

As the Fourier projection showed some disturbing diffraction ripples round the bromine atom due to finite termination of the series, a second Fourier difference projection was prepared with the bromine contributions subtracted. This projection shows much better resolution of the carbon atoms. The structure is shown schematically in Fig. 1. The angle of tilt of the chains is $\tau = 66^\circ$. The subcell is nearly orthorhombic with $a_s = 5.52$, $b_s = 7.02$, $c_s = 2.50$ Å.

The co-ordinates obtained from this projection, referring to all the atoms falling within one asymmetric unit (one-quarter unit cell) but belonging to parts of three separate molecules, are:

Atom	x/a	z/c	Atom	x/a	z/c
Br	0.256	0.0156	C ₆	0.7205	0.2165
N	0.161	0.0278	C ₇	0.2911	0.2438
C ₁	0.1968	0.0650	C ₈	0.1129	0.2178
C ₂	0.4003	0.0860	C ₉	0.1179	0.1800
C ₃	0.3737	0.1258	C ₁₀	0.9315	0.1550
C ₄	0.5563	0.1520	C ₁₁	0.9320	0.1163
C ₅	0.5270	0.1902	C ₁₂	0.7580	0.0900

The consideration of this projection shows that the NH_3^+ groups lie about 0.5 Å out of the planes occupied by the halide ions. This agrees with a similar displacement

observed by King & Lipscomb (1950*b*) for the low-temperature form of *n*-propylammonium chloride.

It is to be noted that the particular crystalline form of the *n*-dodecylammonium chloride and the bromide are approximately isomorphous and have the C-N bond at roughly 90° to the 001 plane, which is near to the value for *n*-propylammonium chloride (space group C_{2h}^2-C2/m). All the three structures, however, are representatives of three different space groups.

In order to obtain more complete information on the packing of the hydrocarbon chains, it will be necessary to prepare the other projections of the unit cell.

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Neutron-diffraction study of the structure of the A-form of the rare earth sesquioxides. By W. C. KOEHLER* and E. O. WOLLAN, Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A.

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In the course of experiments on the paramagnetic

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scattering of neutrons by rare earth ions, the results of which are reported elsewhere (Koehler & Wollan, 1953), neutron-diffraction data from powdered samples of La_2O_3 , Pr_2O_3 and Nd_2O_3 of normal isotopic constitution and Nd_2O_3 enriched in Nd^{142} , Nd^{144} and Nd^{146} were obtained which provide direct evidence in confirmation

Table 1. Values of $j|F|^2$ for La_2O_3 -type structures

Index	Pauling model	Zachariasen model
	2 La in $\pm (\frac{1}{2}, \frac{2}{3}, u)$ 2 O in $\pm (\frac{1}{2}, \frac{2}{3}, v)$ 1 O in (0, 0, 0)	2 La in $\pm (\frac{1}{2}, \frac{2}{3}, u)$ 3 O in $(v, v, 0; \bar{v}, v, 0; v, \bar{v}, 0)$
	$u = 0.25, v = 0.65$	$u = 0.25, v = 0.25$
001	0.0207	6.06
100	$6f_M^2$	$6f_M^2 - 6.96f_M + 2.02$
002	$8f_M^2 - 1.77f_M + 0.0982$	$8f_M^2 - 13.9f_M + 6.07$
101	$36f_M^2 - 33.8f_M + 18.1$	$36f_M^2 + 4.04$
102	$12f_M^2 + 18.2f_M + 18.2$	$12f_M^2 + 13.9f_M + 4.04$
003	5.66	6.06
110	$24f_M^2 + 41.8f_M + 18.2$	$24f_M^2 - 13.9f_M + 10.1$
111	0.124	20.2
103	$36f_M^2 + 12.9f_M + 7.37$	$36f_M^2 + 4.04$
200	$6f_M^2$	$6f_M^2 + 6.96f_M + 2.02$
112	$48f_M^2 - 10.6f_M + 0.589$	$48f_M^2 + 27.8f_M + 20.2$
201	$36f_M^2 - 33.8f_M + 18.1$	$36f_M^2 + 4.04$
004	$8f_M^2 - 2.89f_M + 0.257$	$8f_M^2 + 13.9f_M + 6.06$

Table 2. Comparison of observed and calculated intensities for La_2O_3 -type structures

All intensities (neutrons/min.) are on an absolute scale

Index	La_2O_3		Pr_2O_3		Nd_2O_3		$\text{Nd}_2^{142}\text{O}_3$		$\text{Nd}_2^{144}\text{O}_3$		$\text{Nd}_2^{146}\text{O}_3$	
	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.
001	—	1.0	—	0.4	—	0.7	—	0.3	—	0.4	—	0.2
100	35	36	5	6.5	22	21	17	16	4	3	17	16
002	122	123	50	47	80	77	58	59	48	46	55	53
101	166	164	71	71	111	112	80	84	57	58	67	67
003	—	—	—	—	—	—	—	—	—	—	—	—
110	213	213	86	87	144	146	112	110	66	65	84	88
111	—	—	—	—	—	—	—	—	—	—	—	—
103	—	—	—	—	—	—	—	—	—	—	—	—
200	178	177	48	44	98	105	80	84	31	30	75	77
112	—	—	—	—	—	—	—	—	—	—	—	—
201	—	—	—	—	—	—	—	—	—	—	—	—
	$f_{\text{La}} = 0.83 \times 10^{-12}$ cm.		$f_{\text{Pr}} = 0.44 \times 10^{-12}$		$f_{\text{Nd}} = 0.72 \times 10^{-12}$		$f_{\text{Nd}^{142}} = 0.77 \times 10^{-12}$		$f_{\text{Nd}^{144}} = 0.28 \times 10^{-12}$		$f_{\text{Nd}^{146}} = 0.87 \times 10^{-12}$	

for the accepted structure of the hexagonal form of the rare earth sesquioxides.

The La_2O_3 structure was first investigated by Zachariasen (1926, 1929) and his proposed structure was subsequently criticized by Pauling (1928), who proposed an alternative model on the basis of packing and other physical considerations. More recently, Zachariasen (1949) has pointed out the similarity of the structure of the oxysulfides of La, Ce and Pu to that suggested by Pauling for the hexagonal sesquioxides.

Although Pauling's structure is now accepted for these compounds, the light atom positions have heretofore been determined only indirectly; it was therefore felt that the direct evidence provided by the neutron-scattering data would be of interest.

The atomic positions for the two structures are shown at the top of Table 1, in which are tabulated structure factors calculated for the two models. The oxygen scattering amplitude has been taken as 0.580×10^{-12} cm.; but, since the scattering amplitudes of the rare earth nuclides had not been previously measured, the structure factors are expressed as functions of the metal scattering amplitude.

The structure first proposed can be eliminated without a knowledge of the metal scattering amplitudes by inspection of the diffraction patterns. For example, the reflections (001) and (111) are nearly independent of the metal scattering amplitude, and their intensities are seen to vary markedly from the one model to the other. In the diffraction patterns of all the samples studied the (001) and (111) reflections were immeasurably small, whereas on Zachariasen's model these lines would be among the strongest in the pattern.

An attempt was made to evaluate the parameters of the structure from the absolute intensities observed in the La_2O_3 pattern alone, in order to avoid any possible coherent magnetic scattering effects in the magnetic salts. Since the intensity of the (100) reflection depends only upon the magnitude of the lanthanum scattering amplitude, an approximate value of f_{La} was obtained from this reflection, and by successive approximation the following quantities were evaluated: $f_{\text{La}} = 0.83 \pm 0.01 \times 10^{-12}$ cm., $\theta = 410^\circ \text{ K.}$, $u = 0.245 \pm 0.005$, $v = 0.645 \pm 0.005$. A comparison of the observed and calculated intensities for La_2O_3 and for the oxides of Pr and Nd, assuming the same parameters and characteristic temperature, is given in Table 2 together with the nuclear scattering amplitudes (Koehler & Wollan, 1953) upon which the calculated intensities are based. The agreement is quite satisfactory for the entire series of samples and this suggests that coherent magnetic effects, if any, contribute less than 5% to the intensities observed.

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