distances and angles in Table 2. A stereoview of the unit cell is shown in Fig. 2.

Related literature. A monoclinic structure of Cs_2CdI_4 in polar space group $P2_1$ was assumed by Zandbergen, Verschoor & IJdo (1979). Subsequent measurements of dielectric properties (Gesi, 1985) for the three related compounds Rb_2ZnI_4, Tl_2ZnI_4 and Cs_2HgI_4 with Sr_2GeS_4-type structure indicated a non-polar space group at room temperature. Powder data for α-Cs_2CdI_4, room-temperature phase, were recently reported by Touchard, Louër & Louër (1986). Their results are in good agreement with those of the present work and those of Sjövall & Svensson (1988) on refinement of Cs_2HgI_4. The space group and unit-cell parameters given by Aleksandrov, Mel'nikova & Kokov (1987) do not agree with those in this paper.

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A (2-Amino-2-methylpropanedioato)(Optically Active Cyclen)cobalt(III) Complex*

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Abstract. *cis*-(*SSSR*)-β_1-[(*R*)-2-Amino-2-methylmalonato](2*R*,5*R*,8*R*,11*R*-2,5,8,11-tetraethyl-1,4,7,10-tetraazacyclododecane)cobalt(III) perchlorate 2·5-hydrate, $[Co(C_4H_5NO_4)(C_{16}H_{36}N_4)]ClO_4.2{\cdot}5H_2O$, $M_r = 619{\cdot}00$, triclinic, $P1$, $a = 10{\cdot}455\,(5)$, $b = 31{\cdot}715\,(15)$, $c = 10{\cdot}492\,(7)$ Å, $\alpha = 110{\cdot}50\,(5)$, $\beta = 116{\cdot}74\,(5)$, $\gamma = 80{\cdot}36\,(5)°$, $U = 2910\,(3)$ Å^3, $Z = 4$, $D_m = 1{\cdot}410$, $D_x = 1{\cdot}415$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 0{\cdot}74$ mm^{-1}, $F(000) = 1316$, $T = 296$ K, final $R = 0{\cdot}068$ for 7646 unique reflections with $|F_o| > 3\sigma(|F_o|)$. The geometries of the four independent molecules in the unit cell are essentially the same. In each octahedral molecule, the Co^{III} ion is surrounded by four N of the macrocycle, and by N and O atoms of *pro-R* carboxylate in the amino acid. The uncoordinated carboxyl group forms an intramolecular hydrogen bond to one of the N atoms in the macrocyclic ligand, in molecule 1 [N(1)—H···O(17)2: 2·98 (1) Å, ∠N(1)—H···O(17)2: 159 (12)°].

Experimental. The crystal was obtained from the same reaction product as the monoclinic one whose structure had already been reported (Tsuboyama, Takishima, Sakurai & Tsuboyama, 1987). The density was measured by flotation in CCl_4–benzene. Details of data collection and structure refinement are given in Table 1. Structure solved by direct methods with *MULTAN*78 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1978). Calculations performed using the program system *UNICS*-III (Sakurai & Kobayashi, 1979) on a FACOM M-780. The four independent molecules are labelled 1, 2, 3 and 4. The molecular geometries of these are almost identical to that of the monoclinic crystal. The H atom attached to

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* Part 9 of the series *Metal Complexes of Chiral Cyclen.* Part 8: Tsuboyama, Takishima, Sakurai & Tsuboyama (1987).

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0108-2701/89/040669-04$03.00

Table 1. *Experimental details*

Crystal	Orange-red, pillar, 0·24 × 0·36 × 0·40 mm
Diffractometer used	Rigaku AFC automated four-circle
Monochromator	Graphite
Unit cell	16 reflections, 25·0 > 2θ > 20·0°
Data correction applied	Lorentz and polarization, not absorption
Mode	ω, ω–2θ (2θ > 30°)
Scan rate (deg min^{-1})	4·0
Scan ranges of *h, k, l*	−13→13, −41→41, 0→13
Standards	300, 0,16,0, 29$\bar{3}$, 007
No. of reflections between standards	150, no intensity variation
2θ range (°)	55
Reflections observed	11 812
No. of unobs. reflections	6489 [criterion: $\lvert F_o\rvert > 3\sigma(\lvert F_o\rvert)$]
Parameters refined	1498
R	0·068
wR	0·073
Maximum shift/e.s.d.	0·35*
Max. height in final map (e Å^{-3})	0·7

* Except for disordered ethyl groups and anions.

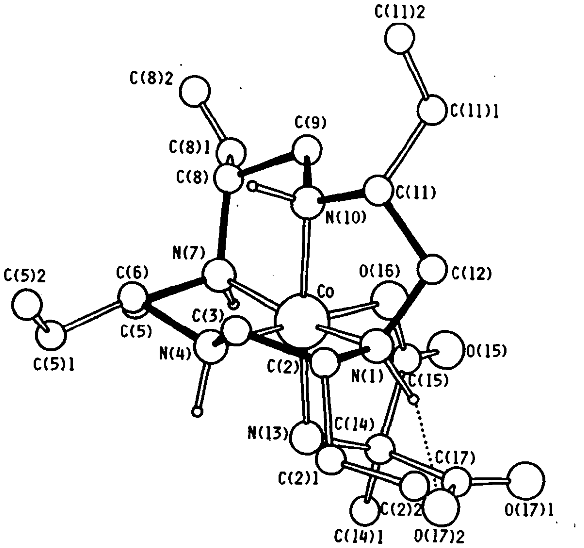

Fig. 1. Molecular structure of molecule 1 with atom numbering. Only the H atoms at the asymmetric nitrogens are attached for clarity.

1N(1) was located in a difference map, the other H-atom coordinates were calculated assuming ideal geometry. Refinement was carried out using a block-diagonal least-squares procedure with anisotropic thermal parameters for all non-hydrogen atoms and isotropic for H atoms. The absolute configurations of the complex cations were assigned from the known configurations of the ligand as an internal reference (Sakurai, Tsuboyama & Tsuboyama, 1980). Scattering factors and corrections for anomalous dispersion from *International Tables for X-ray Crystallography* (1974).

Table 2. *Atomic parameters*

Positional parameters are multiplied by 10^4. The equivalent isotropic temperature factor is defined by $B_{eq} = \frac{4}{3}\sum_i\sum_j\beta_{ij}(\mathbf{a}_i.\mathbf{a}_j)$.

	x	*y*	*z*	B_{eq}(Å^2)
1Co	3029 (2)	4420 (1)	804 (2)	3·4
1N(1)	1242 (10)	4413 (3)	913 (12)	3·5
1C(2)	1416 (15)	4135 (4)	1930 (16)	4·5
1C(3)	2755 (14)	3845 (4)	2152 (16)	4·2
1N(4)	3893 (11)	4108 (3)	2267 (12)	3·7
1C(5)	5163 (16)	3822 (4)	2081 (19)	5·1
1C(6)	5908 (16)	4125 (4)	1753 (19)	5·3
1N(7)	4825 (11)	4279 (4)	507 (14)	4·5
1C(8)	4528 (20)	3946 (5)	−1062 (21)	6·2
1C(9)	2895 (21)	3873 (4)	−1968 (19)	6·5
1N(10)	2370 (13)	3858 (3)	−868 (13)	4·7
1C(11)	802 (19)	3791 (5)	−1418 (18)	6·0
1C(12)	166 (16)	4221 (5)	−687 (17)	5·4
1C(21)	1383 (16)	4473 (5)	3418 (16)	5·0
1C(22)	−112 (19)	4664 (6)	3234 (22)	6·9
1C(51)	6195 (17)	3691 (6)	3487 (21)	6·4
1C(52)	5807 (26)	3274 (9)	3561 (34)	12·1
1C(81)	5241 (35)	4129 (6)	−1814 (29)	12·3
1C(82)	5527 (38)	3820 (12)	−2796 (40)	16·8
1C(111)	−128 (22)	3614 (6)	−3128 (21)	7·9
1C(112)	−138 (32)	3156 (8)	−3771 (25)	12·9
1N(13)	3612 (10)	5020 (3)	2318 (11)	3·3
1C(14)	3005 (13)	5388 (4)	1645 (14)	3·7
1C(15)	2651 (13)	5180 (4)	−57 (15)	3·8
1O(16)	2347 (10)	4767 (2)	−594 (10)	4·0
1O(15)	2565 (10)	5426 (3)	−805 (10)	4·5
1C(141)	3932 (15)	5795 (5)	2416 (17)	4·8
1C(17)	1502 (13)	5538 (3)	1690 (15)	3·7
1O(171)	745 (10)	5791 (3)	944 (12)	5·1
1O(172)	1206 (10)	5395 (3)	2501 (11)	4·9
2Co	296 (2)	1404 (1)	516 (2)	3·4
2N(1)	462 (11)	1410 (3)	−1301 (11)	3·4
2C(2)	1757 (15)	1685 (4)	−862 (17)	4·6
2C(3)	2271 (15)	1984 (5)	796 (16)	4·7
2N(4)	2132 (11)	1718 (3)	1671 (12)	3·8
2C(5)	2218 (17)	1997 (4)	3207 (16)	5·1
2C(6)	1595 (18)	1693 (4)	3678 (17)	5·3
2N(7)	171 (12)	1542 (4)	2410 (11)	4·2
2C(8)	−1069 (19)	1869 (5)	2411 (19)	6·1
2C(9)	−1917 (18)	1948 (4)	874 (23)	6·7
2N(10)	−787 (12)	1970 (3)	390 (14)	4·8
2C(11)	−1258 (16)	2035 (5)	−1131 (19)	5·6
2C(12)	−934 (16)	1611 (5)	−2133 (17)	5·3
2C(21)	2897 (15)	1368 (4)	−1195 (16)	4·6
2C(22)	2512 (21)	1181 (6)	−2867 (20)	6·8
2C(51)	3754 (18)	2135 (6)	4362 (17)	6·3
2C(52)	4302 (28)	2539 (8)	4447 (27)	11·2
2C(81)	−2162 (27)	1718 (7)	2742 (25)	10·0
2C(82)	−1879 (32)	1781 (10)	4097 (33)	13·1
2C(111)	−2759 (21)	2211 (6)	−1828 (26)	8·3
2C(112)	−2963 (25)	2662 (9)	−1401 (40)	14·4
2N(13)	1260 (10)	811 (3)	477 (11)	3·3
2C(14)	197 (13)	438 (4)	−513 (14)	3·5
2C(15)	−1293 (14)	639 (4)	−662 (14)	3·8
2O(16)	−1409 (9)	1060 (2)	−534 (10)	3·9
2O(15)	−2282 (9)	403 (3)	−991 (10)	4·3
2C(141)	588 (15)	24 (4)	7 (15)	4·3
2C(17)	108 (14)	284 (4)	−2179 (14)	3·8
2O(171)	−903 (10)	31 (3)	−3192 (10)	4·8
2O(172)	1060 (10)	430 (3)	−2321 (11)	4·8
3Co	−4787 (2)	−591 (1)	−5246 (2)	4·4
3N(1)	−6813 (13)	−626 (4)	−6594 (13)	5·2
3C(2)	−7626 (17)	−838 (5)	−6071 (17)	5·5
3C(3)	−6614 (16)	−1046 (4)	−4893 (18)	5·0
3N(4)	−5267 (11)	−749 (3)	−3919 (13)	4·1
3C(5)	−3977 (16)	−987 (5)	−2938 (22)	6·3
3C(6)	−2745 (17)	−713 (5)	−2546 (20)	6·0
3N(7)	−2783 (13)	−699 (3)	−4002 (15)	5·4
3C(8)	−2236 (20)	−1138 (5)	−4789 (27)	8·2
3C(9)	−3220 (25)	−1271 (6)	−6488 (31)	10·2
3N(10)	−4708 (15)	−1206 (4)	−6577 (16)	6·1
3C(11)	−5962 (20)	−1298 (4)	−8077 (19)	6·4
3C(12)	−6925 (21)	−866 (5)	−8167 (18)	6·7
3C(21)	−8690 (16)	−499 (5)	−5635 (19)	5·6
3C(22)	−9997 (19)	−440 (6)	−6974 (22)	7·0
3C(51)	−4170 (25)	−1027 (8)	−1631 (25)	9·4
3C(52)	−3845 (46)	−688 (13)	−396 (42)	18·5
3C(81)	−640 (25)	−1099 (7)	−4394 (36)	11·7
3C(82)	24 (33)	−1518 (10)	−4920 (48)	16·0
3C(111)	−5591 (30)	−1473 (8)	−9449 (25)	11·4
3C(112)	−6818 (40)	−1613 (9)	−10881 (30)	14·7
3N(13)	−4739 (11)	60 (3)	−4148 (12)	3·6

Table 2 (*cont.*)

	x	y	z	B_{eq}(Å^2)
3C(14)	−4784 (13)	346 (4)	−5073 (15)	3·6
3C(15)	−4196 (14)	44 (4)	−6188 (15)	3·9
3O(16)	−4248 (11)	−387 (3)	−6488 (11)	5·2
3O(15)	−3768 (11)	211 (4)	−6823 (11)	5·7
3C(141)	−3945 (14)	774 (4)	−4055 (15)	4·0
3C(17)	−6363 (14)	455 (4)	−5984 (14)	3·8
3O(171)	−6566 (10)	710 (4)	−6728 (11)	5·6
3O(172)	−7326 (9)	308 (3)	−5856 (11)	4·7
4Co	9259 (2)	6415 (1)	7714 (2)	4·4
4N(1)	7974 (13)	6457 (4)	5691 (14)	5·1
4C(1)	8727 (17)	6671 (5)	5091 (19)	5·3
4C(3)	10096 (18)	6867 (5)	6302 (18)	5·5
4N(4)	10787 (11)	6583 (3)	7363 (13)	4·4
4C(5)	11982 (19)	6810 (5)	8852 (17)	5·9
4C(6)	12106 (19)	6537 (5)	9835 (19)	6·2
4N(7)	10662 (16)	6523 (4)	9808 (14)	6·0
4C(8)	10231 (25)	6957 (5)	10720 (19)	7·6
4C(9)	8771 (28)	7104 (6)	9932 (24)	9·2
4N(10)	8593 (16)	7027 (4)	8365 (15)	6·0
4C(11)	7183 (21)	7129 (5)	7238 (24)	7·4
4C(12)	6683 (17)	6705 (5)	5845 (22)	6·3
4C(21)	8807 (20)	6319 (6)	3670 (19)	6·3
4C(22)	7363 (20)	6267 (6)	2292 (20)	7·1
4C(51)	13361 (22)	6834 (8)	8714 (25)	8·9
4C(52)	14335 (38)	6473 (11)	8698 (44)	15·9
4C(81)	10701 (35)	6929 (6)	12394 (28)	11·7
4C(82)	10497 (44)	7346 (9)	13408 (31)	15·4
4C(111)	5998 (28)	7309 (8)	7771 (33)	11·5
4C(112)	4574 (32)	7433 (10)	6511 (41)	13·8
4N(13)	9753 (10)	5763 (3)	7081 (11)	3·4
4C(14)	8544 (12)	5479 (4)	6748 (14)	3·3
4C(15)	7700 (14)	5782 (4)	7645 (15)	4·0
4O(16)	7844 (11)	6206 (3)	8002 (12)	5·3
4O(15)	6906 (10)	5612 (3)	7902 (12)	5·0
4C(141)	9132 (14)	5052 (4)	7182 (16)	4·3
4C(17)	7513 (14)	5358 (4)	5021 (16)	4·1
4O(171)	6491 (10)	5116 (4)	4600 (11)	5·7
4O(172)	7763 (10)	5517 (3)	4222 (11)	4·8
1Cl	3300 (6)	2587 (1)	−1256 (6)	7·8
1O(Cl)1	3754 (20)	2946 (4)	−1430 (20)	11·8
1O(Cl)2	2581 (31)	2269 (5)	−2564 (20)	17·7
1O(Cl)3	2446 (21)	2796 (6)	−523 (23)	13·2
1O(Cl)4	4426 (21)	2357 (7)	−470 (29)	15·6
2Cl	103 (6)	3238 (1)	2589 (7)	7·9
2O(Cl)1	−411 (20)	2873 (4)	2690 (20)	11·6
2O(Cl)2	678 (21)	3037 (5)	1557 (22)	13·3
2O(Cl)3	−966 (20)	3538 (5)	2079 (30)	15·7
2O(Cl)4	1195 (25)	3465 (6)	3996 (20)	15·4
3Cl	5367 (10)	7614 (2)	3285 (7)	13·5
3O(Cl)1	5083 (24)	7972 (5)	4193 (25)	14·0
3O(Cl)2	5011 (20)	7201 (5)	3139 (22)	12·8
3O(Cl)3	5433 (34)	7671 (7)	2217 (25)	20·1
3O(Cl)4	6744 (32)	7694 (9)	4531 (28)	19·4
4Cl	9588 (7)	8217 (2)	9630 (9)	11·5
4O(Cl)1	10154 (27)	7849 (5)	9033 (26)	15·2
4O(Cl)2	9880 (22)	8628 (4)	9688 (20)	13·4
4O(Cl)3	8396 (25)	8190 (7)	9997 (34)	18·1
4O(Cl)4	10647 (30)	8159 (9)	11005 (35)	20·3
O(*W*)1	4964 (12)	4720 (4)	−4670 (12)	6·7
O(*W*)2	−3756 (10)	5090 (3)	1201 (11)	4·9
O(*W*)3	4139 (13)	5338 (4)	−2477 (13)	7·3
O(*W*)4	1638 (10)	5720 (3)	5566 (11)	5·0
O(*W*)5	−1824 (11)	5157 (4)	113 (12)	5·9
O(*W*)6	4548 (12)	1103 (4)	2124 (13)	6·5
O(*W*)7	39 (11)	733 (3)	3030 (11)	5·1
O(*W*)8	6137 (12)	486 (4)	693 (12)	7·1
O(*W*)9	−6213 (11)	99 (3)	−2189 (11)	5·4
O(*W*)10	−1081 (11)	672 (4)	−5082 (12)	6·1

The atomic parameters for the structures are given in Table 2,* selected bond lengths and angles for molecule 1 in Table 3. The molecule 1 is shown in Fig. 1. The packing consists of two layers containing two different pairs of cations parallel to the *bc* plane (Fig. 2, in deposited material).

Table 3. *Selected bond distances* (Å), *angles* (°), *and torsion angles* (°) *for molecule* 1

Co—N(1)	1·926 (13)	C(14)—C(15)	1·56 (2)
Co—N(4)	1·917 (12)	C(14)—C(14)1	1·50 (2)
Co—N(7)	1·993 (14)	C(14)—C(17)	1·58 (2)
Co—N(10)	1·967 (9)	C(15)—O(16)	1·26 (1)
Co—N(13)	1·978 (8)	C(15)—O(15)	1·25 (2)
Co—O(16)	1·948 (10)	C(17)—O(17)1	1·25 (2)
N(13)—C(14)	1·48 (2)	C(17)—O(17)2	1·26 (2)
N(1)—Co—N(4)	88·2 (5)	N(7)—Co—N(13)	96·6 (5)
N(1)—Co—N(7)	167·2 (4)	N(7)—Co—O(16)	89·2 (5)
N(1)—Co—N(10)	85·4 (5)	N(10)—Co—N(13)	173·8 (5)
N(1)—Co—N(13)	95·4 (4)	N(10)—Co—O(16)	91·1 (4)
N(1)—Co—O(16)	97·0 (5)	N(13)—Co—O(16)	82·7 (4)
N(4)—Co—N(7)	86·4 (6)	Co—N(13)—C(14)	112·0 (7)
N(4)—Co—N(10)	92·5 (4)	N(13)—C(14)—C(15)	106·7 (9)
N(4)—Co—N(13)	93·7 (4)	C(14)—C(15)—O(16)	114·2 (14)
N(4)—Co—O(16)	174·0 (4)	Co—O(16)—C(15)	117·5 (8)
N(7)—Co—N(10)	83·3 (5)		
C(12)—N(1)—C(2)—C(3)	101 (1)	C(6)—N(7)—C(8)—C(9)	129 (2)
N(1)—C(2)—C(3)—N(4)	37 (2)	N(7)—C(8)—C(9)—N(10)	−39 (2)
C(2)—C(3)—N(4)—C(5)	−165 (1)	C(8)—C(9)—N(10)—C(11)	180 (1)
C(3)—N(4)—C(5)—C(6)	163 (1)	C(9)—N(10)—C(11)—C(12)	−112 (2)
N(4)—C(5)—C(6)—N(7)	−52 (2)	N(10)—C(11)—C(12)—N(1)	−38 (2)
C(5)—C(6)—N(7)—C(8)	−84 (2)	C(2)—N(1)—C(12)—C(11)	−71 (2)

Related literature. The structure of the monoclinic crystal, and the spectral studies and decarboxylation reaction of the title compound have already been published (Tsuboyama, Takishima, Sakurai & Tsuboyama, 1987). For comparison with other complexes containing the amino acid see Glusker, Carrell, Job & Bruice (1974), Yashiro, Ajioka, Yano, Toriumi, Ito & Yoshikawa (1986). The crystal structures, and absorption and circular dichroism spectra of (*R*)- and (*S*)-alanine complexes containing the optically active cyclen have been reported (Tsuboyama, Sakurai & Tsuboyama, 1987).

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* Lists of anisotropic thermal parameters, H-atom coordinates, structure factors, and a projection of the crystal structure (Fig. 2) have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51519 (47 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of Barium Bromate Monohydrate

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Abstract. $Ba(BrO_3)_2.H_2O$, $M_r = 411{\cdot}17$, monoclinic, $I2/c$, $a = 9{\cdot}0696$ (10), $b = 7{\cdot}8952$ (9), $c = 9{\cdot}6295$ (8) Å, $\beta = 93{\cdot}26$ (1)°, $V = 688{\cdot}4$ (2) Å^3, $Z = 4$, $D_m = 3{\cdot}950$, $D_x = 3{\cdot}966$ (1) g cm^{-3}, Mo $K\alpha_1$, $\lambda = 0{\cdot}70930$ Å, $\mu = 172{\cdot}5$ cm^{-1}, $F(000) = 736$, $T = 298$ K, $R = 0{\cdot}016$, $wR = 0{\cdot}020$ for 576 independent reflections with $I > \sigma(I)$. Each Ba atom has eleven O neighbors at distances 2·702 (6) to 3·057 (2) Å; the average Br—O bond length is 1·652 (6) Å, or 1·661 (5) Å if corrected for thermal motion; O···O = 2·832 (4) Å in a hydrogen bond.

Experimental. Crystals were prepared by mixing hot aqueous solutions of barium nitrate and sodium bromate and allowing the mixture to cool. The measured density is quoted from Heydweiller (1920). A crystal 0·043 × 0·055 × 0·25 mm (9 faces, elongated on **c**) was glued to a glass fiber and mounted on an Enraf–Nonius CAD-4 diffractometer equipped with a graphite monochromator. Cell dimensions were derived from 24 reflections in the range $12{\cdot}8 < \theta < 28{\cdot}0°$. Intensities were measured for θ up to 25° at two azimuthal angles [h 0 to 10, k −9 to 0, l −11 to 11] and at one azimuth [h −10 to −1, k −9 to 2, l −11 to 11]. Of 2047 reflections permitted by the space group, 119 were rejected as too weak to measure. After analytical correction for absorption ($2{\cdot}11 < A < 12{\cdot}1$) reflections which were equivalent were averaged giving 582 unique ones with $F^2 > \sigma(F^2)$; $R_{\rm int} = 0{\cdot}031$. Measurements of standard reflections (800, 006, 0$\bar{2}$0) every 3600 s of X-ray exposure were constant within about 1%; no correction was made. Refinement by least squares (on F) with weights $w = [\sigma(F)]^{-2}$, derived from $\sigma(F^2) = \{[\sigma_{\rm cs}(F^2)]^2 + (0{\cdot}03F^2)^2 + 41^2\}^{1/2}$, was started with coordinates of Kartha (1953). Anisotropic thermal parameters were assigned to 6 atoms. The H-atom coordinates and isotropic thermal parameter were refined; the starting position in the hydrogen bond between O2 and O4 was calculated. The 3 strongest reflections (reduced in intensity *ca* 25% by extinction) and 3 others which agreed poorly with the calculated values for unknown reasons were rejected. An empirical isotropic correction for extinction increased the largest remaining F by 12%. The maximum final shift was 0·03σ; extremes of ΔF synthesis were +0·56 and −0·58 e Å^{-3}; GOF = 1·10. Atomic scattering factors, including dispersion terms, for Ba^{2+}, Br, O (for O4), $O^{1/3-}$ (for O1, O2, O3) and H were taken from *International Tables for X-ray Crystallography* (1974). Calculations were made with unpublished local programs. Atomic parameters are listed in Table 1 and

Table 1. *Fractional atomic coordinates and isotropic thermal parameters* (Å^2) *with e.s.d.'s in parentheses*

$$B_{\rm eq} = \textstyle\sum(B_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j)/3.$$

	x	y	z	$B/B_{\rm eq}^*$
Ba	0	0·39194 (3)	0·250	1·03*
O4	0	0·0497 (7)	0·250	3·73*
Br	0·25101 (3)	0·27704 (5)	0·55741 (3)	1·11*
O1	0·07699 (27)	0·3401 (4)	0·56027 (25)	1·64*
O2	0·2566 (3)	0·0980 (3)	0·64701 (28)	1·87*
O3	0·2629 (3)	0·2181 (3)	0·39456 (25)	1·94*
H	0·051 (6)	0·011 (7)	0·215 (5)	2·2 (11)

Table 2. *Interatomic distances* (Å) *and bond angles* (°)

Ba—O1, O1$^{\rm i}$	3·057 (2)	Ba—O3, O3$^{\rm i}$	3·022 (3)
—O1$^{\rm iv}$, O1$^{\rm v}$	2·906 (6)	—O3$^{\rm vi}$, O3$^{\rm vii}$	2·767 (6)
—O2$^{\rm ii}$, O2$^{\rm iii}$	2·874 (6)	—O4	2·702 (6)
Br—O1	1·657 (2), 1·663*	O1—Br—O2	104·4 (1)
—O2	1·655 (3), 1·664*	O1—Br—O3	102·4 (1)
—O3	1·645 (2), 1·655*	O2—Br—O3	104·7 (1)
O4—H, H$^{\rm i}$	0·67 (5)	H—O4—H$^{\rm i}$	125 (9)
O4···O2$^{\rm viii}$, O2$^{\rm ix}$	2·832 (4)	H—O4···O2$^{\rm viii}$	12 (5)

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

* Corrected for thermal motion by riding model.

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