CRYSTAL STRUCTURE OF \$-Ga2O3

TABLE VII. β -Ga₂O₃ powder data (CuK α radiation).

bk/ d d ι ΣΙ ι	bbd	4	4					4		÷.				4			21	
$\frac{1}{200}$ $5,942$ - 0.0 0.0 -	222	1.275	0	0.6	c	0	330	0.982	0	C.1	2.6	0	12.2.1	0.845		1.4		-0
001 5.635 5.62 1.6 1.6 VW	224	1,275	-	0.7	1.3	-	405	0.980	-	0.0	0,1	-	731	0.845	0.845	0.0	1.4	VW.
201 3.677 3.66 (2.0) 2.0 VW	514	1.243	-	0.1	0.4	-	12,0,3	0.977	0.976	0.5	1.8	VW	10,2,2	0.843	0.843	1,2	1.7	WV
110 2.945 2.95 1.1 22.8 VS	911	1.241		0.1			315	0.969	-	0.6	0.6	-	406	0.840		0.1	0.1	
401 2,930 2.92 26.1 26.1 VS 002 2 817 2 81 27.5 hs s vvc	10,0,T	1.223	1.223	0.2	2.1	W	206	0.964	0.964	1.3	2.1	W	13,1,1	0.837	0.025	2.9	12.0	M-5.
207 2.01 2.01 18.0	51 <u>3</u> 621	1.217	-	0.4	1.2	•	406	0.963		0.3			916	0.835	0.835	5.1	12.0	Br.
111 2.549 2.536 50.2 50.2 VVS	712	1.212	1 000	0.1	1.0	VVW.	132	0.957	-	0.1	0.5	-	914	0.833	0.834	2.1	2.6	W,Br.
310 2.412 - 0.2 0.2 -	910	1.211	1.209	0.9	1.0	Br.	623 10,2,1	0.954	0,952	2.1	2.3	w	12,2,0	0.830		2.3		
401 2.403 2.390 17.7 17.7 M-S	620 802	1.206	-	0.2	0.2	-	132	0.944	0.945	0.3	1.1	WWW	134	0.829	0.829	0.0	3.1	₩-₩
202 2.340 2.332 1.1 31.8 S	10,0,2	1.201		0.0			822 _	0.943		0.0	0.0		334	0.829	-	0.4	0.1	
311 2.109 2.100 4.5 8.2 W-M	10,0,0	1.188	•	0.0	0.2		10,2,2	0,943		0.0	0.0		207	0.824		0.0	0.1	-
112 2.098 3.7 5.2 W	422	1.182	-	0.0	0.0	-	606	0.939	0 027	0.2	1.0		425	0.823		0.4		
600 1.980 1.5	622	1.171	1,168	0.4	1.6	WW.	10,2,0	0.936	0.937	0.0	1.0		11,1,3	0.821	-	0.1	0.5	
312 1.978 8.2	804	1.170		0.1			531	0.934	-	0.1	0.1	-	10.0.4	0.819	0.618	1.9	1.9	w
203 1.9273 0.3 -	423	1.159	-	0.6	0.6	-	915	0.932		0.0			14,0,4	0.818	0.817	2.7	3.4	wt
003 1.878 - 0.0 1.1 -	405	1.148		0.1			913	0.930	0.929	1.0	2.9	w,Br.	226	0.816	h	3.9	11 0	
510 1.872 1.865 4.8 4.8 M	714	1. 146	1.146	2.8	4.2	W-W	11,1,4	0.929		0.9			42,5	0.814	0.814	1.0	4.9	Well -
602 1.838 1.831 0.9 3.4 W	913	1.136	· - ·	0.0	0.0	-	42 <u>4</u> 824	0.927	-	0.0	0.1	-	184	0.813		0.2	0.6	-
403 1.791 1.788 1.6 1.6 VW	911	1.134	1,132	0.6	1.9	w	225	0.921	4	0.0			93T	0.812		0.1		-
312 1.714 0.0	223	1.127	-	0.9	0.9	-	804	0.919	-	0.0	0.0	-	14,0,1	0.811	-	0.0	0.1	-
512 1.714 0.1 0.1 511 1.685 1.677 2.8 h.7 w.4	10.0.1	1,111	-	0.0	0.1		425	0.916		0.1	0.1		533	0.806	-	0.4	0.6	-
203 1.680 1.677 1.9 1.7 mm	605	1.098	1.098	1.7	1.7	W	10,0,3	0.911		0.6		<	732	0.804		0.1		
313 1.598 1.595 13.2 13.2 M-S	623	1.089	1.086	2.2	2.2	WVW	532	0.911	0.910	0.0	3.8	W,Br.	932 930	0.804	-	0.0	.0.7	-
603 1,560 1,559 3.7 3.7 W	821	1.077	1.075	3.6	5.7	₩-M,	516	0.910		1.3			12,0,3	0.801	-	0.2	0.5	
80T 1.528 . cor 5.9 .c h .M-S.	115	1.074	1.013	2.1	5.1	Br.	531	0.906		0.5	0.5		317	0.800		0.1		-
020 1.520 1.525 10.5 10.4 Br.	205	1.062	1.061	1.0	1.0	VW	133	0.905		0.0			626 12,2,1	0.799	0.798	0.9	8.8	м
800 1.485 1 479 0.2 3 5 W-W	515	1.057		1.0			10,2,1	0.897		0.2			10,2,5	0.797	0 796	6.3	h q	wT
710 1.482 1.473 3.3 5.5 1.4	822	1.055	-	0.0	1.1		11,1,2	0.896	0.895	0.1	1.8	WVW,	807	0.790	0.789	1.5	9.6	Ч
513 1.470 0.1 021 1.468 - 0.0 0.2 -	803	1.050	1.048	0.5	5.6	м	13,1,2	0.895		0.2		86.	117	0.788	0.103	8.1	0.0	
602 1.465 0.1 802 1.465 0.0	423	1.046	-	0.7	0.7	-	515	0.895		0.1			15,1,2	0.787	-	0.0	0.3	-
204 1.450 1.449 7.9 7.9 M	11,1,1	1.043	1.043	1.3	1,3	VVW	333	0.892	0.892	2.8	7.3	M,Br.	12.2.4	0.786	-	0.0	5.0	-
<u>221 1.446 - 0.2 0.2 -</u>	10,0,4	1.038	-	0.0	0.2	-	133	0.882	0.880	2.9	3.3	w	334	0.784		1.6		
512 1.440 1.436 14.9 31.9 VS	514 914	1.037		2.5			715	0.880	01000	0.3			734 15,1,T	0.784	0.784	5.1	13.3	M-S
0.2	912	1.034	1.033	2.7	10.0	M-S,	13,1,0	0.875	-	0.1	0.2	-	516	0.783		0.9		t
404 1.409 - 0.1 0.4 - 221 1.405 0.1	024 424	1.033		0.1		Br.	13,1,3	0.873	-	0.3	0,3	-	13,1,5	0.783	0.782	3.3	8.4	W,Br.
313 1.388 - 0.4 0.4 -	115	1.033		1.2	0.1		14,0,2	0.872	0 870	0.8	h 7	м	933	0.781		0.1		
801 1.359 3.5	11,1,0	1.018	1 015	0.5	1.1		14,0,1	0.870	0.010	0.0			931	0.780	-	0.0	1.6	-
420 1.353 1.355 1.7 9.2 M,Br. 421 1.349 4.0	12,0,T	1.017	1.015	0.6	1.1		533	0.868	-	0.0	0.0	-	12,0,6	0.780		0.1		
022 1.338 1.336 2.4 5.6 W-M	10,0,2	1.012	1.011	0.2	3.6	W	823	0.864	-	1.0	1.0	-	717	0.778	-	0.1	0.1	-
803 1.328 0.7 0.7 -	130	1.010		0.0			532 732	0.861	0.861	4.7	9.8	M-S, Br.	15,1,3	0.775	0.775	15.7	15.7	M-S
204 1.303 2.1 604 1.303 0.8	715 82 <u>3</u>	1.003	1.000	0.1	1.3	vw	624 10.2.4	0.857	-	0.0	0.8	-						
713 1.302 1.301 0.6 3.8 W-M	131	0.997		0.6			11,1,5	0.856		0.4				e e				
314 1.301 0.3	131	0.990	0.989	2.5	8.3	M-S,	14,0,3	0.853	-	0.5	0.5	-						
421 1.285 1.281 4.1 4.1 W	224 624	0.989		1.9		Br.	333	0.850	-	0.2	0.4	-						
							825	0.848		0.2		-						

* Beginning with this line the α_1 , α_2 doublet on the powder photograph was resolved.

 $\dagger \alpha_2$ Line from previous reflection overlaps α_1 of this reflection.

that there are six interactions of a tetrahedrally coordinated ion with octahedrally coordinated ions and six interactions of an octahedrally coordinated ion with tetrahedrally coordinated ions. Thus there would be six important magnetic interactions per magnetic ion. From the recent paper by Gilleo,²⁸ one would estimate a Néel temperature of about 700°K for an Fe₂O₃ phase isostructural with β -Ga₂O₃.

Now, the facts that: (1) the β -Ga₂O₃ structure appears to be favorable to antiferromagnetic interaction, (2) that Fe³⁺ ion has a crystal chemistry similar

to that of Ga³⁺ ion, and (3) that the Fe³⁺ ion would prefer octahedral sites if substituted for Ga³⁺ in yttriumgallium garnet, all would immediately indicate the possibility of producing a ferrimagnetic material from solid solutions of Fe₂O₃ in β -Ga₂O₃. However, experiments made by Remeika *prior* to the determination of this structure, indicated that not much Fe³⁺ ion could be made to dissolve in β -Ga₂O₃ by solid-solid reaction,³⁰ not enough, that is, to produce strong enough interac-

³⁰ J. P. Remeika (private communication).

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