



# Crystal structure of barium perchlorate anhydrate, $\text{Ba}(\text{ClO}_4)_2$ , from laboratory X-ray powder data

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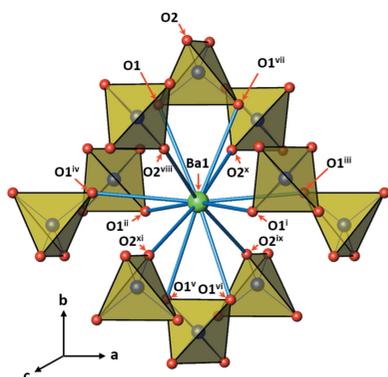
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The previously unknown crystal structure of barium perchlorate anhydrate, determined and refined from laboratory X-ray powder diffraction data, represents a new structure type. The title compound was obtained by heating hydrated barium perchlorate  $[\text{Ba}(\text{ClO}_4)_2 \cdot x\text{H}_2\text{O}]$  at 423 K *in vacuo* for 6 h. It crystallizes in the orthorhombic space group *Fddd*. The asymmetric unit contains one Ba (site symmetry  $222$  on special position  $8a$ ), one Cl (site symmetry  $2$  on special position  $16f$ ) and two O sites (on general positions  $32h$ ). The structure can be described as a three-dimensional polyhedral network resulting from the corner- and edge-sharing of  $\text{BaO}_{12}$  polyhedra and  $\text{ClO}_4$  tetrahedra. Each  $\text{BaO}_{12}$  polyhedron shares corners with eight  $\text{ClO}_4$  tetrahedra, and edges with two  $\text{ClO}_4$  tetrahedra. Each  $\text{ClO}_4$  tetrahedron shares corners with four  $\text{BaO}_{12}$  polyhedra, and an edge with the other  $\text{BaO}_{12}$  polyhedron.

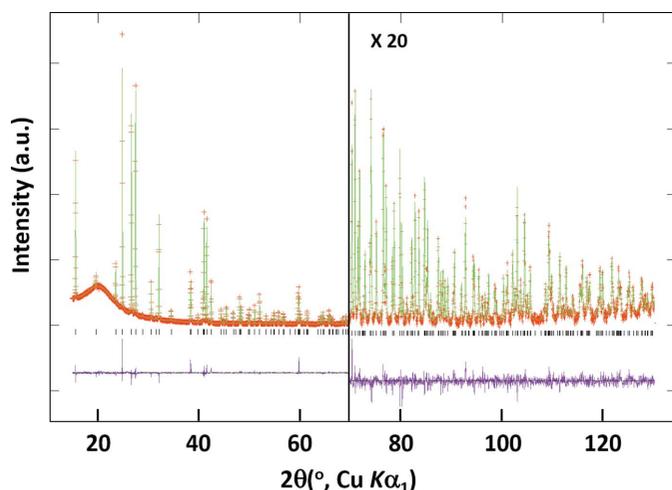
## 1. Chemical context

The alkaline earth metal ions (Mg, Ca, Sr and Ba) have been of increasing interest as ion carriers for post Li ion batteries (Wang *et al.*, 2013), and their perchlorates are often used as conventional organic electrolyte salts for electrochemical cells such as magnesium (Amatucci *et al.*, 2001; Levi *et al.*, 2010) and calcium ion batteries (Padigi *et al.*, 2015). Since such salts adsorb water easily from the atmosphere and the water causes unwanted side reactions in the electrochemical cells, removing water from the salts and its confirmation before use would be very important. However, due to the difficulty in growing a single crystal of such anhydrous perchlorates, no crystal structure had ever been solved before we first identified the magnesium perchlorate structure from powder X-ray diffraction data (Lim *et al.*, 2011). Barium perchlorate is a very strong oxidizing agent due to the high oxidation state of chlorine VII, and it is commonly stabilized as hydrate forms in the atmosphere. Several different forms of the hydrates are expected to exist, as observed in the magnesium analogues (Robertson & Bish, 2010; West, 1935). The crystal structure of the trihydrate form was determined from single-crystal data (Gallucci & Gerkin, 1988), but the anhydrous form,  $\text{Ba}(\text{ClO}_4)_2$ , has not been reported to date. We present here its crystal structure, as determined and refined from laboratory powder X-ray diffraction data (Fig. 1). This is the second crystal structure reported among the anhydrate alkaline earth metal perchlorates.



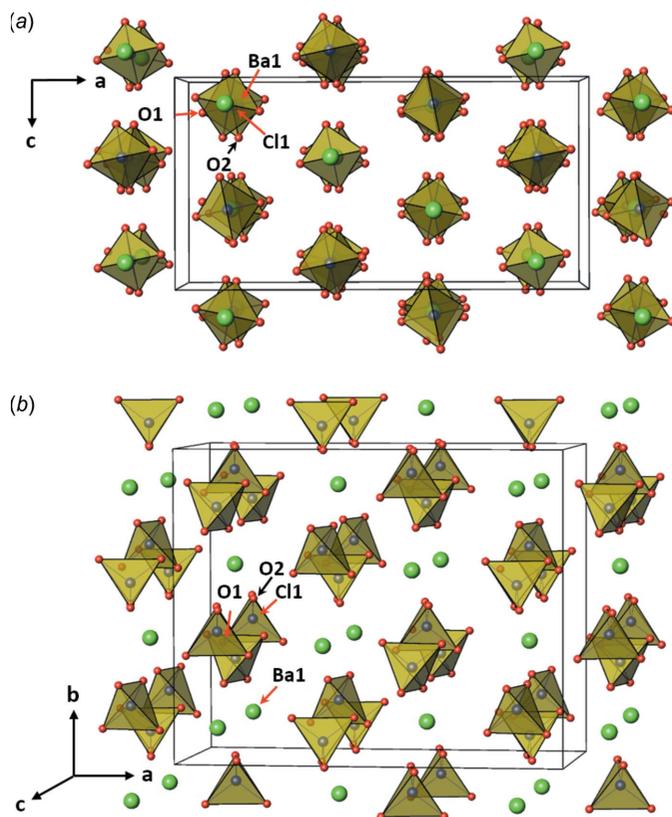
## 2. Structural commentary

Anhydrous  $\text{Ba}(\text{ClO}_4)_2$  crystallizes in a new structure type in terms of atomic ratios (1:2:8) and its polyhedral network is, to



**Figure 1**  
X-ray Rietveld refinement profiles for  $\text{Ba}(\text{ClO}_4)_2$  recorded at room temperature. Crosses mark experimental points (red) and the solid line is the calculated profile (green). The bottom trace shows the difference curve (purple) and the ticks denote expected peak positions.

our knowledge, unique. The asymmetric unit contains one Ba (site symmetry 222 on special position  $8a$ ), one Cl (site symmetry 2 on special position  $16f$ ) and two O sites (on general positions  $32h$ ). The crystal structure is illustrated in



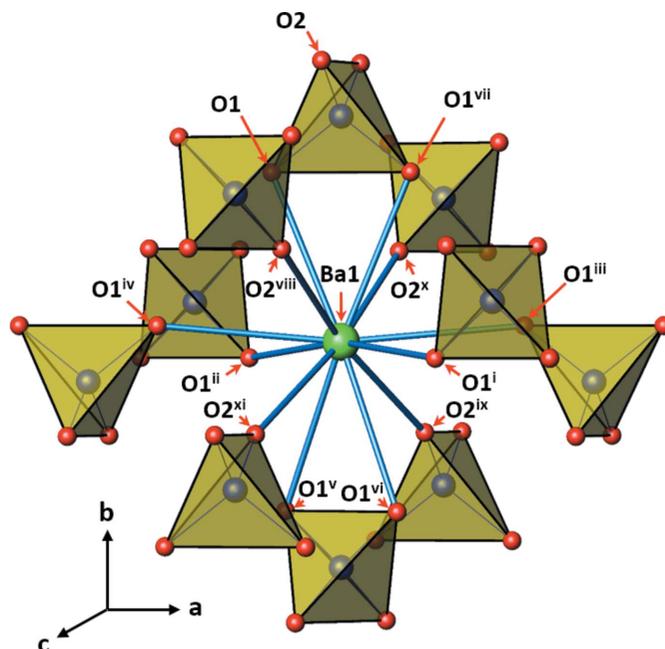
**Figure 2**  
The unit cell structures for  $\text{Ba}(\text{ClO}_4)_2$  with  $(\text{ClO}_4)$  tetrahedra (yellow) and Ba atoms (green), showing (a) the  $[010]$  view and (b) the  $[001]$  view.

**Table 1**  
Selected bond lengths ( $\text{\AA}$ ).

Ba1—O1	2.901 (4)	Ba1—O2 <sup>iii</sup>	2.903 (4)
Ba1—O1 <sup>i</sup>	2.939 (4)	Cl1—O1	1.441 (4)
Ba1—O1 <sup>iii</sup>	2.901 (4)	Cl1—O2	1.437 (4)

Symmetry codes: (i)  $x + \frac{1}{4}, y - \frac{1}{4}, -z + \frac{1}{2}$ ; (ii)  $x, -y + \frac{1}{4}, -z + \frac{1}{4}$ ; (iii)  $x, -y + \frac{3}{4}, -z + \frac{3}{4}$ .

Fig. 2, where two different views along  $[010]$  and  $[001]$  are presented for better visualization. The crystal structure is represented with  $\text{ClO}_4$  tetrahedra and Ba atoms in Fig. 2a and 2b. The local environment around the Ba atom is presented in Fig. 3. It is clearly seen that there are chains of  $[(\text{ClO}_4)\text{—Ba}(\text{ClO}_4)]_\infty$  parallel to the  $b$ -axis direction. Along each chain, the barium atom is placed between the two  $\text{ClO}_4$  tetrahedra, bonded to two oxygen atoms at each tetrahedron. The  $[010]$  view in Fig. 2a clearly shows the two-dimensional arrangement of the chains. The chains are interconnected through Ba—O bonds. Each chain is surrounded by six neighboring ones that are shifted parallel to  $b$ -axis in such a way that a barium atom of the central chain is connected to the oxygen atoms of eight  $\text{ClO}_4$  tetrahedra of six neighboring chains. Four tetrahedra are from four chains, one from each. The other four tetrahedra are from two other chains, two from each. The structure may also be described as a three-dimensional polyhedral network resulting from the corner- and edge-sharing of  $\text{BaO}_{12}$  polyhedra and  $\text{ClO}_4$  tetrahedra. Each  $\text{BaO}_{12}$  polyhedron shares corners with eight  $\text{ClO}_4$  tetrahedra, and edges with two  $\text{ClO}_4$  tetrahedra. Each  $\text{ClO}_4$  tetrahedron shares corners with four  $\text{BaO}_{12}$  polyhedra, and an edge with the other  $\text{BaO}_{12}$  poly-



**Figure 3**  
The local environment of the  $\text{Ba}^{2+}$  cation (green sphere) surrounded by  $(\text{ClO}_4)$  tetrahedra (yellow). [Symmetry codes: (i)  $x + \frac{1}{4}, y - \frac{1}{4}, -z + \frac{1}{2}$ ; (ii)  $-x, y - \frac{1}{4}, z - \frac{1}{4}$ ; (iii)  $x + \frac{1}{4}, -y + \frac{1}{2}, z - \frac{1}{4}$ ; (iv)  $-x, -y + \frac{1}{2}, -z + \frac{1}{2}$ ; (v)  $x, -y + \frac{1}{4}, -z + \frac{1}{4}$ ; (vi)  $-x + \frac{1}{4}, -y + \frac{1}{4}, z$ ; (vii)  $-x + \frac{1}{4}, y, -z + \frac{1}{4}$ ; (viii)  $x, -y + \frac{3}{4}, -z + \frac{3}{4}$ ; (ix)  $x, y - \frac{1}{2}, z - \frac{1}{2}$ ; (x)  $-x + \frac{1}{4}, -y + \frac{3}{4}, z - \frac{1}{2}$ ; (xi)  $-x + \frac{1}{4}, y - \frac{1}{2}, -z + \frac{3}{4}$ ]

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	Ba(ClO <sub>4</sub> ) <sub>2</sub>
<i>M<sub>r</sub></i>	336.23
Crystal system, space group	Orthorhombic, <i>Fddd</i>
Temperature (K)	298
<i>a</i> , <i>b</i> , <i>c</i> (Å)	14.304 (9), 11.688 (7), 7.2857 (4)
<i>V</i> (Å <sup>3</sup> )	1218.1 (11)
<i>Z</i>	8
Radiation type	Cu <i>Kα</i> <sub>1</sub> , λ = 1.54059 Å
Specimen shape, size (mm)	Flat sheet, 20 × 20
Data collection	
Diffractometer	PANalytical Empyrean
Specimen mounting	Packed powder
Data collection mode	Reflection
Scan method	Step
2θ values (°)	2θ <sub>min</sub> = 14.992 2θ <sub>max</sub> = 129.964 2θ <sub>step</sub> = 0.026
Refinement	
<i>R</i> factors and goodness of fit	<i>R<sub>p</sub></i> = 0.041, <i>R<sub>wp</sub></i> = 0.060, <i>R<sub>exp</sub></i> = 0.045, <i>R</i> ( <i>F</i> <sup>2</sup> ) = 0.05733, χ <sup>2</sup> = 1.769
No. of data points	4423
No. of parameters	25

Computer programs: *X'Pert Data Collector* and *X'Pert HighScore-Plus* (PANalytical, 2011), *GSAS* (Larson & Von Dreele, 2000), *SHELXS97* (Sheldrick, 2008), *CRYSTALS* (Betteridge *et al.*, 2003) and *ATOMS* (Dowty, 2000).

hedron. The oxygen atoms in a ClO<sub>4</sub> tetrahedron consist of two O1 and two O2 ones. O1 is bonded to three atoms, one Cl and two Ba atoms, forming an almost planar environment. On the other hand, O2 is bonded to only two atoms, Cl and Ba. Selected bond lengths are given in Table 1.

It is interesting to see the significant difference in crystal structures between Ba(ClO<sub>4</sub>)<sub>2</sub> and Mg(ClO<sub>4</sub>)<sub>2</sub> due to the difference in the cation radii, 1.61 Å for Ba<sup>2+</sup> and 0.72 Å for Mg<sup>2+</sup> (Shannon, 1976). The much bigger cation, Ba<sup>2+</sup>, is coordinated by eight ClO<sub>4</sub> tetrahedra, while the magnesium is coordinated by only six. Accordingly, the repulsion between two cations of Ba<sup>2+</sup>–Cl<sup>7+</sup> must be much weaker than that of the magnesium compound since the interatomic Ba–Cl distances of 3.55–4.06 Å are much longer than that (3.3 Å) of Mg–Cl for the same charges. This might be a reason why magnesium perchlorate is much more highly reactive with water when exposed to the atmosphere.

The empirical expression for bond valence, which has been widely adopted to estimate valences in inorganic solids (Brown, 2002), was used to check the Ba(ClO<sub>4</sub>)<sub>2</sub> crystal structure. The bond-valence sums (Brown & Altermatt, 1985; Brese & O'Keeffe, 1991) calculated with the program *Valence* (Hormillosa *et al.*, 1993) [given in v.u. (valence units): Ba 2.20, Cl 6.89, O1 2.04 and O2 1.73] match the expected charges of the ions reasonably well.

### 3. Synthesis and crystallization

The anhydrous form of barium perchlorate was prepared by dehydration from Ba(ClO<sub>4</sub>)<sub>2</sub>·xH<sub>2</sub>O (97%, Aldrich). The

powder was thoroughly ground in an agate mortar and put into the bottom of a fused-silica tube with the other end sealed with a rubber septum. The tube was inserted into a box furnace through a hole on top of the furnace so that the bottom of the tube was at the center of the furnace inside, and the other end outside connected to a vacuum pump through a needle stuck into the septum. It was heated at a rate of 4K/min up to 423K for 6 h under continuous vacuum. After furnace cooling, powder sampling for X-ray measurement was processed in an Ar atmosphere glove-box, and a tightly sealed dome-type X-ray sample holder commercially available from Bruker was used to prevent hydration during measurement.

### 4. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 2. The powder X-ray diffraction (XRD) data were collected at room temperature on a Bragg–Brentano diffractometer (PANalytical Empyrean) with a Cu *Kα*<sub>1</sub> X-ray tube, a focusing primary Ge (111) monochromator (λ = 1.54059 Å), and a position-sensitive PIXcel 3D 2x2 detector, the angular range of 15 ≤ 2θ ≤ 130°, step 0.0260 and total measurement time of 13 h at room temperature. The structure determination from the powder XRD data was performed using a combination of the powder profile refinement program *GSAS* (Larson & Von Dreele, 2000) and the single-crystal structure refinement program *CRYSTALS* (Betteridge *et al.*, 2003). For a three-dimensional view of the Fourier density maps, *MCE* was used (Rohlíček & Hušák, 2007). The XRD pattern was indexed using the program *TREOR90* (Werner, 1990) run in *CRYSFIRE* (Shirley, 2002) via the positions of 20 diffraction peaks, resulting in an orthorhombic unit cell. The systematic absences suggested the space group *Fddd*. The structure determination was performed in the same way as in our previous work (Lee & Hong, 2008) where the details were described. At the beginning, a structural model with only a dummy atom at an arbitrary position in the unit cell was used. Structure factors were extracted from the powder data, then direct methods were used for the initial solution of the structure using *SHELXS97* (Sheldrick, 2008) run in *CRYSTALS*, which yielded a couple of atom positions. However, not all the atoms could be identified at once. The partial model at this stage replaced the initial dummy-atom model, and was used for a Le Bail fit in *GSAS*. Then, improved structure factors were extracted, which were used for the improved data in the refinement in *CRYSTALS*. These processes were iterated until a complete and satisfactory structural model was obtained. Finally, Rietveld refinement was employed to complete the structure determination, resulting with reasonable temperature factors and an *R<sub>wp</sub>* factor of 0.06.

### Acknowledgements

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## References

- Amatucci, G. G., Badway, F., Singhal, A., Beaudoin, B., Skandan, G., Bowmer, T., Plitz, I., Pereira, N., Chapman, T. & Jaworski, R. (2001). *J. Electrochem. Soc.* **148**, A940–A950.
- Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
- Brese, N. E. & O'Keeffe, M. (1991). *Acta Cryst.* **B47**, 192–197.
- Brown, I. D. (2002). In *The Chemical Bonds in Inorganic Chemistry*. Oxford University Press.
- Brown, I. D. & Altermatt, D. (1985). *Acta Cryst.* **B41**, 244–247.
- Dowty, E. (2000). *ATOMS for Windows*. Shape Software, Kingsport, Tennessee, USA.
- Gallucci, J. C. & Gerkin, R. E. (1988). *Acta Cryst.* **C44**, 1873–1876.
- Hormillosa, C., Healy, S., Stephen, T. & Brown, I. D. (1993). *Bond Valence Calculator*. McMaster University, Canada. <http://CCP14.ac.uk> and [http://www.CCP14.ac.uk/solution/bond\\_valence/](http://www.CCP14.ac.uk/solution/bond_valence/).
- Larson, A. C. & Von Dreele, R. B. (2000). *General Structure Analysis System (GSAS)*. Report LAUR 86-748. Los Alamos National Laboratory, New Mexico, USA.
- Lee, E.-J. & Hong, S.-T. (2008). *J. Solid State Chem.* **181**, 2930–2934.
- Levi, E., Gofer, Y. & Aurbach, D. (2010). *Chem. Mater.* **22**, 860–868.
- Lim, H.-K., Choi, Y. S. & Hong, S.-T. (2011). *Acta Cryst.* **C67**, i36–i38.
- Padigi, P., Goncher, G., Evans, D. & Solanki, R. (2015). *J. Power Sources*, **273**, 460–464.
- PANalytical (2011). *X'Pert Data Collector and X'Pert Highscore-Plus*. PANalytical BV, Almelo, The Netherlands.
- Robertson, K. & Bish, D. (2010). *Acta Cryst.* **B66**, 579–584.
- Rohlíček, J. & Hušák, M. (2007). *J. Appl. Cryst.* **40**, 600–601.
- Shannon, R. D. (1976). *Acta Cryst.* **A32**, 751–767.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Shirley, R. (2002). *The Crysfire 2002 System for Automatic Powder Indexing: User's Manual*. Guildford, England: The Lattice Press.
- Wang, R. Y., Wessells, C. D., Huggins, R. A. & Cui, Y. (2013). *Nano Lett.* **13**, 5748–5752.
- Werner, P. E. (1990). *TREOR90*. Stockholm, Sweden.
- West, C. D. (1935). *Z. Kristallogr.* **91**, 480–493.

## supporting information

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## Crystal structure of barium perchlorate anhydrate, Ba(ClO<sub>4</sub>)<sub>2</sub>, from laboratory X-ray powder data

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### Computing details

Data collection: *X'Pert Data Collector* (PANalytical, 2011); cell refinement: *GSAS* (Larson & Von Dreele, 2000); data reduction: *X'Pert HighScore-Plus* (PANalytical, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008) and *CRYSTALS* (Betteridge *et al.*, 2003); program(s) used to refine structure: *GSAS* (Larson & Von Dreele, 2000); molecular graphics: *ATOMS* (Dowty, 2000); software used to prepare material for publication: *GSAS* (Larson & Von Dreele, 2000).

### Barium perchlorate anhydrate

#### Crystal data

Ba(ClO<sub>4</sub>)<sub>2</sub>

$M_r = 336.23$

Orthorhombic, *Fddd*

Hall symbol: -F 2uv 2vw

$a = 14.304$  (9) Å

$b = 11.688$  (7) Å

$c = 7.2857$  (4) Å

$V = 1218.1$  (11) Å<sup>3</sup>

$Z = 8$

$F(000) = 1232.0$

$D_x = 3.667$  Mg m<sup>-3</sup>

Cu  $K\alpha_1$  radiation,  $\lambda = 1.54059$  Å

$T = 298$  K

white

flat sheet, 20 × 20 mm

#### Data collection

PANalytical Empyrean  
diffractometer

Radiation source: sealed X-ray tube,  
PANalytical Cu Ceramic X-ray tube

Specimen mounting: packed powder

Data collection mode: reflection

Scan method: step

$2\theta_{\min} = 14.992^\circ$ ,  $2\theta_{\max} = 129.964^\circ$ ,  $2\theta_{\text{step}} =$   
 $0.026^\circ$

Refinement

Least-squares matrix: full

$R_p = 0.041$

$R_{wp} = 0.060$

$R_{exp} = 0.045$

$R(F^2) = 0.05733$

$\chi^2 = 1.769$

4423 data points

Profile function: CW Profile function number 3  
with 19 terms Pseudovoigt profile coefficients  
as parameterized in P. Thompson, D.E. Cox &  
J.B. Hastings (1987). J. Appl. Cryst.,20,79-83.  
Asymmetry correction of L.W. Finger, D.E. Cox  
& A. P. Jephcoat (1994). J. Appl.  
Cryst.,27,892-900. #1(GU) = 0.000 #2(GV) =  
0.000 #3(GW) = 0.000 #4(GP) = 4.256 #5(LX)  
= 1.263 #6(LY) = 7.277 #7(S/L) = 0.0005  
#8(H/L) = 0.0005 #9(trns) = -1.26 #10(shft)=  
1.5725 #11(stec) = 4.60 #12(pte) = 1.24  
#13(sfec) = 0.00 #14(L11) = -0.018 #15(L22) =  
-0.022 #16(L33) = -0.202 #17(L12) = 0.017  
#18(L13) = 0.017 #19(L23) = 0.000 Peak tails  
are ignored where the intensity is below 0.0010  
times the peak Aniso. broadening axis 0.0 0.0  
1.0

25 parameters

0 restraints

$(\Delta/\sigma)_{max} = 0.01$

Background function: GSAS Background  
function number 1 with 36 terms. Shifted  
Chebyshev function of 1st kind 1: 567.648 2:  
-857.136 3: 662.653 4: -377.264 5: 131.512 6:  
59.5938 7: -169.995 8: 206.701 9: -185.404 10:  
133.783 11: -68.7256 12: 6.71856 13: 43.4515  
14: -72.2732 15: 82.7653 16: -73.3661 17:  
50.0183 18: -22.8495 19: -2.57480 20: 20.6662  
21: -29.1651 22: 28.9267 23: -24.2542 24:  
14.4066 25: -5.32227 26: -4.03875 27: 10.7050  
28: -13.4416 29: 11.1646 30: -9.08855 31:  
2.53787 32: -0.292410 33: -1.46976 34:  
0.544854 35: -1.31862 36: 0.893355

Preferred orientation correction: March-Dollase  
AXIS 1 Ratio= 0.97385 h= 1.000 k= 0.000 l=  
0.000 Preferred orientation correction range:  
Min= 0.96103, Max= 1.08275

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{iso}^*/U_{eq}$
Ba1	0.125	0.125	0.125	0.0139 (2)*
Cl1	0.125	0.42875 (18)	0.125	0.0160 (7)*
O1	0.0471 (3)	0.3533 (3)	0.1575 (5)	0.0162 (11)*
O2	0.1412 (3)	0.5016 (4)	0.2807 (4)	0.0170 (12)*

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

Ba1—O1	2.901 (4)	Ba1—O2 <sup>viii</sup>	2.903 (4)
Ba1—O1 <sup>i</sup>	2.939 (4)	Ba1—O2 <sup>ix</sup>	2.903 (4)
Ba1—O1 <sup>ii</sup>	2.939 (4)	Ba1—O2 <sup>x</sup>	2.903 (4)
Ba1—O1 <sup>iii</sup>	2.939 (4)	Ba1—O2 <sup>xi</sup>	2.903 (4)
Ba1—O1 <sup>iv</sup>	2.939 (4)	Cl1—O1	1.441 (4)

Ba1—O1 <sup>v</sup>	2.901 (4)	Cl1—O1 <sup>vii</sup>	1.441 (4)
Ba1—O1 <sup>vi</sup>	2.901 (4)	Cl1—O2	1.437 (4)
Ba1—O1 <sup>vii</sup>	2.901 (4)	Cl1—O2 <sup>vii</sup>	1.437 (4)
O1—Ba1—O1 <sup>i</sup>	110.93 (10)	O1 <sup>i</sup> —Ba1—O2 <sup>ix</sup>	110.87 (10)
O1—Ba1—O1 <sup>ii</sup>	78.56 (7)	O1 <sup>i</sup> —Ba1—O2 <sup>x</sup>	125.15 (10)
O1—Ba1—O1 <sup>iii</sup>	106.64 (7)	O1 <sup>i</sup> —Ba1—O2 <sup>xi</sup>	63.76 (10)
O1—Ba1—O1 <sup>iv</sup>	63.56 (12)	O1 <sup>vi</sup> —Ba1—O1 <sup>vii</sup>	134.82 (15)
O1—Ba1—O1 <sup>v</sup>	134.82 (15)	O2 <sup>xii</sup> —Ba1—O2 <sup>ix</sup>	170.85 (15)
O1—Ba1—O1 <sup>vi</sup>	170.64 (14)	O2 <sup>viii</sup> —Ba1—O2 <sup>x</sup>	120.42 (15)
O1—Ba1—O1 <sup>vii</sup>	46.25 (15)	O2 <sup>viii</sup> —Ba1—O2 <sup>xi</sup>	60.43 (15)
O1—Ba1—O2 <sup>viii</sup>	60.21 (10)	O1—Cl1—O1 <sup>vii</sup>	104.5 (3)
O1—Ba1—O2 <sup>ix</sup>	123.92 (10)	O1—Cl1—O2	110.96 (19)
O1—Ba1—O2 <sup>x</sup>	65.35 (10)	O1—Cl1—O2 <sup>vii</sup>	111.6 (2)
O1—Ba1—O2 <sup>xi</sup>	110.84 (10)	O2—Cl1—O2 <sup>vii</sup>	107.3 (3)
O1 <sup>i</sup> —Ba1—O1 <sup>ii</sup>	170.09 (14)	Ba1—O1—Ba1 <sup>xiii</sup>	116.44 (12)
O1 <sup>i</sup> —Ba1—O1 <sup>iii</sup>	66.21 (14)	Ba1—O1—Cl1	104.6 (2)
O1 <sup>i</sup> —Ba1—O1 <sup>iv</sup>	114.73 (14)	Ba1 <sup>xiii</sup> —O1—Cl1	133.1 (2)
O1 <sup>i</sup> —Ba1—O2 <sup>viii</sup>	60.66 (10)	Ba1 <sup>viii</sup> —O2—Cl1	164.5 (2)

Symmetry codes: (i)  $x+1/4, y-1/4, -z+1/2$ ; (ii)  $-x, y-1/4, z-1/4$ ; (iii)  $x+1/4, -y+1/2, z-1/4$ ; (iv)  $-x, -y+1/2, -z+1/2$ ; (v)  $x, -y+1/4, -z+1/4$ ; (vi)  $-x+1/4, -y+1/4, z$ ; (vii)  $-x+1/4, y, -z+1/4$ ; (viii)  $x, -y+3/4, -z+3/4$ ; (ix)  $x, y-1/2, z-1/2$ ; (x)  $-x+1/4, -y+3/4, z-1/2$ ; (xi)  $-x+1/4, y-1/2, -z+3/4$ ; (xii)  $x, -y+7/4, -z+11/4$ ; (xiii)  $-x, y+1/4, z+1/4$ .