determines the relative position of its main levels S = 0, 1, 2, 3 and of the lines of the N_2 series.

In the N_1-pair model proposed in [6] (third neighbors), the Cr^{3+} ions entering into the pair occupy places with opposite signs of the odd trigonal field. This leads to cancellation of the dipole moments in both the ground state of the pair and in its excited state (owing to resonant excitation transfer between the ions). There should therefore be no linear level shift in an electric field, in agreeement with the experimentally observed absence of a noticeable influence of the field on the N_1-pair spectrum.

Thus, the results of our investigation confirm fully the classification given in [1,2] for the lines and the N_1- and N_2-pair model considered in [6].** In qualitative agreement with the theory of [5], experiment indicates that the directions of the odd trigonal field at the ion locations of the exchange-linked Cr^{3+} - Cr^{3+} pair plays a decisive role in the behavior of its spectrum in an electric field.***

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*The positions of all lines belonging to pairs, indicated in Fig. 1, have been measured on samples of Al_2O_3 with 1.6% Cr, and differ from the data of [2], which were obtained with samples having 0.5% Cr, by an average long-wave shift of about 0.5 Å.

**The lines 6973, 6969, and 6962 Å, which split in the field into doublets, form a sequence with intervals close to those of the N_2 series. This suggests a connection between the lines and transitions to the levels S = 0, 1, 2 of the N_2 pair from one of the higher radiative levels (14381 cm^{-1}).

*** Preliminary experiments reveal that the field has likewise no influence on the 7451 Å ruby emission line that belongs [6] to the chromium pair of second neighbors with opposite directions of the odd-field components.

STRUCTURE OF α MODIFICATION OF OXYGEN

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Neutron-diffraction investigations of solid oxygen at 27, 20.4 and 4.2°K yielded reliable Debyegrams of the β and α modifications of O_2 [1].

A neutron-diffraction pattern obtained with α-O_2 is shown in Fig. 1 (where a small-scale Debyegram of β-O_2 is also shown). There is no corresponding analog among the hitherto published

sets of diffraction lines ascribed to the α phase of oxygen [2-5]. In all the earlier results, the data pertained to a mixture of the β and α modifications, due to unfavorable experimental conditions wherein the precipitated oxygen samples had a considerable temperature gradient overlapping the interval from the bath temperature (20, 16, 20.5 and 20°K) to the temperature of the α → β transition (23.88°K).

In the present investigation, the procedure for which was described earlier [1], the diffraction patterns obtained at 20.4 and 4.2°K are identical and belong to the α modification; on the other hand, their general structure is quite similar to that observed in the β phase at 27°K.

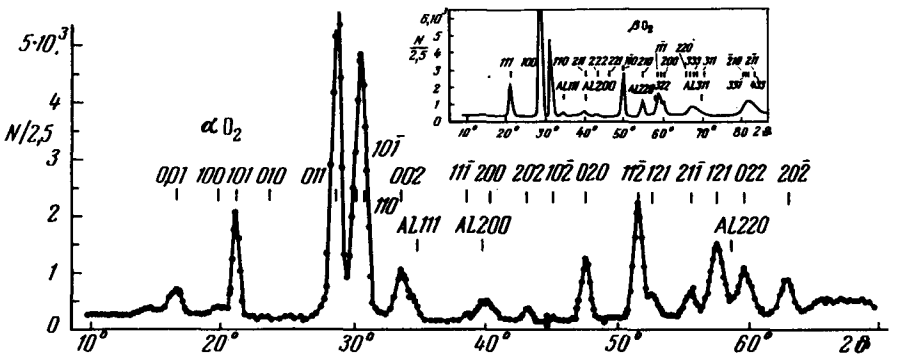

Fig.1

This pertains both the the line position and to the character of the distribution of the intensity among the lines (see Fig. 1).

A detailed comparison of the neutron patterns highlights the constance of the two lines at 21°11' and 43°16', and also the appearance of new reflections in the Debyegram of α-O_2 (16°45', 19°45', 33°39', and 47°33') and the decreased density of the dense reflection group at angles larger than 50°.

The fact that the neutron patterns contain invariant reflections, and also the general similarity of the diffraction patterns of both modifications has served as a useful methodological attribute making it possible to determine the structure of the α modification of oxygen. We started from the hypothesis that the β → α transition is accompanied by an insignificant shift of the oxygen molecules from the positions they occupy in the rhombohedron of β-O_2 (0: ±(u,u,u), u = 0.055). The approach to the solution of the problem of the structure of α-O_2 is shown schematically in Fig. 2, where the rhombohedral grid of β-O_2 is drawn in three projections.

In the center are shown four neighboring rhombohedral cells, the symmetry planes of which coincide with the plane of the figure. The line labeled 1-2-3 separates two pairs of cells along (100) planes perpendicular to the plane of the figure. A view from the side of the (100) planes (side view) is shown in the upper left corner of the figure, where two rhombi show the relative positions of the cells inside the pair. The projection shown in the lower part of the figure (top view of the cell) is along the rhombohedral axis with sections through three neighboring basal planes at the levels marked 1, 2, 3.

Inscribed in the above rhombohedral lattice is another lattice marked in Fig. 2 with

heavy lines. The (110) planes of the two cells located along the diagonal and bounded pairwise by planes of the (211) and (110) type produce a new cell, which, as can be seen from the construction, should be monoclinic body-centered with spatial symmetry of type I^2/m, and in the customary notation (with a different construction variant) - C^3_{2h} - C^2/m.

Table

βO_2			αO_2		
hkl	2*d*	*d*	*d*	2*d*	*hkl*
110	5.108		4.773		001
211	4.016		4.024		100
111		3.752	3.782		101
110	3.308			3.448	020
			2.795		011

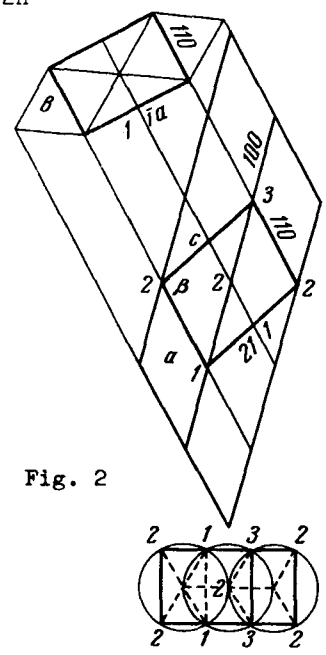

Fig. 2

Bearing in mind the proposed β → α transition scheme and examining simultaneously the Debyegrams of the β and α modifications, we can now index part of the reflections of the α-O_2 neutron diffraction pattern.

It follows from the construction of the cell that d_{001}, d_{010}, and d_{100} of α-O_2 should be practically double the values of d_{110}, $d_{1\bar{1}0}$, and d_{211} of β-O_2. The table lists the values of $2d(\beta\text{-}O_2)$ and the interplanar α-O_2 distances calculated from the positions of the first four peaks.

The maximum $d(\alpha\text{-}O_2)$ corresponding to the first peak ($2\theta = 16°45$) of the neutron pattern differs from $2d_{110}(\beta\text{-}O_2)$ by 65%. The next peak (19°54') has very low intensity, but its position agrees well with $2d_{211}(\beta\text{-}O_2)$. The table shows further a comparison of the interplanar distances of the peak which remains outwardly unchanged in the β → α transition and indicate its indices that follow from the cell construction. Finally, the third term of the family {110}(010), as will be explained, is missing from the α-O_2 neutron pattern. There are no reflections that give a value of d sufficiently close to $2d_{1\bar{1}0}$ $(\beta\text{-}O_2)$. During the course of the interpretation we made use here of the fact that besides vanishing of the structural nuclear factor we have here vanishing of the (010) magnetic structural factor (unlike (001) and (100)).

We were, however, able to determine the value of d_{011} by using the reflections at larger scattering angles, having in mind the (020) reflection. Among the peaks near 50° there are observed two reflections (47°33' and 51°33'), for which the values of 2d are respectively 3.448 and 3.197. The choice fell on the first of these values, for in this case the theoreti-

cal value d_{011} = 2.794 (which follows from the order of the interplanar distance of the monoclinic lattice) is in splendid agreement with the observed value. In our case such a criterion is fully justified since the (011) reflection is the most intense one of the neutron pattern.

Having the set of data listed in the table, it is not difficult to find the unit-cell parameters of the α modification of oxygen: a = 4.284 ± 0.009, b = 3.448 ± 0.007, c = 3.081 ± 0.011, β = 110°4' ± 11'.

The indices of all the succeeding reflections followed the sequence indicated over the reflections of Fig. 1.

The cells contain two oxygen molecules, and the density at 20.4°K is 1.489 g/cm^3. Consequently, practically no change in density takes place in the β → α transition, unlike the γ → β transition, where the density increases 13%.

Preliminary calculations of the coordinates of the oxygen atoms have confirmed the assumed model of the β → α transition, in which the axis of the O_2 molecule is fixed along the rhombohedral axis of β-O_2.

A universal determination of the coordinates of the atoms was carried out jointly with E. B. Vul and Yu. G. Fedorov [6] by the nonlocal-search method used earlier for x-ray structure analysis [7].

During the course of the search, which was made in the entire region of possible values of the atom coordinates, we established uniqueness of the obtained solution, namely, we obtained the following values of the oxygen-atom coordinates: ±(x, 0, z) and ±(1/2 + x, 1/2, 1/2 + z), where x = 0.104, z = 0.044, and R = 5.9%.

The magnetic structure of the α modification of oxygen, as follows from the neutron pattern that contains reflections with an odd sum of indices, is antiferromagnetic with magnetic moments oriented along the crystal axis and perpendicular to the molecule axis.

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PHONON SPECTRUM OF THE SUPERCONDUCTING MODIFICATION OF BISMUTH

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It is known [1,2] that bismuth condensed on a surface cooled to 2 - 4°K froms a new crystallographic modification, in which the metal is a superconductor with a critical temperature 6°K. We have investigated bismuth by the tunnel-effect method to be able (i) to measure the gap Δ_0 in the electron spectrum of this superconductor and (ii) to obtain information on the phonon spectrum distribution density.