bone packing occurs: the molecule forms an angle of 25·2° with the *a* axis and the molecules related by the *a* glide in the **b** direction form angles of 50·4° with each other. Intermolecular contact distances within the *x*, *y* layers are normal (Table 3). Molecules in adjacent layers are aligned head-to-tail and make contact through pairs of Cl···H(6) interactions of 3·02 Å about the center of symmetry at $(0,0,\frac{1}{2})$. In addition, there is a rather short Cl···Cl interaction of 3·44 Å across the center of symmetry at $(\frac{1}{2},0,\frac{1}{2})$. This structure differs fundamentally from those of the centrosymmetric chlorodioxins, 2,7-dichlorodibenzo-*p*-dioxin (Boer & North, 1972), 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (Boer, van Remoortere, North & Neuman, 1972), and octachlorodibenzo-*p*-dioxin (Neuman, North & Boer, 1972), where the molecules are stacked along very short lattice periods of about 3·8 Å.

References

ANILINE, O. (1972). To be published.

BOER, F. P. & NORTH, P. P. (1972). *Acta Cryst.* B**28**, 1613.

BOER, F. P., VAN REMOORTERE, F. P., NORTH, P. P. & NEUMAN, M. A. (1972). *Acta Cryst.* B**28**, 1023.

CANTRELL, J. S., WEBB, N. C. & MABIS, A. J. (1969). *Acta Cryst.* B**25**, 150.

International Tables for X-ray Crystallography (1962). Vol. III, p. 202–16. Birmingham: Kynoch Press.

NEUMAN, M. A., NORTH, P. P. & BOER, F. P. (1972). *Acta Cryst.* B**28**, 2313.

ROWE, V. K., NORRIS, J. M., SPARSCHU, G. L., SCHWETZ, B. H. & GEHRING, P. J. (1971). Symposium on the Origin and Fate of the Chlorodioxins, 162nd National American Chemical Society Meeting, Washington, D. C., Sept. 16–17.

STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175.

Acta Cryst. (1972). B**28**, 2880

Sodium Rubidium Dichromate and Sodium Caesium Dichromate

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Abstract. Sodium rubidium dichromate is monoclinic, space group $P2_1/c$, $a=12{\cdot}947$ (15), $b=11{\cdot}133$ (11), $c=10{\cdot}037$ (18) Å, $\beta=93{\cdot}42$ (8)°, formula $NaRbCr_2O_7$, $Z=8$, $D_x=2{\cdot}98$. Prepared from a melt of a 1:1 mixture of $Na_2Cr_2O_7$ and $Rb_2Cr_2O_7$. The structure contains blocks of composition $(RbCr_2O_7)_4$ which are similar to those found in $Rb_2Cr_2O_7$ structures. The Na atoms all lie between the blocks. Sodium caesium dichromate, $NaCsCr_2O_7$, is isotypic with $a=12{\cdot}98$ (2), $b=11{\cdot}58$ (2), $c=10{\cdot}10$ (2) Å, $\beta=93{\cdot}8$ (2)°.

Introduction. The crystals are hygroscopic and were sealed in quartz capillaries under dry nitrogen.

The crystal size was approximately 0·2 mm across, μ(Mo $K\alpha$) = 10·2 mm^{-1}. Cell constants were determined from the angular settings of 14 low angle reflexions measured with Mo $K\alpha$ radiation (λ = 0·71069 Å) on a Syntex diffractometer. Systematic absences were observed for $h0l$ reflexions with l odd and $0k0$ reflexions with k odd. Intensities measured on the Syntex diffractometer with Mo $K\alpha$ radiation included all in the range $5<2\theta<55°$ and some in the range $55<2\theta<65°$ for the quadrant of reciprocal space with k and $l\geq 0$. In all, 3200 reflexions of a possible 5200 were measured and 1406 of these were within three standard deviations (counting statistics) of zero after correction for absorption (the crystal shape was defined by 12 faces). Lorentz and polarization corrections were then applied. The structure was solved by Patterson methods and refined by least squares to give an unweighted residual ($R_1=\sum(|F_o|-|F_c|)/\sum|F_o|$) of 0·046 and a weighted residual $\{R_2=[\sum w(F_o-F_c)^2/\sum wF_o^2]^{1/2}\}$ of 0·058 where $w=(17{\cdot}710-0{\cdot}3817|F_o|+$

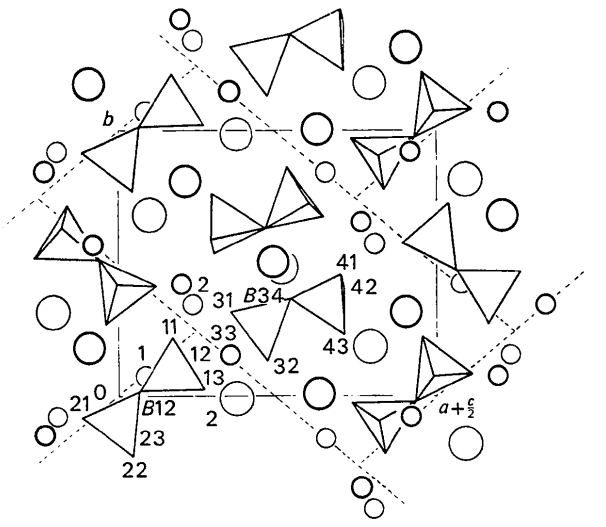

Fig. 1. Projection of $NaRbCr_2O_7$ perpendicular to $(20\bar{1})$. The dichromate groups are shown by linked tetrahedra, the sodium atoms by small circles, the rubidium atoms by large circles. The $(RbCr_2O_7)_4$ units are outlined. The cations all lie above and below the plane of the dichromate ions.

$0{\cdot}0042|F_o|^2)^{-1}$. Further details of the structure determination have been given by Panagiotopoulos (1972). Final atomic coordinates are given in Table 1 and bond lengths and angles are given in Table 2. A list of structure factors is obtainable as Supplementary Publication No. SUP 30010 (6pp.).*

* This table has been deposited with the National Lending Library, England. Copies may be obtained through the Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 1. *Atomic positional and thermal coordinates*

Standard errors in the last figures quoted as given by final round of least-squares analysis are shown in parentheses. The temperature factors were calculated using the expression

$$\exp\left[2\pi 10^{-4}(u_{11}h^2a^{*2}+u_{22}k^2b^{*2}+u_{33}l^2c^{*2}+2u_{12}hka^*b^*+2u_{23}klb^*c^*+2u_{13}hla^*c^*)\right].$$

	x	y	z
Cr(1)	0·1579 (1)	0·1037 (2)	0·3862 (2)
Cr(2)	−0·0032 (1)	−0·0952 (2)	0·2545 (2)
O(11)	0·1294 (8)	0·2195 (9)	0·4705 (10)
O(12)	0·2025 (7)	0·1393 (10)	0·2450 (9)
O(13)	0·2424 (8)	0·0265 (9)	0·4705 (10)
O(21)	−0·1275 (7)	−0·0812 (9)	0·2396 (10)
O(22)	0·0314 (8)	−0·2247 (9)	0·3155 (10)
O(23)	0·0441 (7)	−0·0781 (9)	0·1099 (9)
O(*B*12)	0·0432 (8)	0·0178 (11)	0·3644 (9)
Cr(3)	0·4398 (1)	0·2710 (2)	0·4696 (2)
Cr(4)	0·6642 (1)	0·3644 (2)	0·6089 (2)
O(31)	0·3332 (7)	0·3204 (10)	0·5189 (11)
O(32)	0·4592 (8)	0·1341 (9)	0·5228 (10)
O(33)	0·4354 (8)	0·2717 (11)	0·3069 (9)
O(41)	0·6671 (9)	0·4575 (10)	0·7315 (11)
O(42)	0·7408 (8)	0·4056 (11)	0·4972 (11)
O(43)	0·6960 (8)	0·2321 (9)	0·6596 (12)
O(*B*34)	0·5364 (8)	0·3666 (10)	0·5368 (12)
Na(1)	0·1521 (4)	0·0765 (5)	0·0161 (5)
Na(2)	0·2817 (4)	0·3440 (5)	0·1800 (5)
Rb(1)	0·1483 (1)	0·6833 (1)	0·0862 (1)
Rb(2)	0·4171 (1)	−0·0087 (1)	0·2603 (1)

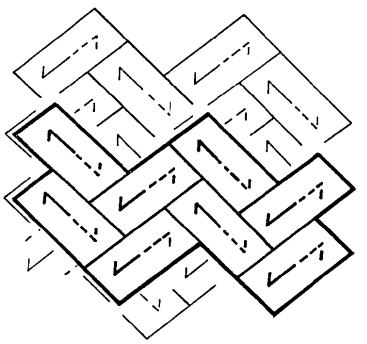

Fig. 2. The packing of $(RbCr_2O_7)_4$ blocks.

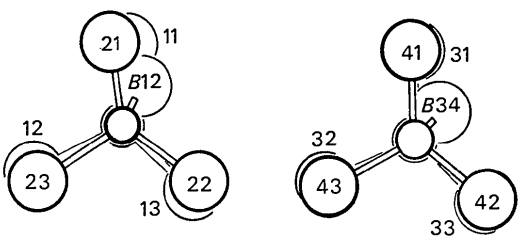

Fig. 3. The conformations of the dichromate groups.

Discussion. This structure determination was undertaken as part of a study of the structure and polymorphism of alkali metal dichromates. The dichromate ions are similar to those found in $Na_2Cr_2O_7$ (Panagiotopoulos & Brown, 1972) and $Rb_2Cr_2O_7$ (Panagiotopoulos & Brown, 1970; Löfgren, 1971; Löfgren & Waltersson, 1971) with Cr–O–Cr angles of 135·9 (6) and 141·4 (6)°.

Table 1 (*cont.*)

	u_{11}	u_{22}	u_{33}	u_{12}	u_{13}	u_{23}
Cr(1)	215 (9)	199 (11)	197 (10)	−34 (9)	10 (7)	−18 (8)
Cr(2)	146 (8)	280 (11)	209 (9)	−15 (9)	−19 (7)	− 9 (9)
O(11)	466 (57)	340 (58)	393 (58)	5 (48)	48 (45)	−133 (49)
O(12)	379 (53)	573 (68)	202 (47)	−102 (51)	29 (40)	72 (49)
O(13)	420 (57)	398 (64)	375 (53)	58 (50)	−49 (43)	244 (50)
O(21)	203 (42)	398 (58)	402 (56)	−73 (44)	17 (37)	2 (50)
O(22)	435 (57)	401 (60)	360 (55)	151 (51)	3 (44)	91 (48)
O(23)	332 (52)	356 (58)	329 (55)	−60 (46)	58 (42)	14 (48)
O(*B*12)	353 (54)	762 (82)	267 (49)	−288 (58)	72 (41)	−223 (56)
Cr(3)	182 (9)	243 (11)	200 (10)	− 1 (9)	−34 (7)	14 (9)
Cr(4)	192 (9)	246 (11)	284 (11)	−36 (9)	−28 (8)	−12 (9)
O(31)	331 (52)	537 (70)	545 (66)	− 7 (50)	135 (48)	67 (59)
O(32)	531 (62)	210 (50)	348 (55)	−122 (49)	−134 (46)	31 (46)
O(33)	567 (65)	628 (76)	186 (46)	86 (59)	−17 (43)	77 (50)
O(41)	686 (73)	334 (61)	456 (63)	−31 (57)	−90 (54)	−185 (54)
O(42)	508 (65)	524 (74)	452 (69)	56 (58)	230 (53)	3 (58)
O(43)	424 (55)	307 (56)	617 (72)	−15 (49)	28 (50)	201 (57)
O(*B*34)	361 (56)	304 (59)	798 (85)	−19 (49)	−321 (55)	56 (60)
Na(1)	345 (27)	264 (29)	291 (27)	18 (24)	−64 (21)	33 (24)
Na(2)	343 (27)	308 (30)	344 (29)	98 (24)	12 (22)	7 (25)
Rb(1)	369 (7)	274 (7)	338 (7)	12 (6)	24 (5)	−36 (6)
Rb(2)	329 (6)	275 (7)	338 (7)	36 (6)	14 (5)	3 (6)

Table 2. *Interatomic distances in* $NaRbCr_2O_7$

	Distance (Å)		Angles (°)		
	Uncorrected	Corrected*	O(12)	O(13)	O(*B*12)
Cr(1)–O(11)	1·597	1·61	112	109	106
O(12)	1·611	1·63		109	112
O(13)	1·593	1·61			109
O(*B*12)	1·769	1·79			
			O(22)	O(23)	O(*B*12)
Cr(2)–O(21)	1·615	1·62	112	110	107
O(22)	1·618	1·64		109	109
O(23)	1·620	1·63			110
O(*B*12)	1·755	1·78			
Cr(1)–O(B12)–Cr(2) = 135·9°					
			O(32)	O(33)	O(*B*34)
Cr(3)–O(31)	1·593	1·61	110	109	106
O(32)	1·630	1·64		109	111
O(33)	1·630	1·65			111
O(B34)	1·746	1·77			
			O(42)	O(43)	O(*B*34)
Cr(4)–O(41)	1·607	1·63	111	111	106
O(42)	1·608	1·63		109	108
O(43)	1·604	1·62			111
O(*B*34)	1·767	1·79			
Cr(3)–O(*B*34)–Cr(4) = 141·4°					

* Corrected for thermal motion assuming O riding on Cr (Busing & Levy, 1964).

Na–O distances less than 3·0 Å

Na(1)–O(11)	2·332	Na(2)–O(21)	2·351
O(42)	2·362	O(33)	2·434
O(23)	2·442	O(41)	2·458
O(12)	2·452	O(31)	2·556
O(21)	2·568	O(13)	2·576
O(31)	2·608	O(12)	2·598
O(23)	2·770	O(32)	2·874
		O(11)	2·884

Rb–O distances less than 3·4 Å

Rb(1)–O(13)	2·908	Rb(2)–O(32)	2·972
O(23)	2·994	O(43)	3·019
O(42)	3·004	O(32)	3·097
O(22)	3·008	O(33)	3·164
O(22)	3·065	O(33)	3·198
O(*B*12)	3·152	O(13)	3·208
O(43)	3·293	O(*B*34)	3·214
O(41)	3·316	O(12)	3·226
O(43)	3·323	O(41)	3·316
O(*B*12)	3·385	O(31)	3·337
		O(42)	3·338
		O(*B*34)	3·377

Standard errors indicated by the least-squares refinement Cr–O = 0·010 Å, Na–O = 0·010 Å, Rb–O = 0·010 Å, O–Cr–O = 1°, Cr–O–Cr = 0·6°.

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References

Busing, W. R. & Levy, H. A. (1964). *Acta Cryst.* **17**, 142.

Löfgren, P. (1971). *Acta Chem. Scand.* **25**, 44.

Löfgren, P. & Waltersson, K. (1971). *Acta Chem. Scand.* **25**, 35.

Panagiotopoulos, N. C. (1972). Ph.D. Thesis, McMaster University, Hamilton, Ontario, Canada. pp. 57–68.

Panagiotopoulos, N. C. & Brown, I. D. (1970). *Canad. J. Chem.* **48**, 537.

Panagiotopoulos, N. C. & Brown, I. D. (1972). *Acta Cryst.* B**28**, 1352.