The Vibrational Spectra of Strontium Chromate ($SrCrO_4$) and Lead Chromate ($PbCrO_4$)

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(Z. Naturforsch. **25 a**, 1856—1862 [1970]; received 21 September 1970)

The Raman spectra of the monoclinic compounds strontium chromate, lead chromate and of the mineral crocoite ($PbCrO_4$) have been recorded at 300 °K and 77 °K. The spectrum of the orthorhombic modification of lead chromate has also been recorded. The spectra of the monoclinic and of the orthorhombic $PbCrO_4$ were found to be indistinguishable, whereas the spectra of the isomorphous monoclinic salts $SrCrO_4$ and $PbCrO_4$ are remarkably different. Inversion doubling was observed in $SrCrO_4$ but less distinctly in monocrystalline crocoite.

I. Introduction

$SrCrO_4$ and $PbCrO_4$ were investigated as a part of a comprehensive study of the Raman effect in inorganic chromates and dichromates. The particular interest in these substances is in an attempt to shed some light on the influence of the crystal field on the vibrational spectra of anions. It is known that monoclinic [1] $SrCrO_4$ and $PbCrO_4$ have almost identical unit cell dimensions. $PbCrO_4$ exists also in an orthorhombic [2] modification. No detailed analysis has thus far been undertaken to study the influence of phase transition and isomorphism of chromates by means of the Raman effect.

II. Experimental

1. Apparatus

Raman spectra were recorded on a photoelectrically recording spectrometer described elsewhere [3, 4]. Wave numbers quoted in this paper are accurate to within $\pm 2\ \mathrm{cm}^{-1}$.

For the low temperature work two types of cryostats were used. The first type was a conventional cryostat as used in IR transmission work adapted for 90° scattering experiments by means of a copper cold finger protruding horizontally from the cryostat. A cylindrical Pyrex tube covers the cold finger. This cryostat was used for $SrCrO_4$ only. The lowest temperature which could be reached with liquid nitrogen as coolant and with the thermocouple embedded in the sample was 110 °K. Since the sample is kept under vacuum and cooled by conduction only, decomposition of $PbCrO_4$ by the focussed laser beam ($\lambda = 6328$ Å, $P = 180$ mW) could not be prevented.

The second type of cryostat simply consists of one Pyrex tube (150 mm × 10 mm i. d.) surrounded by another (100 mm × 20 mm o. d.). The space between the tubes, when properly evacuated, serves as a thermal insulation. The sample is put into the centre of the inner tube. Liquid nitrogen is fed into the inner Pyrex tube. A thermocouple pushed in from the other side is used to monitor the temperature. This double-walled Pyrex cryostat has two advantages. Firstly, liquid nitrogen temperature is easily reached and any temperature between 300 °K and 77 °K can be obtained by controlling the N_2 gas flow. Secondly, the sample is cooled by convection at the actual scattering area, so that any heating effect of the absorbed laser radiation is minimised. In the case of $PbCrO_4$ no decomposition occurs at 77 °K and 160 mW of focussed laser power (power density approximately 10^4 W/cm^2).

2. Sample Preparation

Strontium chromate was prepared by precipitation from aqueous solutions of Merck extra pure potassium chromate and Analar reagent strontium chloride, and dried at 200 °C. The X-ray powder pattern of this material was taken and found to be consistent with the one given by PISTORIUS [1].

Monoclinic lead chromate was prepared by precipitation from aqueous solutions of Merck extra pure potassium chromate and Merck extra pure lead acetate, and dried at 200 °C. The X-ray powder pattern of this compound also was found to be consistent with the one given by PISTORIUS [1].

Lead chromate in its orthorhombic modification was prepared by precipitation from aqueous solutions of

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[1] C. W. F. T. PISTORIUS and M. C. PISTORIUS, Z. Krist. **117,** 4 [1962].

[2] G. COLLOTTI, L. CONTI, and M. ZOCCHI, Acta Cryst. **12,** 416 [1959].

[3] W. SCHEUERMANN and G. J. RITTER, Z. Naturforsch. **24 a,** 408 [1969].

[4] W. SCHEUERMANN and G. J. RITTER, J. Mol. Structure **6,** 240 [1970].

Merck extra pure potassium chromate and Merck extra pure lead nitrate and dried at 25 °C in vacuum. The X-ray powder pattern was found to be consistent with the one given by COLLOTTI, CONTI, and ZOCCHI[2].

The samples of crocoite of approx. 1 × 1 × 4 mm^3 were of Tasmanian origin.

III. Crystal Structure of $SrCrO_4$ and $PbCrO_4$

Space groups and unit cells of $SrCrO_4$ and the two modifications of $PbCrO_4$ are given in Table 1. The structure of $SrCrO_4$ has not been determined yet although BRAGG and CLARINGBULL[5] predicted $SrCrO_4$ to fall in the barite group which is orthorhombic with space group $\text{Pnma} - D_{2h}^{16}$, $Z = 4$. The structure of the mineral crocoite ($PbCrO_4$) has been established[6, 7].

BRODY[6] could, for crocoite, only determine the positions of the lead and chromium atoms while Quareni and De Pieri managed to determine the positions of the oxygen atoms and later presented refined data[7]. The structure is as follows. The chromium atom is surrounded by an approximate tetrahedron of oxygen atoms at an average distance of 1.65 Å with bond angles varying from 105.7° to 113.1°. The lead atom is surrounded by seven CrO_4 tetrahedra, with Pb – Cr distances in the range 3.32 Å to 4.15 Å. The lead atom is also surrounded by ten oxygen atoms with Pb – O distances ranging from 2.53 to 3.44 Å; all the other Pb – O distances are greater than 4.03 Å.

The structure of orthorhombic lead chromate $PbCrO_4$ has also been worked out[2].

The positions of the atoms were calculated by means of a method based on trial and error. This was done under the assumption of regular CrO_4 tetrahedra. It will be shown in this work that the tetrahedra in $SrCrO_4$ and both modifications of $PbCrO_4$ are in fact distorted.

The structure of synthetic monoclinic $PbCrO_4$ remains to be determined.

IV. Results and Discussion

1. Strontium Chromate

The Raman spectra of strontium chromate at 300 °K and 110 °K were obtained by focussing the laser beam on the powder pellet at an angle of approximately 45° and observing the scattered light perpendicular to the incident beam. Results are listed in Table 2 together with the Raman data of GRIFFITH[8]. The infrared data are taken from AFREMOW and VANDEBERG[9]. The low temperature Raman spectrum is shown in Fig. 1.

A regular CrO_4 tetrahedron possesses T_d symmetry. The optically active vibrations are $\nu_1: A_1(R)$, $\nu_2: E(R)$, $\nu_3: F_2(R, IR)$, $\nu_4: F_2(R, IR)$. Neglecting the observed splitting in the first instance, it appears that the spectra can only be explained under the assumption of lifted degeneracies due to a distorted tetrahedron since 7 IR bands and 9 Raman bands have been observed. The total number of 9 Raman bands fits perfectly with the allowed number of vibrations for a five-atomic ion. However, 6 of these are split by 5 to 13 cm^{-1} in the Raman and 2 bands are split by 10 and 12 cm^{-1} in the IR. There is a strong indication that the observed splitting is due to inversion doubling of two coupled CrO_4 ions since the splitting of the Raman bands is smaller than that of the corresponding IR bands as demanded by theory[10], viz.,

$$\begin{aligned} &\text{R}(857/866\ \text{cm}^{-1}; \quad \Delta\nu = 9\ \text{cm}^{-1}),\\ &\text{IR}(845/855\ \text{cm}^{-1}; \quad \Delta\nu = 10\ \text{cm}^{-1}),\\ &\text{R}(889/893\ \text{cm}^{-1}; \quad \Delta\nu = 4\ \text{cm}^{-1}),\\ &\text{IR}(875/887\ \text{cm}^{-1}; \quad \Delta\nu = 12\ \text{cm}^{-1}). \end{aligned}$$

Substance	Ref.	System	Space group	*Z*	*a*	*b*	*c*	*β*
$SrCrO_4$	1	monoclinic	$P2_1/n - C_{2h}^5$	4	7,081	7,388	6,771 Å ± 0,01 Å	103°25′ ± 5′
$PbCrO_4$	1	monoclinic	$P2_1/n - C_{2h}^5$	4	7,118	7,434	6,794 Å ± 0,004 Å	102°25½′ ± 2′
crocoite	7	monoclinic	$P2_1/n - C_{2h}^5$	4	7,12	7,43	6,79 Å	102°25′
$PbCrO_4$	2	orthorhombic	$\text{Pnma} - D_{2h}^{16}$	4	8,67 ± 0,03	5,59 ± 0,01	7,13 Å ± 0,02 Å	

Table 1. Space groups and unit cells of $SrCrO_4$ and $PbCrO_4$.

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[5] L. BRAGG and G. F. CLARINGBULL, Crystal Structure of Minerals, Bell, London 1965.

[6] S. B. BRODY, J. Chem. Phys. **10**, 650 [1942].

[7] S. QUARENI and R. DE PIERI, Acta Cryst. **19**, 287 [1965].

[8] W. P. GRIFFITH, J. Chem. Soc. (A), **286** [1970].

[9] L. C. AFREMOW and J. T. VANDENBERG, J. Paint Techn. **38**, (No. 495) 169 [1966].

[10] G. HERZBERG, Infra-Red and Raman Spectra of Polyatomic Molecules, D van Nostrand, Inc., New York 1945.

Infra red Ref. [9]		Raman Ref. [8]		Powder 300 °K			Powder 110 °K			Assignment
ν [cm^{-1}]	I	ν [cm^{-1}]	I	ν [cm^{-1}]	Raman I	Slit: 2 cm^{-1} HW [cm^{-1}]	ν [cm^{-1}]	Raman I	Slit: 1 cm^{-1} HW [cm^{-1}]	T_d
		344	(2)	366	116	6.1	337	140	2.4	d, $\nu_2(E)$
350	vw b	354	(3)	348.7	121	7.6	348	145	2.8	
				354	46	4.2	354	50	4.3	d, $\nu_2(E)$
				367 sh	40	4.7	367	38	4.7	
		380	(6)	373	146	13.2	373	115	8.8	$\nu_4(F_2)$
				401	66	3.8	401	65	2.3	d, $\nu_4(F_2)$
410	w sp	407	(4)	406	66	3.6	406	72	2.0	
				425	13	3.8	429	15	3.3	d, $\nu_4(F_2)$
431	w sp	437	(2)	432	14	6.6	436	18	3.3	
845	s sp	864	(5)	857	555	5.5	860	750	2.7	d, $\nu_1(A_1)$
855	vw sp sh	870	(10)	866	1030	4.9	867	1250	2.8	
875	vw sp sh			889	600	3.5	892	800	2.1	d, $\nu_3(F_2)$
887	s sp	898	(9)	893	850	4.4	897	950	3.3	
912	s m			915	180	4.9	920	295	2.5	$\nu_3(F_2)$
927	s sp			928	70	4.7	934	100	2.3	$\nu_3(F_2)$

I Intensities are peak values in arbitrary units, cannot be transferred from one spectrum to another and are not corrected for spectral response. d doublet.

Table 2. Vibrational data of $SrCrO_4$.

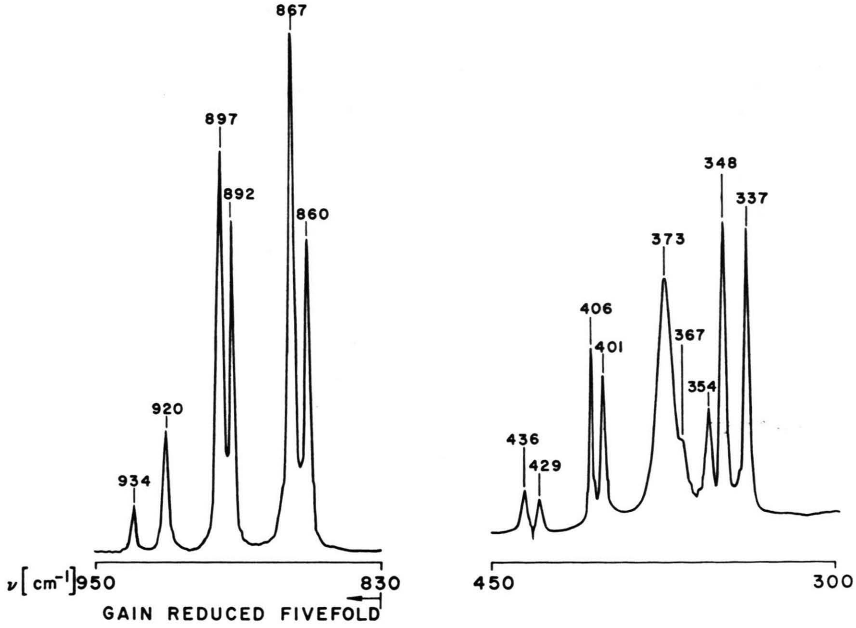

Fig. 1. Low temperature Raman spectrum of $SrCrO_4$ powder pellet in reflection with 6328 Å/180 mW excitation. $\Theta = 110$ °K; $s = 50\ \mu = 1$ cm^{-1}; $T = 0.3$ sec; $v = 5$ Å/min.

It is reasonable to assume that the strongest band in the Raman spectrum (860/867 cm^{-1} doublet) is the totally symmetric A_1 vibration. The splitting of this band cannot be explained by means of factor group analysis as can be seen from Fig. 2 where the correlation diagram for the possible site symmetry C_2 is shown.

The other phonons observed in the region between 892 and 934 cm^{-1} must originate from the triply degenerate $\nu_3(F_2)$ vibration. One component was found split (892/897 cm^{-1} doublet), the others are single.

The wave number region 337 to 436 cm^{-1} contains the phonons originating from the $\nu_2(E)$ and

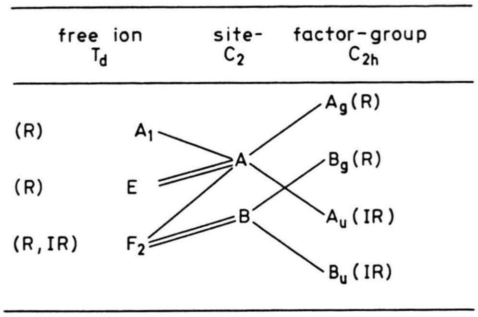

Fig. 2. Correlation diagram for C_{2h} factor group.

$\nu_4(F_2)$ vibrations. Since in tetrahedral ions with a heavy central atom, such as chromium, the doubly degenerate E vibration is usually of lower energy than the triply degenerate F_2 vibration, the two doublets (337/348 and 354/367 cm^{-1}) are assigned to the E vibrations. The remaining phonon at 373 and the doublets at (401/406 and 429/436 cm^{-1}) are assigned to the three F_2 vibrations. The rather large half-width (8.8 cm^{-1}) of the 373 cm^{-1} band indicates the accidental degeneracy of the two components of one F_2 vibration.

The assigment is listed in Table 2 with reference to a regular tetrahedron.

Another explanation for the observed splittings could be given if two crystallographically and energetically distinct CrO_4^{2-} ions are present in the lattice, giving rise to distinct vibrations. The rule of mutual exclusion would then not be applicable and corresponding bands should occur at the same energies in the infrared and Raman spectra. It can be seen by inspecting Table 2 that this is clearly not the case.

Judging from the vibrational data, it would appear that the structure of $SrCrO_4$ contains distorted CrO_4^{2-} tetrahedra (symmetry C_2 or C_1) with the Cr atoms in general positions related pairwise by a center of symmetry.

2. *Lead Chromate*

2.1. Synthetic Lead Chromate

Raman spectra at 300 °K and 77 °K of the monoclinic and at 77 °K of the orthorhombic modification were obtained in the same manner as in the case of $SrCrO_4$. The results are listed in Table 3 and the low temperature spectrum is shown in Fig. 3.

Although monoclinic strontium and lead chromates belong to the same space group and possess

$PbCrO_4$ infra red Ref.[9]		Crocoite Raman Ref.[8]		Powder 300 °K			Powder 77 °K		
				Raman			Raman		
ν [cm^{-1}]	I	ν [cm^{-1}]	I	ν [cm^{-1}]	I	Slit: 1 cm^{-1} HW [cm^{-1}]	ν [cm^{-1}]	I	Slit: 1 cm^{-1} HW [cm^{-1}]
		180	(1)						
		324	(2)	325	30	6.5	325	48	2.4
		327	(3)						
		337	(5)	337	58	6.5	337	124	2.4
		355	(3)	347	24	5.7	348	40	2.6
		360	(3)	358	150	8.5	358	332	3.1
		377	(4)	377	54	6.5	377	112	2.6
397	m vb, sh	398	(2)	400	22	6.5	401	60	2.2
≈ 790	? sp, sh	795	(3)	n.o.			n.o.		
				n.r.			820	200	5.5
		824	(2)	823 sh			829	200	5.5
833	w m	840	(10)	839	470	13	840	2200	2.5
				n.r.			849 sh	200	5.5
				n.r.			853 sh	100	
858	s m, sh	855	(3)	854 sh			859	320	4.3
≈ 905	w vb								

I Intensities are peak values in arbitrary units, cannot be transferred from one spectrum to another and are not corrected for spectral response.

n. o. Not observed.

n. r. Not resolved.

Table 3. Vibrational data of $PbCrO_4$ monoclinic.

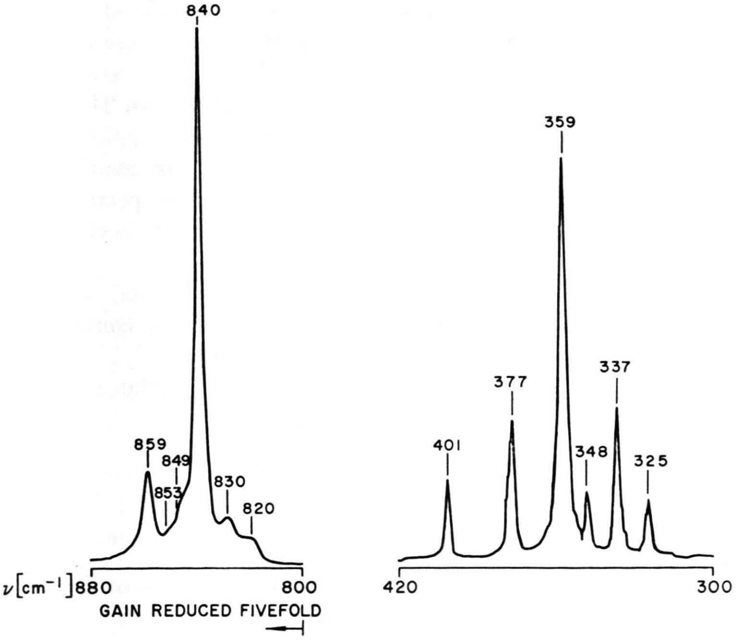

Fig. 3. Low temperature Raman spectrum of $PbCrO_4$ powder pellet in reflection with 6328 Å/180 mW excitation. $\Theta = 77$ °K; $s = 50\ \mu = 1\ cm^{-1}$; $T = 0.3$ sec; $v = 5$ Å/min.

almost identical unit cells, their vibrational spectra are quite different. On the other hand, the spectra of monoclinic crocoite, monoclinic synthetic lead chromate and orthorhombic synthetic lead chromate are almost indistinguishable. The only significant difference in the Raman spectra of monoclinic and orthorhombic lead chromate lies in the scattering efficiency. The bands of the monoclinic form are approximately eight times as intense as those of the orthorhombic form. This can partly be due to the influence of different particle size in the sample.

The total number of 12 bands in the R and of 5 bands in the IR spectra suggests again that the CrO_4^{2-} ion is a distorted tetrahedron causing all degeneracies to be lifted.

2.2. Crocoite, $PbCrO_4$

Single crystal Raman spectra of this mineral were taken at 300 °K and 77 °K. In order to obtain meaningful results[11] from a monoclinic crystal with an extraordinary high birefringence ($N_X = 2.31$ Li, $N_Y = 2.37$, $N_Z = 2.66$; optic plane: 010; $Z \wedge c = -5.5°$)[12], it is necessary to choose an arrangement where neither the incident nor the scattered radiation becomes depolarized. Therefore, the crocoite specimen was cut normal to the *c* axis and polished to 1 mm thickness. The crystal was then examined in transmission with the incident and scattered radiation parallel to the *c* axis. This setup was checked by determining the depolarization ratio of the Rayleigh line; it was found to be $\varrho_s = 0.01$, with the collecting lens set at 1 : 4 aperture for this and all the single crystal measurements.

The results of these single crystal measurements are listed in Table 4 together with the assignments. The first column gives the wave number of the observed bands, the following four columns give the relative intensities and half width in four meaningful scattering-configurations. The symbol $c(b \perp b)\, c$ indicates[13] that the incident and scattered radiation propagate along the *c* axis, the incident radiation being polarized parallel to the *b* axis and the scattered radiation being analysed normal to the *b* axis. It should be noted that the direction $\perp b$ is not coincident with the *a* axis.

The significance of the low temperature single crystal spectrum can be seen in the excellent resolu-

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[11] I. R. BEATTIE and T. R. GILSON, Proc. Roy. Soc. London A **307**, 407 [1968].

[12] A. N. WINCHELL and H. WINCHELL, Elements of Optical Mineralogy, Part II, Description of Minerals, 4-th Ed., J. Wiley, New York 1956.

[13] T. C. DAMEN, S. P. S. PORTO, and B. TELL, Phys. Rev. **142**, 570 [1966].

ν[cm^{-1}]		$c(b\,b)c$				$c(\perp b\,b)c$				$c(\perp b \perp b)c$				$c(b \perp b)c$				Assignment	
300 °K	77°K	300°K		77 °K		300 °K		77 °K		300 °K		77 °K		300 °K		77 °K		C_{2h}	T_d
		I	HW	*I*	HW	*I*	HW	*I*	HW	*I*	HW	*I*	HW	*I*	HW	*I*	HW		
325	325	4	*	20	3.3	93	6.1	250	2.8	3	*	15	3.3	35	5.2	300	3.0	Bg	E
337	337	133	5.2	280	3.2	6	*	20	3.0	81	5.1	470	3.0	5	*	25	3.3	Ag	E
347	348	52	5.7	140	2.8	58	4.8	180	2.8	17	5.2	40	3.8	21	4.0	170	2.6	Ag + Bg	F_2
358	358	70	7	250	3.9	6	*	10	*	15	6.1	70	4.3	*	*	5	*	Ag	E
377	377	12	5.7	30	3.8	29	4.5	100	2.8	17	4.3	110	3.0	9	3.9	65	3.0	Ag + Bg	F_2
400	401	58	4.5	220	2.8	33	4.7	110	2.8	6	4.8	35	4.3	9	4.0	90	2.8	Ag + Bg	F_2
+	820			160	4.3			45	4.9			360	3.7			25	4.3	Ag	F_2
823 sh	829	70	+	180	4.9	10	+	15	4.4	46	10	60	3.2	*	*	*	*	Ag	F_2
839	840	1270	8.5	7000	2.7	70	9	380	2.6	145	11	1000	2.9	29	10	200	2.8	Ag	A_1
+	847			60	+			150	3.7			30	+			85	4.3	Bg	F_2
854 sh	859	115	+	540	3.2	46	14	170	4.2	133	13	1400	3.2	19	13	90	4.6	Ag	F_1
863 sh	867	20	+	30	*	40	12	220	7.5	15	+	30	*	19	12	170	7.1	Bg	F_2
880 sh	883	*	*	*	*	25	11	20	5.3	*	*	*	*	9	11	20	5.3	Bg	F_2

I Peak intensities in arbitrary units; same scale for 300 °K and 77 °K spectra; not corrected for spectral response; accuracy ±20%.
HW Half width [cm^{-1}] measured with 2 cm^{-1} spectral slit width; accuracy ±20%.
sh Shoulder.
* Too weak to be measured; $^+$ too overlapped to be measured.

Table 4. Single crystal Raman data of Crocoite $PbCrO_4$.

tion obtained, especially in the region from 820 to 883 cm^{-1}. At 300 °K all bands marked sh had to be deduced from their envelopes by graphical methods. The intensities and half width of these bands are, therefore, subject to a larger error.

Considering the Raman tensor of the monoclinic class $2/m - C_{2h}$ given by LOUDON[14] the assignment of most of the bands is straightforward. Only a few bands show mixed $A_g + B_g$ character.

The connection of the assignment obtained from single crystal measurements with the vibrations of the distorted tetrahedron is done on the basis of the T_d point group. The most intense band in the 820 to 883 cm^{-1} region is assigned to the $\nu_1(A_1)$ stretching vibration. The only other vibration which can be possibly active in this region is the $\nu_3(F_2)$ bending vibration which is triply degenerate. In order to account for the observed three A_g and three B_g phonons, it must be concluded that the degeneracy of the $\nu_3(F_2)$ vibration is lifted and that each component is split into an A_g and B_g component.

In the region from 325 to 401 cm^{-1} the doubly degenerate $\nu_2(E)$ bending and the triply degenerate $\nu_4(F_2)$ bending vibration can be expected. Since nine phonons are observed, if the three bands showing mixed character are counted as six separate phonons, the assignment follows the same pattern as above. All degeneracies are lifted and each component appears split into A_g and B_g. One B_g phonon remains unobserved. The division of the observed phonons into a group originating from E and F_2 vibrations, respectively, can only be made tentatively under the assumption that the E vibration is of lower energy than the F_2 vibration.

3. *Inter-ionic Forces*

It is interesting to note that the wave number of the totally symmetric stretching vibration $\nu_1(A_1)$ is significantly lower in $PbCrO_4$ (840 cm^{-1}) than in $SrCrO_4$ (860/867 cm^{-1}). The weakening of the chromium-oxygen bond can be understood under the assumption of a strengthened lead-oxygen bond which means that the character of the lead-oxygen bond has become partly covalent.

If one allows the insolubility of a chromate to be considered as a measure of bond strength between cation and anion, the conclusion may follow that for the chromate with the highest solubility the wave number of $\nu_1(A_1)$ is also highest and the character of the cation-anion bond has greater ionic character.

In Table 5 wave numbers of vibrations $\nu_1(A_1)$ are listed for a number of chromates, together with the solubilities of these compounds in water[15].

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[14] R. LOUDON, Adv. Phys. **13**, 423 [1964].

[15] Handbook of Chemistry and Physics, 40th ed., Chemical Rubber Publishing Co., Cleveland, Ohio 1958.

[16] J. S. STEPHENS and D. W. J. CRUICKSHANK, Acta Cryst. B **26**, 222 [1970].

	$CaCrO_4 \cdot 2H_2O$	$SrCrO_4$	$BaCrO_4$	$PbCrO_4$
$\nu_1(A_1)$ at 300 °K	880	857/866	863	839
solubility [g/100 ml] at °C	22.4°	$0{,}12^{15}$	$0{,}00034^{16}$	$0{,}0000058^{25}$

Table 5. Wave number of $\nu_1(A_1)$ versus solubility at °C for various chromates.

It can also be argued that the deviation[16] of the Cr – O – Cr bond angle from the ideal value 109.5° observed in crocoite originates from a strengthened Pb – O bond thus causing a decreased bonding power of the narrow tetrahedral d^3s orbitals of chromium. This, in turn, would lead to a decrease in the $\nu_1(A_1)$ frequency as observed.

Acknowledgements

The authors are indebted to Miss C. G. RÜMKE, Geological Survey of South Africa and to Dr. E. B. FÖRTSCH, University of Pretoria, for the gift of the crocoite samples, and to Dr. J. P. R. DE VILLIERS, N.P.R.L., for valuable discussions.

Partielle Interferenz- und partielle Atomverteilungsfunktionen sowie elektrischer Widerstand von geschmolzenen Magnesium—Zinn-Legierungen *

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(Z. Naturforsch. **25 a**, 1862—1867 [1970]; eingegangen am 7. Oktober 1970)

From measured intensity functions, published in a previous paper, partial interference functions, partial pair correlation functions, partial atomic distribution functions, and partial coordination numbers were calculated and discussed. According to the theory of Faber and Ziman, the electrical resistivity of molten Mg—Sn alloys was calculated from the partial interference functions and from pseudopotentials reported by Animalu and Heine. The calculated values, being normalized to the resistivity of the molten components, are in good agreement with values measured by a rotating field method.

The partial interference functions are derived by the assumption of independency of concentration. This assumption is proved by discussion of the partial coordination numbers and the results of electrical resistivity determinations.

Für die Berechnungen des elektrischen Widerstandes geschmolzener Legierungen aus Röntgen-Beugungsdaten nach FABER und ZIMAN[1] ist neben der Kenntnis der Pseudopotentiale[2] die der partiellen Interferenzfunktionen notwendig. Die partiellen Interferenzfunktionen wurden bisher für die Systeme Cu-Sn[3], Ag-Mg[4], sowie Au-Sn und Ag-Sn[5–7] angegeben. In vorliegender Arbeit werden die partiellen Interferenzfunktionen für das System Mg-Sn aus den in[8] publizierten Röntgen-Beugungsexperimenten berechnet. Außerdem werden durch Fouriertransformation der partiellen Interferenzfunktionen die partiellen Atomverteilungsfunktionen und Teilkoordinationszahlen berechnet. Mit Hilfe der Interferenzfunktionen erfolgt die Berechnung des elektrischen Widerstandes, der außerdem mit direkt gemessenen Werten[8] verglichen wird.

Sonderdruckanforderungen an Priv.-Doz. Dr. S. STEEB, Max-Planck-Institut für Metallforschung, Institut für Sondermetalle, *D-7000 Stuttgart 1*, Seestraße 92.

* Teil der Dissertation von H. F. BÜHNER.

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