

ment, within experimental errors, with the values observed in the *s-facial* isomer (Kobayashi, Marumo & Saito, 1972). All the observed Co–N distances are normal for Co(III) complexes of linear aliphatic polyamines. The chelate rings formed by a dien ligand in the complex cation *A* have eclipsed envelope and symmetrical skew conformations, while those in the complex cation *B* are both eclipsed envelope conformations. They are shown in Fig. 3. The Newman projections along the C–C bonds are illustrated in Fig. 4. All the dihedral angles N–C–C–N are in the range 43–45° and are much smaller than that in a typical *gauche* structure. The bond distances and angles in the hexacyanocobaltate(III) anion are listed in Table 5. They may be compared with those observed in $(-)_{589}\text{-}[\text{Co}(\text{penten})][\text{Co}(\text{CN})_6]\cdot 2\text{H}_2\text{O}$ (Muto, Marumo & Saito, 1970). The closest approach between complex cations and anions occurs between the terminal nitrogen atom of the cation and the nitrogen atom of the anion: N(3)···N(12) and N(4)···N(9) are 2.918 and 3.086 Å respectively. The positions of hydrogen atoms attached to N(3) and N(4) suggest that N(3)···N(12) and N(4)···N(9) are hydrogen bonds. The water molecules are surrounded by two nitrogen atoms of the anion and a terminal nitrogen atom of the cation as indicated by broken lines in Fig. 2. These N···O distances are mostly less than 3 Å. Other interatomic distances less than 3.5 Å between complexes are listed in Table 6.

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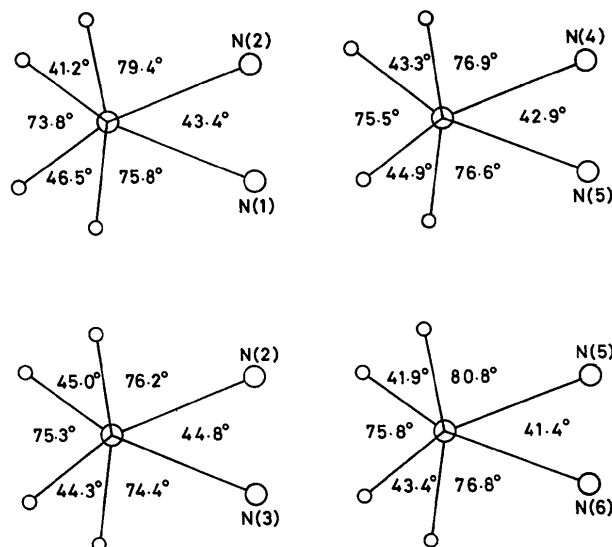


Fig. 4. Newman projections along the C–C bonds in the chelate ring.

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The Crystal Structure of CsMnCl_3

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The crystal structure of CsMnCl_3 , determined from Weissenberg data, is trigonal, space group $R3m$. The hexagonal cell contains 9 molecules and has dimensions $a = 7.29$ (1) and $c = 27.48$ (5) Å. The c parameter accommodates 9 close-packed layers of composition CsCl_3 and the Mn ions are octahedrally coordinated by Cl ions. The structure is closely related to that of CsNiCl_3 .

Introduction

Many complex halides of composition CsMCl_3 , where M represents a metal ion in the first transition series, have the same structure as CsNiCl_3 (Tishchenko, 1955), which consists of hexagonally close-packed CsCl_3 layers with Ni octahedrally coordinated by Cl ions

such that the Ni–Cl octahedra share opposite faces to form infinite chains of composition $(\text{NiCl}_3)_n^{n-}$ parallel to c , the space group being $P6_3/mmc$ with $a \approx 7.2$ Å, $c/a \approx 0.82$ and $Z = 2$. Recent work (Goodyear & Kennedy, 1972) has shown that CsMnBr_3 also has this structure.

An investigation of the unit cell of CsMnCl_3 by Kes-

tigian, Croft & Leipziger (1967) using a powder diffractometer technique indicated a hexagonal cell with $a = 7.288$ and $c = 27.44$ Å, and an observed density of 3.48 g cm⁻³ required 9 molecules per unit cell. The a parameter of this cell is very similar to that of CsNiCl₃ and suggests that this structure also contains CsCl₃ close-packed layers; but the axial ratio, which is approximately $4\frac{1}{2}$ times that of the CsNiCl₃ cell, would require a different stacking sequence of such layers.

In the present work, a Weissenberg study of CsMnCl₃ has confirmed the unit-cell data found by Kestigian, Croft & Leipziger and a consideration of a suitable stacking arrangement of CsCl₃ layers to explain the large c parameter has enabled the crystal structure to be determined.

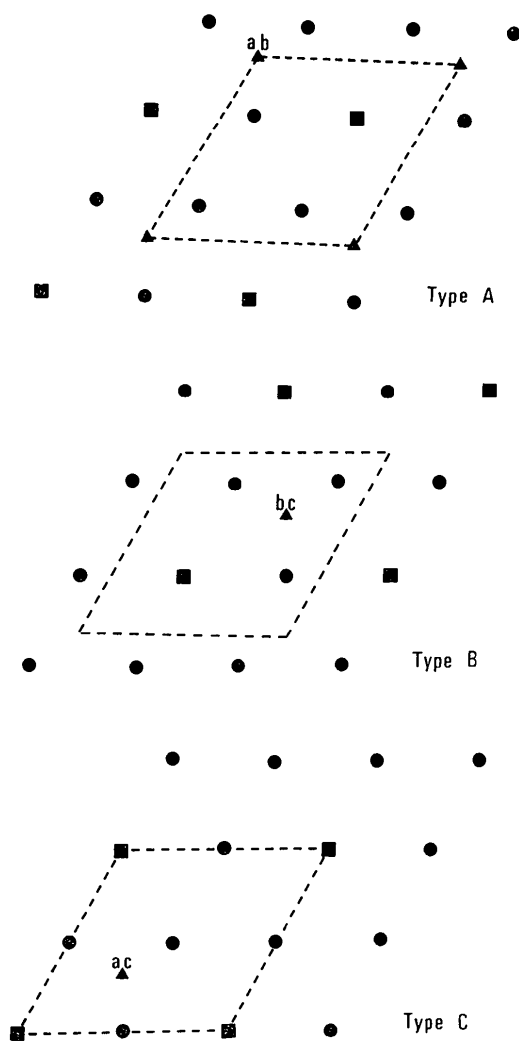


Fig. 1. Close-packed CsCl₃ layers classified according to the position of the unit cell (broken line). The circles and squares represent Cl and Cs atoms respectively. The triangles show possible sites for Mn atoms between different pairs of layers; ab , bc and ac are sites between types A and B , B and C , A and C respectively.

Experimental

Single crystals of CsMnCl₃ were prepared by heating an equimolar mixture of MnCl₂ and CsCl in a sealed evacuated silica tube to a temperature above the melting point and then cooling the specimen to room temperature at a rate of about 5°C per hour. Because of the extremely hygroscopic nature of the material, single crystals suitable for X-ray examination were selected and examined in a stream of dry nitrogen and were then mounted in Lindemann-glass capillary tubes containing P₂O₅.

The unit-cell dimensions were determined from Cu $K\alpha$ Weissenberg photographs, taken about the a axis, using the method of Main & Woolfson (1963). The density was determined by weighing a sample of the material quickly in air and in toluene, and agreement between the observed and calculated densities was obtained by assigning 9 molecules of CsMnCl₃ per unit cell. The complete crystal data are shown in Table 1.

Table 1. Crystal data

Formula, CsMnCl ₃	F.W. 294.20
Hexagonal cell	$a = 7.29$ (1), $c = 27.48$ (5) Å
	$Z = 9$, $D_o = 3.48$, $D_x = 3.48$ g cm ⁻³
Mean r (cm)	0.0037
μ (cm ⁻¹)	102 ($\lambda = 0.7107$ Å)

Intensity data were collected from equi-inclination Weissenberg photographs taken about the a axis with Mo $K\alpha$ radiation. The intensities of 687 reflexions from layer lines 0 to 6 were measured from multiple film exposures using a Joyce-Loebl flying-spot microdensitometer, although the intensities of a few very weak reflexions had to be estimated visually against a calibrated scale; 251 reflexions were unobserved. These data were corrected for the Lorentz-polarization factor and for absorption using the factors given by Bond (1959) for a cylindrical specimen.

The observed reflexions all satisfied the condition $-h + k + l = 3n$, pointing to a rhombohedral primitive cell and $R\bar{3}m$, $R3m$, $R32$, $R\bar{3}$ and $R3$ as possible space groups.

Determination and description of the structure

The initial structure was determined by considering a stacking arrangement of CsCl₃ layers which would explain a c parameter of the order of 27 Å. In the CsNiCl₃ structure, the c parameter accommodates two close-packed layers, indicating a layer separation of about 3 Å and thus suggesting 9 layers in the unit cell of CsMnCl₃. This is also consistent with the assignment of 9 molecules per cell.

Since each Cs atom must be in contact with 12 Cl atoms, there are three possible positions of a layer in relation to the outline of the unit cell; these correspond

to the types *A*, *B* and *C* of Fig. 1. The stacking sequence for a 9 layer structure would then be

BABACACBC ..., or *(chh)*₃ in the usual nomenclature. In the CsNiCl₃ structure the layers are hexagonally close-packed, *i.e.* *BABA* ...

In a close-packed array of CsCl₃ layers only one quarter of the octahedral sites are bounded exclusively by Cl atoms and each of these must be occupied by a Mn atom in order to obtain the correct compositional formula. The triangular motifs in Fig. 1 indicate these sites in the unit cell between different pairs of layers; for example that labelled *ab* is such a site between *A* and *B*-type layers.

The idealized structure based on this reasoning is shown in Fig. 2, which is drawn in three parts to show the relation between the proposed structure and that of CsNiCl₃. The section between $z = -\frac{1}{6}$ and $z = \frac{1}{6}$ consists of a slice of CsNiCl₃-type structure $1\frac{1}{2}$ unit cells high. The next section, between $z = \frac{1}{6}$ and $z = \frac{1}{2}$, is a similar slice which is displaced $-a/3$ parallel to *X* and $a/3$ parallel to *Y*, whilst the section between $z = \frac{1}{2}$ and $z = \frac{5}{6}$ represents a third similar slice displaced $a/3$ parallel to *X* and $-a/3$ parallel to *Y* relative to the first slice.

The idealized positional parameters are consistent with the most symmetrical of the possible space groups, $R\bar{3}m$, and initially the model was tested by means of a block-diagonal three-dimensional least-squares refinement in this space group using individual isotropic temperature factors with Cs at equipoints 6(*c*) and 3(*b*), Mn at 6(*c*) and 3(*a*) and Cl at 18(*h*) and 9(*d*). In these calculations the atomic scattering factors given in *International Tables for X-ray Crystallography* (1962) for Cs⁺, Mn²⁺ and Cl⁻ were used and interlayer scaling was achieved by scaling the observed to the calculated structure factors. With the idealized positional coordinates and temperature factors similar to those found for the

Table 2. Refined temperature factors in the space group $R\bar{3}m$

	Equipoint	Coordinates	<i>B</i> (Å ²)
Mn(1)	3(<i>a</i>)	0,0,0	2.99
Mn(2)	6(<i>c</i>)	0,0, <i>z</i>	0.38
Cs(1)	3(<i>b</i>)	0,0, $\frac{1}{2}$	4.18
Cs(2)	6(<i>c</i>)	0,0, <i>z</i>	1.04
Cl(1)	9(<i>d</i>)	$\frac{1}{2}$,0, $\frac{1}{2}$	3.43
Cl(2)	18(<i>h</i>)	<i>x</i> ,2 <i>x</i> , <i>z</i>	0.62

CsMnBr₃ structure, the initial *R* value, $\frac{\sum |F_o| - |F_c|}{\sum |F_o|}$, was as low as 20%. After about 10 cycles of refinement *R* decreased to 11.6%, at which stage

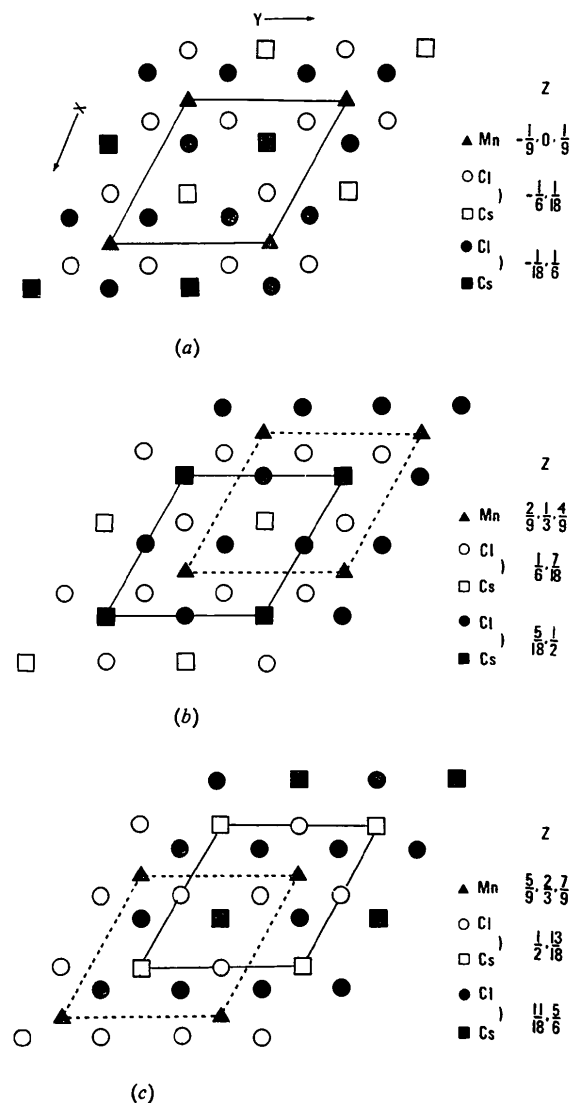


Fig. 2. Projection along the *c* axis of the idealized structure of CsMnCl₃, showing its relation to the CsNiCl₃ structure. The full line represents the base of the cell and the broken line indicates the base of a subcell of CsNiCl₃-type structure; in (a) the unit cell and subcell coincide.

Table 3. Final atomic parameters

Standard deviations are given in parentheses.

	Equipoint	<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	<i>B</i> (Å ²)
Mn(1)	3(<i>a</i>)	0	0	-0.0002 (7)	1.17 (8)
Mn(2)	3(<i>a</i>)	0	0	0.1160 (3)	1.34 (12)
Mn(3)	3(<i>a</i>)	0	0	-0.1159 (3)	0.89 (9)
Cs(1)	3(<i>a</i>)	0	0	0.2817 (1)	2.09 (5)
Cs(2)	3(<i>a</i>)	0	0	-0.2816 (1)	2.04 (5)
Cs(3)	3(<i>a</i>)	0	0	0.4968 (2)	1.86 (4)
Cl(1)	9(<i>b</i>)	0.1608 (6)	0.3216 (6)	0.0571 (3)	1.34 (9)
Cl(2)	9(<i>b</i>)	-0.1558 (5)	-0.3116 (5)	-0.0573 (2)	0.97 (8)
Cl(3)	9(<i>b</i>)	-0.1606 (9)	-0.3212 (9)	0.1675 (5)	1.38 (7)

the shifts in the positional parameters were all less than $\frac{1}{10}$ of the estimated standard deviations. However, the refined temperature factors were not too satisfactory, since for each type of atom the temperature factor of an atom in a fixed position differed greatly from that of an atom in a position for which z could vary, as can be seen in Table 2.

Table 4. Magnitudes of observed and calculated structure factors

hkl	F _o	F _c	hkl	F _o	F _c	hkl	F _o	F _c	hkl	F _o	F _c	hkl	F _o	F _c
0 0 0	0	0	0 0 0	0	0	0 0 0	0	0	0 0 0	0	0	0 0 0	0	0
0 0 1	193	193	0 0 1	193	193	0 0 1	193	193	0 0 1	193	193	0 0 1	193	193
0 0 2	386	386	0 0 2	386	386	0 0 2	386	386	0 0 2	386	386	0 0 2	386	386
0 0 3	579	579	0 0 3	579	579	0 0 3	579	579	0 0 3	579	579	0 0 3	579	579
0 0 4	772	772	0 0 4	772	772	0 0 4	772	772	0 0 4	772	772	0 0 4	772	772
0 0 5	965	965	0 0 5	965	965	0 0 5	965	965	0 0 5	965	965	0 0 5	965	965
0 0 6	1158	1158	0 0 6	1158	1158	0 0 6	1158	1158	0 0 6	1158	1158	0 0 6	1158	1158
0 0 7	1351	1351	0 0 7	1351	1351	0 0 7	1351	1351	0 0 7	1351	1351	0 0 7	1351	1351
0 0 8	1544	1544	0 0 8	1544	1544	0 0 8	1544	1544	0 0 8	1544	1544	0 0 8	1544	1544
0 0 9	1737	1737	0 0 9	1737	1737	0 0 9	1737	1737	0 0 9	1737	1737	0 0 9	1737	1737
0 0 10	1930	1930	0 0 10	1930	1930	0 0 10	1930	1930	0 0 10	1930	1930	0 0 10	1930	1930
0 0 11	2123	2123	0 0 11	2123	2123	0 0 11	2123	2123	0 0 11	2123	2123	0 0 11	2123	2123
0 0 12	2316	2316	0 0 12	2316	2316	0 0 12	2316	2316	0 0 12	2316	2316	0 0 12	2316	2316
0 0 13	2509	2509	0 0 13	2509	2509	0 0 13	2509	2509	0 0 13	2509	2509	0 0 13	2509	2509
0 0 14	2702	2702	0 0 14	2702	2702	0 0 14	2702	2702	0 0 14	2702	2702	0 0 14	2702	2702
0 0 15	2895	2895	0 0 15	2895	2895	0 0 15	2895	2895	0 0 15	2895	2895	0 0 15	2895	2895
0 0 16	3088	3088	0 0 16	3088	3088	0 0 16	3088	3088	0 0 16	3088	3088	0 0 16	3088	3088
0 0 17	3281	3281	0 0 17	3281	3281	0 0 17	3281	3281	0 0 17	3281	3281	0 0 17	3281	3281
0 0 18	3474	3474	0 0 18	3474	3474	0 0 18	3474	3474	0 0 18	3474	3474	0 0 18	3474	3474
0 0 19	3667	3667	0 0 19	3667	3667	0 0 19	3667	3667	0 0 19	3667	3667	0 0 19	3667	3667
0 0 20	3860	3860	0 0 20	3860	3860	0 0 20	3860	3860	0 0 20	3860	3860	0 0 20	3860	3860
0 0 21	4053	4053	0 0 21	4053	4053	0 0 21	4053	4053	0 0 21	4053	4053	0 0 21	4053	4053
0 0 22	4246	4246	0 0 22	4246	4246	0 0 22	4246	4246	0 0 22	4246	4246	0 0 22	4246	4246
0 0 23	4439	4439	0 0 23	4439	4439	0 0 23	4439	4439	0 0 23	4439	4439	0 0 23	4439	4439
0 0 24	4632	4632	0 0 24	4632	4632	0 0 24	4632	4632	0 0 24	4632	4632	0 0 24	4632	4632
0 0 25	4825	4825	0 0 25	4825	4825	0 0 25	4825	4825	0 0 25	4825	4825	0 0 25	4825	4825
0 0 26	5018	5018	0 0 26	5018	5018	0 0 26	5018	5018	0 0 26	5018	5018	0 0 26	5018	5018
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0 0 29	5597	5597	0 0 29	5597	5597	0 0 29	5597	5597	0 0 29	5597	5597	0 0 29	5597	5597
0 0 30	5790	5790	0 0 30	5790	5790	0 0 30	5790	5790	0 0 30	5790	5790	0 0 30	5790	5790
0 0 31	5983	5983	0 0 31	5983	5983	0 0 31	5983	5983	0 0 31	5983	5983	0 0 31	5983	5983
0 0 32	6176	6176	0 0 32	6176	6176	0 0 32	6176	6176	0 0 32	6176	6176	0 0 32	6176	6176
0 0 33	6369	6369	0 0 33	6369	6369	0 0 33	6369	6369	0 0 33	6369	6369	0 0 33	6369	6369
0 0 34	6562	6562	0 0 34	6562	6562	0 0 34	6562	6562	0 0 34	6562	6562	0 0 34	6562	6562
0 0 35	6755	6755	0 0 35	6755	6755	0 0 35	6755	6755	0 0 35	6755	6755	0 0 35	6755	6755
0 0 36	6948	6948	0 0 36	6948	6948	0 0 36	6948	6948	0 0 36	6948	6948	0 0 36	6948	6948
0 0 37	7141	7141	0 0 37	7141	7141	0 0 37	7141	7141	0 0 37	7141	7141	0 0 37	7141	7141
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0 0 39	7527	7527	0 0 39	7527	7527	0 0 39	7527	7527	0 0 39	7527	7527	0 0 39	7527	7527
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0 0 41	7913	7913	0 0 41	7913	7913	0 0 41	7913	7913	0 0 41	7913	7913	0 0 41	7913	7913
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0 0 44	8492	8492	0 0 44	8492	8492	0 0 44	8492	8492	0 0 44	8492	8492	0 0 44	8492	8492
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0 0 46	8878	8878	0 0 46	8878	8878	0 0 46	8878	8878	0 0 46	8878	8878	0 0 46	8878	8878
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0 0 58	11194	11194	0 0 58	11194	11194	0 0 58	11194	11194	0 0 58	11194	11194	0 0 58	11194	11194
0 0 59	11387	11387	0 0 59	11387	11387	0 0 59	11387	11387	0 0 59	11387	11387	0 0 59	11387	11387
0 0 60	11580	11580	0 0 60	11580	11580	0 0 60	11580	11580	0 0 60	11580	11580	0 0 60	11580	11580
0 0 61	11773	11773	0 0 61	11773	11773	0 0 61	11773	11773	0 0 61	11773	11773	0 0 61	11773	11773
0 0 62	11966	11966	0 0 62	11966	11966	0 0 62	11966	11966	0 0 62	11966	11966	0 0 62	11966	11966
0 0 63	12159	12159	0 0 63	12159	12159	0 0 63	12159	12159	0 0 63	12159	12159	0 0 63	12159	12159
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0 0 66	12738	12738	0 0 66	12738	12738	0 0 66	12738	12738	0 0 66	12738	12738	0 0 66	12738	12738
0 0 67	12931	12931	0 0 67	12931	12931	0 0 67	12931	12931	0 0 67	12931	12931	0 0 67	12931	12931
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0 0 72	13896	13896	0 0 72	13896	13896	0 0 72	13896	13896	0 0 72	13896	13896	0 0 72	13896	13896
0 0 73	14089	14089	0 0 73	14089	14089	0 0 73	14089	14089	0 0 73	14089	14089	0 0 73	14089	14089
0 0 74	14282	14282	0 0 74	14282	14282	0 0 74	14282	14282	0 0 74	14282	14282	0 0 74	14282	14282
0 0 75	14475	14475	0 0 75	14475	14475	0 0 75	14475	14475	0 0 75	14475	14475	0 0 75	14475	14475
0 0 76	14668	14668	0 0 76	14668	14668	0 0 76	14668	14668	0 0 76	14668	14668	0 0 76	14668	14668
0 0 77	14861	14861	0 0 77	14861	14861	0 0 77	14861	14861	0 0 77	14861	14861	0 0 77	14861	14861
0 0 78	15054	15054	0 0 78	15054	15054									

Table 5. *Bond lengths and angles*

Standard deviations, attributable to e.s.d.'s in the positional and cell parameters, are given in parentheses.

		Multiplicity			
Mn(1)-Cl octahedron					
Mn—Cl(1 ⁱ)	3	2.570 (14) Å	Cl(1 ⁱ)-Mn-Cl(1 ⁱ)	86.3 (4)°	
Mn—Cl(2 ⁱ)	3	2.516 (13)	Cl(2 ⁱ)-Mn-Cl(2 ⁱ)	85.3 (4)	
Cl(1 ⁱ)-Cl(1 ⁱ)	3	3.517 (14)	Cl(1 ⁱ)-Mn-Cl(2 ⁱ)	94.2 (4)	
Cl(2 ⁱ)-Cl(2 ⁱ)	3	3.408 (12)			
Cl(1 ⁱ)-Cl(2 ⁱ)	6	3.726 (11)			
Mn(2)-Cl octahedron					
Mn—Cl(1 ⁱ)	3	2.596 (10)	Cl(1 ⁱ)-Mn-Cl(1 ⁱ)	85.3 (2)	
Mn—Cl(3 ⁱ)	3	2.472 (13)	Cl(3 ⁱ)-Mn-Cl(3 ⁱ)	90.5 (4)	
Cl(1 ⁱ)-Cl(1 ⁱ)	3	3.517 (14)	Cl(1 ⁱ)-Mn-Cl(3 ⁱ)	92.1 (3)	
Cl(3 ⁱ)-Cl(3 ⁱ)	3	3.512 (20)			
Cl(1 ⁱ)-Cl(3 ⁱ)	6	3.649 (16)			
Mn(3)-Cl octahedron					
Mn—Cl(2 ⁱ)	3	2.543 (8)	Cl(2 ⁱ)-Mn-Cl(2 ⁱ)	84.2 (2)	
Mn—Cl(3 ⁱⁱ)	3	2.577 (13)	Cl(3 ⁱⁱ)-Mn-Cl(3 ⁱⁱ)	94.3 (4)	
Cl(2 ⁱ)-Cl(2 ⁱ)	3	3.408 (12)	Cl(2 ⁱ)-Mn-Cl(3 ⁱⁱ)	90.6 (3)	
Cl(3 ⁱⁱ)-Cl(3 ⁱⁱ)	3	3.778 (20)			
Cl(2 ⁱ)-Cl(3 ⁱⁱ)	6	3.639 (15)			
Cs(1)-Cl distances					
Cs-Cl(1 ⁱ)	3	3.699 (9)			
Cs-Cl(2 ⁱ)	6	3.651 (5)			
Cs-Cl(3 ⁱⁱ)	3	3.736 (14)			
Cs(2)-Cl distances					
Cs-Cl(1 ⁱ)	6	3.649 (5)			
Cs-Cl(2 ⁱ)	3	3.741 (8)			
Cs-Cl(3 ⁱ)	3	3.857 (14)			
Cs(3)-Cl distances					
Cs-Cl(1 ⁱ)	3	3.645 (10)			
Cs-Cl(2 ⁱⁱ)	3	3.820 (9)			
Cs-Cl(3 ⁱ)	6	3.648 (5)			

Location of atoms [see Fig. 2(a) and (b)]:

Mn(1) at (0, 0, 0); Mn(2) at (0, 0, $\frac{1}{2}$); Mn(3) at (0, 0, $-\frac{1}{2}$).Cs(1) at ($\frac{1}{2}$, $\frac{1}{2}$, $-\frac{1}{8}$); Cs(2) at ($\frac{2}{3}$, $\frac{1}{3}$, $\frac{1}{8}$); Cs(3) at ($\frac{1}{3}$, $\frac{2}{3}$, $\frac{1}{8}$).Cl(1ⁱ) at $z = \frac{1}{8}$; Cl(2ⁱ) at $z = -\frac{1}{8}$; Cl(2ⁱⁱ) at $z = \frac{5}{8}$; Cl(3ⁱ) at $z = \frac{1}{6}$; Cl(3ⁱⁱ) at $z = -\frac{1}{6}$.

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