

long and short O—O distances of the LiO_6 octahedra and $r(\text{O}^{2-})$ is the ionic radius of the O^{2-} ion. For $r(\text{O}^{2-}) = 1.36 \text{ \AA}$, $R = 0.38 (1) \text{ \AA}$; for $r(\text{O}^{2-}) = 1.31 \text{ \AA}$, $R = 0.43 (1) \text{ \AA}$. The bottleneck radius is therefore quite small, although in four coordination the Li^+ ionic radius has dropped to 0.59 \AA . The structural data suggest that fast Li^+ -ion transport may be found even when the bottleneck to motion appears too small. The almost perfect cation ordering facilitates such motion because the presence of highly charged Co^{III} atoms in the lithium layer would impede the motion in a manner similar to that of interlayer Ti atoms in the CdI_2 structure of $\text{Ti}_{1+x}\text{S}_2$ (Whittingham & Gamble, 1975).

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References

- BACON, G. E. (1975). *Neutron Diffraction*, 3rd ed., pp. 39–41. Oxford Univ. Press.
 HEWAT, A. W. (1979). *Acta Cryst.* A35, 248.
 JOHNSTON, W. D., HEIKES, R. R. & SESTRICH, D. (1958). *J. Phys. Chem. Solids*, 7, 1–13.
 MIZUSHIMA, K., GOODENOUGH, J. B. & WISEMAN, P. J. (1980). US Patent No. 06/135222.
 MIZUSHIMA, K., JONES, P. C., WISEMAN, P. J. & GOODENOUGH, J. B. (1980). *Mater. Res. Bull.* 15, 783–789.
 RIETVELD, H. M. (1969). *J. Appl. Cryst.* 2, 65–71.
 SHANNON, R. D. (1976). *Acta Cryst.* A32, 751–767.
 THOMAS, M. G. S. R. & WISEMAN, P. J. (1984). In preparation.
 WHITTINGHAM, M. S. & GAMBLE, R. R. (1975). *Mater. Res. Bull.* 10, 363–371.

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Dicesium Magnesium Bis(chromate) Hexahydrate, $\text{Cs}_2\text{Mg}(\text{CrO}_4)_2 \cdot 6\text{H}_2\text{O}^*$

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Abstract. $M_r = 630.2$, monoclinic, $P2_1/a$, $a = 9.621 (5)$, $b = 12.968 (5)$, $c = 6.375 (3) \text{ \AA}$, $\beta = 106.17 (4)^\circ$, $V = 763.9 (5) \text{ \AA}^3$, $Z = 2$, $D_m(\text{floatation}) = 2.70$, $D_x = 2.740 \text{ Mg m}^{-3}$, $F(000) = 588$, $\lambda(\text{Mo K}\alpha) = 0.71069 \text{ \AA}$, $\mu = 6.35 \text{ mm}^{-1}$, $T = 295 \text{ K}$. The structure which is isomorphous with the corresponding diammonium nickel chromate has been determined by refinement of diffractometer data to a final R value of 0.069 for 1340 observed reflexions. The metal–water distances are 2.098 (3), 2.093 (3) and 2.057 (3) \AA .

Introduction. In the continuing study of the variations of hexaaqua ions of the first transition group of elements (Montgomery, 1980), the structure of the title compound has been determined.

Experimental. Crystal $0.26 \times 0.19 \times 0.40 \text{ mm}$ from aqueous solution at room temperature, mounted along c , PDP-11-controlled Picker four-circle diffractometer, Zr-filtered $\text{MoK}\alpha$ radiation; accurate cell dimensions by least-squares fitting of eight pairs of reflexions, $2\theta = 24$ to 41° ; intensity measurements in the $\theta/2\theta$ scan mode, 60 steps of 0.04° in 2θ , counting 1 s/step and for 30s at

each end of the scan; three standard reflexions recorded for every 50 observed reflexions; $2\theta \leq 45^\circ$, $h = -11$ to 10, $k = 0$ to 15, $l = 0$ to 7, 1475 nonequivalent reflexions measured, 1340 observed at $3\sigma(I)$ level, corrected for Lorentz and polarization effects and for absorption by the method of Coppens, Leiserowitz & Rabinovich (1965). Initial atomic parameters taken from diammonium nickel chromate (Montgomery, 1979), least squares on $\sum w(|F_o| - |F_c|)^2$, $w = (A + B|F_o| + C|F_o|^2 + D|F_o|^3)^{-1}$, $A = 4.9272$, $B = 2.65394$, $C = -0.08266$, $D = 0.00183$; computer programs of Penfold (1969); scattering factors from *International Tables for X-ray Crystallography* (1974) and those for H from Stewart, Davidson & Simpson (1965), anomalous dispersion (real and imaginary) included for Cs, Mg and Cr; final pair of cycles run varying only the H-atom positions and individual isotropic temperature factors ($B = 5.0 \text{ \AA}^2$ initially); † final $R = 0.069$, $R_w = 0.086$; $(\Delta/\sigma)_{\text{max}} = 0.2$; difference-map excursions $< 0.3 \text{ e \AA}^{-3}$; no correction for secondary extinction.

† Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38842 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

* Tutton's Salts. XII.

Discussion. The atom numbering in the complex is shown in Fig. 1. The structure closely follows that of isostructural sulfates, chromates, selenates and tetrafluoroberyllates [Tables 1, 2, 3; Montgomery (1980, and references therein)]. The Mg–water distances are 2.098 (3), 2.093 (3) and 2.057 (3) Å and the average is very close (within 0.7%) to that recorded (Margulis & Templeton, 1962) for diammonium magnesium sulfate hexahydrate. Apparently the differences between the size of the Cs⁺ (1.70 Å) and the NH₄⁺ ion (1.42 Å) and between the chromate group (Cr–O = 1.65 Å) and the sulfate group (S–O = 1.48 Å) make no difference in the metal coordination sphere. The Cr–O distances in the chromate ion are regular (mean 1.650 Å), as in Cs₂CrO₄ (Morris, Kennard, Moore, Smith & Montgomery, 1981).

The hydrogen bonding also differs only slightly (1% on average) from the corresponding ammonium sulfate. Differences in individual interatomic distances seem to be more a function of the absence of the ammonium ion. In diammonium nickel chromate (Montgomery, 1979), for example, the hydrogen bonding very closely follows that of the diammonium magnesium sulfate (Table 3; 0.3% difference on average).

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Table 1. Fractional coordinates ($\times 10^4$, $\times 10^3$ for H) and isotropic temperature factors

$$B_{eq} = \frac{4}{3} \sum_i \sum_j \beta_{ij} a_i a_j$$

	x	y	z	$B_{eq}/B(\text{Å}^2)$
Mg	0	0	0	1.5
Cr	3928 (1)	1461 (1)	7416 (2)	1.4
Cs	1212 (0.5)	3543 (0.5)	3462 (1)	2.5
O(3)	4111 (6)	2438 (4)	5863 (8)	2.7
O(4)	5448 (5)	796 (4)	8080 (9)	2.9
O(5)	2617 (5)	709 (4)	5982 (8)	2.3
O(6)	3549 (6)	1885 (4)	9640 (7)	2.4
O(7)	1533 (5)	1093 (4)	1620 (8)	2.4
O(8)	–1655 (5)	1030 (4)	102 (9)	2.6
O(9)	–69 (5)	–623 (4)	2936 (8)	2.1
H(15) O(7)	172 (16)	87 (10)	256 (22)	3.6 (2)
H(16) O(7)	230 (16)	132 (8)	86 (23)	3.1 (2)
H(17) O(8)	–249 (10)	108 (7)	–72 (15)	3.1 (2)
H(18) O(8)	–144 (31)	152 (14)	–101 (46)	13.0 (3)
H(19) O(9)	–75 (10)	–60 (6)	311 (14)	4.1 (2)
H(20) O(9)	18 (7)	–119 (5)	362 (10)	3.2 (2)

Table 2. Bond lengths (Å) and angles (°)

Cr–O(3)	1.647 (3)	O(3)–Cr–O(4)	108.7 (2)
Cr–O(4)	1.649 (3)	O(3)–Cr–O(5)	108.3 (2)
Cr–O(5)	1.653 (3)	O(3)–Cr–O(6)	110.2 (2)
Cr–O(6)	1.653 (3)	O(4)–Cr–O(5)	108.6 (2)
		O(4)–Cr–O(6)	110.2 (2)
		O(5)–Cr–O(6)	110.7 (2)
O(7)–Mg–O(8)	89.4 (1)		
O(7)–Mg–O(9)	90.8 (1)		
O(8)–Mg–O(9)	90.3 (1)		

Table 3. Interatomic distances (Å) in two double salts of magnesium and in diammonium nickel chromate

	Cesium chromate	Ammonium sulfate	Diammonium nickel chromate	Relative position of second atom*
Mg–O(7)	2.098 (3)	2.073 (5)		x, y, z
Mg–O(8)	2.093 (3)	2.083 (5)		$x, y, z-1$
Mg–O(9)	2.057 (3)	2.051 (5)		$x-1, y, z-1$
Hydrogen bonding				
O(7)···O(5)	2.730 (5)	2.792	2.787 (5)	x, y, z
O(7)···O(6)	2.788 (5)	2.844	2.827 (5)	$x, y, z-1$
O(8)···O(4)	2.743 (5)	2.722	2.720 (5)	$x-1, y, z-1$
O(8)···O(6)	2.733 (5)	2.756	2.741 (5)	$x-\frac{1}{2}, \frac{1}{2}, y, z-1$
O(9)···O(3)	2.714 (5)	2.713	2.731 (5)	$-x, -y, 1-z$
O(9)···O(5)	2.728 (5)	2.777	2.744 (5)	$\frac{1}{2}-x, y-\frac{1}{2}, 1-z$

* Transformation relating each second atom of cesium magnesium chromate to the corresponding atom in the original asymmetric unit.

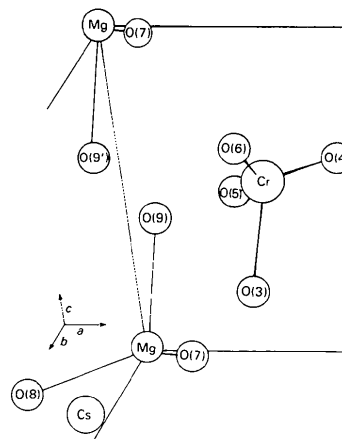


Fig. 1. Part of the unit-cell contents showing the atom numbering.

References

- COPPENS, P., LEISEROWITZ, L. & RABINOVICH, D. (1965). *Acta Cryst.* **18**, 1035–1038.
- International Tables for X-ray Crystallography* (1974). Vol. IV. Birmingham: Kynoch Press.
- MARGULIS, T. N. & TEMPLETON, D. H. (1962). *Z. Kristallogr.* **117**, 344–357.
- MONTGOMERY, H. (1979). *Acta Cryst.* **B35**, 155–156.
- MONTGOMERY, H. (1980). *Acta Cryst.* **B36** 2121–2123.
- MORRIS, A. J., KENNARD, C. H. L., MOORE, F. H., SMITH, G. & MONTGOMERY, H. (1981). *Cryst. Struct. Commun.* **10**, 529–532.
- PENFOLD, B. R. (1969). Crystallographic programs (versions of ORFLS and ORFFE). Univ. of Canterbury, Christchurch, New Zealand.
- STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.