528 (8)	Cl2—Ba2^{xii}	3.2921 (9)
Ba1—Ba1^{iii}	4.1528 (8)	Cl2—Ba2^{iv}	3.2921 (9)
Ba1—Pb1^{i}	4.1528 (8)	Cl2—Ba2^{i}	3.2922 (9)
Ba2—F4^{iv}	2.531 (15)	Cl2—Ba2^{xiii}	3.2922 (9)
Ba2—F1^{v}	2.559 (7)	Cl2—Ba2^{xiv}	3.2922 (9)
Ba2—F1^{vi}	2.559 (7)	F1—Pb2^{vii}	2.559 (7)
Ba2—F3^{vi}	2.560 (13)	F1—Ba2^{vii}	2.559 (7)
Ba2—F4	2.746 (14)	F1—Pb2^{xv}	2.559 (7)
Ba2—F2^{iii}	3.001 (11)	F1—Ba2^{xv}	2.559 (7)
Ba2—F2	3.001 (11)	F1—Pb1^{x}	2.670 (12)
Ba2—Cl2	3.2922 (9)	F1—Ba1^{x}	2.670 (12)
Ba2—Cl2^{iii}	3.2922 (9)	F2—Ba3^{i}	2.870 (11)
Ba2—Ba3	3.9297 (12)	F2—Ba2^{i}	3.001 (11)
Ba2—Pb2^{i}	4.1528 (8)	F3—Pb2^{vii}	2.560 (13)
Ba3—F3^{vii}	2.549 (15)	F3—Ba2^{vii}	2.560 (13)
Ba3—F3	2.549 (15)	F3—Ba1^{iii}	2.618 (8)
Ba3—F3^{vi}	2.549 (15)	F3—Pb1^{iii}	2.618 (8)
Ba3—F2	2.870 (11)	F4—Pb2^{xiv}	2.531 (15)
Ba3—F2^{v}	2.870 (11)	F4—Ba2^{xiv}	2.531 (15)
Ba3—F2^{viii}	2.870 (11)	F4—Pb1^{iii}	2.683 (8)
Ba3—F2^{vii}	2.870 (11)	F4—Ba1^{iii}	2.683 (8)

F3—Ba1—F3^{i}	105.0 (5)	F3^{vii}—Ba3—F2^{vi}	69.4 (4)
F3—Ba1—F2	72.7 (4)	F3—Ba3—F2^{vi}	133.7 (2)
F3^{i}—Ba1—F2	72.7 (4)	F3^{vi}—Ba3—F2^{vi}	70.2 (4)
F3—Ba1—F1^{ii}	127.5 (2)	F2—Ba3—F2^{vi}	73.4 (4)
F3^{i}—Ba1—F1^{ii}	127.5 (2)	F2^{v}—Ba3—F2^{vi}	92.7 (5)
F2—Ba1—F1^{ii}	120.7 (4)	F2^{viii}—Ba3—F2^{vi}	139.61 (17)
F3—Ba1—F4^{i}	148.1 (4)	F2^{vii}—Ba3—F2^{vi}	73.4 (4)
F3^{i}—Ba1—F4^{i}	67.8 (4)	F2^{iii}—Ba3—F2^{vi}	139.61 (17)
F2—Ba1—F4^{i}	75.6 (3)	Ba1^{ix}—Cl1—Ba1^{x}	76.95 (3)
F1^{ii}—Ba1—F4^{i}	68.0 (3)	Ba1^{ix}—Cl1—Ba1^{ii}	133.912 (9)
F3—Ba1—F4	67.8 (4)	Ba1^{x}—Cl1—Ba1^{ii}	85.38 (2)
F3^{i}—Ba1—F4	148.1 (4)	Ba1^{ix}—Cl1—Ba1^{xi}	85.38 (2)
F2—Ba1—F4	75.6 (3)	Ba1^{x}—Cl1—Ba1^{xi}	133.912 (9)
F1^{ii}—Ba1—F4	68.0 (3)	Ba1^{ii}—Cl1—Ba1^{xi}	76.95 (3)
F4^{i}—Ba1—F4	101.4 (4)	Ba1^{ix}—Cl1—Ba1^{iii}	85.38 (2)
F3—Ba1—F1	67.7 (3)	Ba1^{x}—Cl1—Ba1^{iii}	133.911 (9)
F3^{i}—Ba1—F1	67.7 (3)	Ba1^{ii}—Cl1—Ba1^{iii}	133.909 (9)
F2—Ba1—F1	112.2 (4)	Ba1^{xi}—Cl1—Ba1^{iii}	85.38 (2)
F1^{ii}—Ba1—F1	127.1 (4)	Ba1^{ix}—Cl1—Ba1	133.911 (10)
F4^{i}—Ba1—F1	129.3 (2)	Ba1^{x}—Cl1—Ba1	85.38 (2)
F4—Ba1—F1	129.3 (2)	Ba1^{ii}—Cl1—Ba1	85.38 (2)
F3—Ba1—Cl1^{i}	133.6 (3)	Ba1^{xi}—Cl1—Ba1	133.909 (9)

F3^{i}—Ba1—Cl1^{i}	72.7 (3)	Ba1^{iii}—Cl1—Ba1	76.95 (3)
F2—Ba1—Cl1^{i}	141.26 (4)	Ba2^{xii}—Cl2—Ba2^{iv}	78.21 (3)
F1^{ii}—Ba1—Cl1^{i}	70.1 (2)	Ba2^{xii}—Cl2—Ba2	134.340 (9)
F4^{i}—Ba1—Cl1^{i}	75.6 (3)	Ba2^{iv}—Cl2—Ba2	84.45 (2)
F4—Ba1—Cl1^{i}	135.6 (3)	Ba2^{xii}—Cl2—Ba2^{i}	84.45 (2)
F1—Ba1—Cl1^{i}	69.12 (19)	Ba2^{iv}—Cl2—Ba2^{i}	134.340 (9)
F3—Ba1—Cl1	72.7 (3)	Ba2—Cl2—Ba2^{i}	78.21 (3)
F3^{i}—Ba1—Cl1	133.6 (3)	Ba2^{xii}—Cl2—Ba2^{xiii}	84.45 (2)
F2—Ba1—Cl1	141.26 (4)	Ba2^{iv}—Cl2—Ba2^{xiii}	134.339 (9)
F1^{ii}—Ba1—Cl1	70.1 (2)	Ba2—Cl2—Ba2^{xiii}	134.337 (9)
F4^{i}—Ba1—Cl1	135.6 (3)	Ba2^{i}—Cl2—Ba2^{xiii}	84.45 (2)
F4—Ba1—Cl1	75.6 (3)	Ba2^{xii}—Cl2—Ba2^{xiv}	134.339 (9)
F1—Ba1—Cl1	69.12 (19)	Ba2^{iv}—Cl2—Ba2^{xiv}	84.45 (2)
Cl1^{i}—Ba1—Cl1	76.95 (3)	Ba2—Cl2—Ba2^{xiv}	84.450 (19)
F4^{iv}—Ba2—F1^{v}	72.1 (3)	Ba2^{i}—Cl2—Ba2^{xiv}	134.337 (9)
F4^{iv}—Ba2—F1^{vi}	72.1 (3)	Ba2^{xiii}—Cl2—Ba2^{xiv}	78.20 (3)
F1^{v}—Ba2—F1^{vi}	108.5 (5)	Pb2^{vii}—F1—Ba2^{vii}	0.00 (10)
F4^{iv}—Ba2—F3^{vi}	115.8 (4)	Pb2^{vii}—F1—Pb2^{xv}	108.5 (5)
F1^{v}—Ba2—F3^{vi}	71.7 (3)	Ba2^{vii}—F1—Pb2^{xv}	108.5 (5)
F1^{vi}—Ba2—F3^{vi}	71.7 (3)	Pb2^{vii}—F1—Ba2^{xv}	108.5 (5)
F4^{iv}—Ba2—F4	126.1 (5)	Ba2^{vii}—F1—Ba2^{xv}	108.5 (5)
F1^{v}—Ba2—F4	125.7 (2)	Pb2^{xv}—F1—Ba2^{xv}	0.00 (10)
F1^{vi}—Ba2—F4	125.7 (2)	Pb2^{vii}—F1—Pb1^{x}	109.6 (3)
F3^{vi}—Ba2—F4	118.2 (4)	Ba2^{vii}—F1—Pb1^{x}	109.6 (3)
F4^{iv}—Ba2—F2^{iii}	135.8 (2)	Pb2^{xv}—F1—Pb1^{x}	109.6 (3)
F1^{v}—Ba2—F2^{iii}	67.5 (3)	Ba2^{xv}—F1—Pb1^{x}	109.6 (3)
F1^{vi}—Ba2—F2^{iii}	137.7 (4)	Pb2^{vii}—F1—Ba1^{x}	109.6 (3)
F3^{vi}—Ba2—F2^{iii}	67.1 (4)	Ba2^{vii}—F1—Ba1^{x}	109.6 (3)
F4—Ba2—F2^{iii}	69.3 (4)	Pb2^{xv}—F1—Ba1^{x}	109.6 (3)
F4^{iv}—Ba2—F2	135.8 (2)	Ba2^{xv}—F1—Ba1^{x}	109.6 (3)
F1^{v}—Ba2—F2	137.7 (4)	Pb1^{x}—F1—Ba1^{x}	0.00 (5)
F1^{vi}—Ba2—F2	67.5 (3)	Pb2^{vii}—F1—Ba1	108.1 (3)
F3^{vi}—Ba2—F2	67.1 (4)	Ba2^{vii}—F1—Ba1	108.1 (3)
F4—Ba2—F2	69.3 (4)	Pb2^{xv}—F1—Ba1	108.1 (3)
F2^{iii}—Ba2—F2	87.6 (4)	Ba2^{xv}—F1—Ba1	108.1 (3)
F4^{iv}—Ba2—Cl2	70.5 (2)	Pb1^{x}—F1—Ba1	112.9 (4)
F1^{v}—Ba2—Cl2	139.3 (3)	Ba1^{x}—F1—Ba1	112.9 (4)
F1^{vi}—Ba2—Cl2	74.6 (3)	Ba1—F2—Ba3	102.5 (4)
F3^{vi}—Ba2—Cl2	140.896 (13)	Ba1—F2—Ba3^{i}	102.5 (4)
F4—Ba2—Cl2	68.3 (2)	Ba3—F2—Ba3^{i}	92.7 (5)
F2^{iii}—Ba2—Cl2	137.3 (3)	Ba1—F2—Ba2^{i}	103.7 (4)
F2—Ba2—Cl2	82.1 (3)	Ba3—F2—Ba2^{i}	153.7 (6)
F4^{iv}—Ba2—Cl2^{iii}	70.5 (2)	Ba3^{i}—F2—Ba2^{i}	83.99 (13)
F1^{v}—Ba2—Cl2^{iii}	74.6 (3)	Ba1—F2—Ba2	103.7 (4)
F1^{vi}—Ba2—Cl2^{iii}	139.3 (3)	Ba3—F2—Ba2	83.99 (13)
F3^{vi}—Ba2—Cl2^{iii}	140.896 (13)	Ba3^{i}—F2—Ba2	153.7 (6)
F4—Ba2—Cl2^{iii}	68.3 (2)	Ba2^{i}—F2—Ba2	87.6 (4)
F2^{iii}—Ba2—Cl2^{iii}	82.1 (3)	Ba3—F3—Pb2^{vii}	100.6 (5)

F2—Ba2—Cl2^{iii}	137.3 (3)	Ba3—F3—Ba2^{vii}	100.6 (5)
Cl2—Ba2—Cl2^{iii}	78.21 (3)	Pb2^{vii}—F3—Ba2^{vii}	0.000 (6)
F3^{vii}—Ba3—F3	120.0	Ba3—F3—Ba1	113.2 (4)
F3^{vii}—Ba3—F3^{vi}	120.0	Pb2^{vii}—F3—Ba1	112.6 (4)
F3—Ba3—F3^{vi}	120.0	Ba2^{vii}—F3—Ba1	112.6 (4)
F3^{vii}—Ba3—F2	133.7 (2)	Ba3—F3—Ba1^{iii}	113.2 (4)
F3—Ba3—F2	70.2 (4)	Pb2^{vii}—F3—Ba1^{iii}	112.6 (4)
F3^{vi}—Ba3—F2	69.4 (4)	Ba2^{vii}—F3—Ba1^{iii}	112.6 (4)
F3^{vii}—Ba3—F2^{v}	69.4 (4)	Ba1—F3—Ba1^{iii}	105.0 (5)
F3—Ba3—F2^{v}	133.7 (2)	Ba3—F3—Pb1^{iii}	113.2 (4)
F3^{vi}—Ba3—F2^{v}	70.2 (4)	Pb2^{vii}—F3—Pb1^{iii}	112.6 (4)
F2—Ba3—F2^{v}	139.61 (17)	Ba2^{vii}—F3—Pb1^{iii}	112.6 (4)
F3^{vii}—Ba3—F2^{viii}	70.2 (4)	Ba1—F3—Pb1^{iii}	105.0 (5)
F3—Ba3—F2^{viii}	69.4 (4)	Ba1^{iii}—F3—Pb1^{iii}	0.00 (6)
F3^{vi}—Ba3—F2^{viii}	133.7 (2)	Pb2^{xiv}—F4—Ba2^{xiv}	0.00 (5)
F2—Ba3—F2^{viii}	139.61 (17)	Pb2^{xiv}—F4—Pb1^{iii}	110.1 (4)
F2^{v}—Ba3—F2^{viii}	73.4 (4)	Ba2^{xiv}—F4—Pb1^{iii}	110.1 (4)
F3^{vii}—Ba3—F2^{vii}	70.2 (4)	Pb2^{xiv}—F4—Ba1^{iii}	110.1 (4)
F3—Ba3—F2^{vii}	69.4 (4)	Ba2^{xiv}—F4—Ba1^{iii}	110.1 (4)
F3^{vi}—Ba3—F2^{vii}	133.7 (2)	Pb1^{iii}—F4—Ba1^{iii}	0.00 (5)
F2—Ba3—F2^{vii}	73.4 (4)	Pb2^{xiv}—F4—Ba1	110.1 (4)
F2^{v}—Ba3—F2^{vii}	139.61 (17)	Ba2^{xiv}—F4—Ba1	110.1 (4)
F2^{viii}—Ba3—F2^{vii}	92.7 (5)	Pb1^{iii}—F4—Ba1	101.4 (4)
F3^{vii}—Ba3—F2^{iii}	133.7 (2)	Ba1^{iii}—F4—Ba1	101.4 (4)
F3—Ba3—F2^{iii}	70.2 (4)	Pb2^{xiv}—F4—Ba2	113.9 (5)
F3^{vi}—Ba3—F2^{iii}	69.4 (4)	Ba2^{xiv}—F4—Ba2	113.9 (5)
F2—Ba3—F2^{iii}	92.7 (5)	Pb1^{iii}—F4—Ba2	110.3 (4)
F2^{v}—Ba3—F2^{iii}	73.4 (4)	Ba1^{iii}—F4—Ba2	110.3 (4)
F2^{viii}—Ba3—F2^{iii}	73.4 (4)	Ba1—F4—Ba2	110.3 (4)
F2^{vii}—Ba3—F2^{iii}	139.61 (17)		

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