TABLE 2

Guinier Diffraction Data for Some Rare Earth Orthoaluminates.

	Eu		Gd		Tb		Dy		Ho		Er		Tm		Yb		Lu	
hkℓ	d_o	d_c	d_o	d_c	d_o	d_c	d_o	d_c	d_o	d_c	d_o	d_c	d_o	d_c	d_o	d_c	d_o	d_c
101													4.215 vw	4.211	4.203 vw	4.197	4.180 vw	4.181
110	3.735 m	3.734	3.731 m	3.731	3.729 m	3.727	3.722 m	3.720	3.714 s	3.713	3.709 m	3.706	3.700 ms	3.700	3.696 s	3.695	3.685 ms	3.686
002		3.731	3.726 w	3.723	3.711 wm	3.710	3.699 m	3.698	3.688 ms	3.687	3.679 m	3.677	3.667 m	3.667	3.655 ms	3.657	3.651 wm	3.650
111			3.337 w	3.335	3.330 w	3.330	3.325 wm	3.323	3.316 m	3.316	3.310 m	3.310	3.303 m	3.304	3.298 m	3.298	3.291 m	3.290
020	2.647 w	2.647	2.651 w	2.651	2.653 w	2.655	2.659 wm	2.659	2.662 wm	2.661	2.663 wm	2.664	2.663 m	2.664	2.665 m	2.666	2.665 wm	2.666
112	2.639 s	2.639	2.635 s	2.635	2.628 s	2.629	2.622 vs	2.622	2.617 vs	2.616	2.611 s	2.610	2.603 s	2.605	2.598 vs	2.599	2.593 vs	2.594
200		2.634	2.626 w	2.625	2.616 w	2.616	2.603 wm	2.603	2.591 m	2.591	2.579 wm	2.580	2.572 m	2.572	2.562 m	2.563	2.550 wm	2.551
021			2.499 vvw	2.497	2.500 vw	2.500	2.502 wm	2.502	2.503 wm	2.503	2.505 m	2.504	2.503 m	2.504	2.503 m	2.504	2.503 m	2.504
211											2.214 w	2.214	2.208 w	2.209	2.202 w	2.202	2.194 w	2.194
103												2.214						
022	2.158 wm	2.159	2.159 w	2.159	2.159 w	2.159	2.158 m	2.159	2.159 m	2.158	2.158 wm	2.157	2.154 m	2.155	2.154 m	2.154	2.153 m	2.153
202	2.151 wm	2.151	2.145 w	2.145	2.138 w	2.138	2.128 m	2.128	2.120 m	2.120	2.113 wm	2.112	2.104 m	2.105	2.098 ms	2.099	2.091 m	2.091
113					2.060 vw	2.061	2.055 vw	2.055	2.050 w	2.050	2.044 w	2.045	2.039 wm	2.040	2.035 m	2.035	2.030 m	2.031
122									1.992 vw	1.992					1.986 vw	1.986		
220	1.865 wm	1.867	1.865 wm	1.865	1.864 wm	1.863	1.860 m	1.860	1.856 m	1.856	1.854 wm	1.853	1.850 m	1.850	1.848 m	1.847	1.843 m	1.843
004		1.865			1.855 w	1.855	1.849 m	1.849	1.843 m	1.844	1.839 wm	1.838	1.833 wm	1.833	1.828 m	1.829	1.824 wm	1.825
023	1.815 w	1.812			1.808 w	1.810	1.805 wm	1.807	1.805 w	1.806	1.803 vw	1.804	1.802 wm	1.801	1.799 wm	1.799	1.797 wm	1.797
221		1.811				1.807		1.804	1.800 wm	1.800	1.797 m	1.797	1.795 wm	1.794	1.791 m	1.791	1.787 m	1.787
222	1.668 w	1.669	1.665 wm	1.668	1.665 vw	1.665	1.661 vw	1.661	1.658 w	1.658	1.654 wm	1.655	1.652 w	1.652	1.649 w	1.649	1.645 wm	1.645
114		1.668		1.666	1.661 vw	1.661	1.655 w	1.656	1.652 wm	1.651	1.647 wm	1.647	1.643 wm	1.643	1.639 wm	1.639	1.635 m	1.636
310					1.657 vw	1.657	1.649 vw	1.649	1.643 vw	1.643	1.637 m	1.637	1.636 m	1.636	1.628 w	1.627	1.620 w	1.620
131			1.634 w	1.634	1.635 vw	1.635	1.636 wm	1.636	1.636 wm	1.637				1.632	1.636 m	1.636	1.635 m	1.636
311													1.593 w	1.593	1.589 vw	1.588		
132			1.527 w	1.527	1.528 w	1.528	1.528 wm	1.528	1.527 wm	1.528	1.527 wm	1.527	1.527 wm	1.526	1.526 wm	1.526	1.526 w	1.525
024					1.520 w	1.521	1.518 wm	1.518	1.515 wm	1.515			1.510 wm	1.510	1.508 wm	1.508	1.506 wm	1.506
204	1.522 w	1.522	1.518 wm	1.519	1.512 m	1.513	1.507 m	1.507	1.502 w	1.502	1.497 wm	1.497	1.493 w	1.493	1.489 w	1.489	1.485 wm	1.484
312		1.521		1.518		1.513		1.506	1.500 m	1.501	1.495 m	1.495	1.491 m	1.491	1.487 m	1.486	1.482 wm	1.481
223											1.478 w	1.478	1.476 wm	1.475	1.473 wm	1.472	1.470 w	1.469
133							1.387 w	1.387	1.386 wm	1.386	1.384 m	1.385	1.384 m	1.384	1.383 wm	1.383	1.382 wm	1.382
115															1.360 vw	1.360		
041											1.310 w	1.310	1.310 vw	1.310	1.312 w	1.311		
224	1.320 w	1.319			1.315 w	1.315	1.311 m	1.311	1.308 m	1.308	1.305 m	1.305	1.302 wm	1.302	1.300 wm	1.300	1.297 m	1.297
314															1.215 wm	1.215		
331									1.220 w	1.221								
332							1.178 m	1.176					1.169 wm	1.170	1.168 wm	1.167		
043														1.169				
241													1.167 w	1.167				
116	1.179 w	1.180											1.160 wm	1.161	1.158 w	1.158		
420		1.179																
225													1.149 w	1.149	1.148 w	1.147		
135														1.104				
422													1.105 wm	1.104				
206														1.104				

coordination between $TbFeO_3$ and $NdFeO_3$. At the extremities of the series this approximation breaks down. For $LuFeO_3$ the seventh and eighth nearest oxygen atoms are becoming second nearest neighbors, while for $LaFeO_3$ the ninth nearest oxygen is too close to be considered a next nearest-neighbor. This change in coordination number governs the behavior of the b parameter.

It seems likely that a similar mechanism applies in the case of the $REAlO_3$ series. However, it is important to note that the orthorhombic series begins with $SmAlO_3$ where the coordination number of Sm^{3+} is very nearly twelve, compared to eight for its iron counterpart. Also, the non-linear variation of the c parameter and the significant change in slope of the b parameter between Sm and Tb in Fig. 1 suggest a rapid decrease in the coordination numbers of the rare earth ions. Between $DyAlO_3$ and $LuAlO_3$ the coordination number does not appear to decrease as drastically. However, without a detailed knowledge of the structure of at least several more $REAlO_3$ members, it is difficult to ascertain how the rare earth polyhedron varies across the series.

Another interesting point is that starting with Ho one needs high pressures to synthesize single phase rare earth orthoaluminates. $LuAlO_3$ was easily formed at 32 kbar but no attempt was made to find the minimum pressure necessary for this synthesis. We suspect that 32 kbar exceeds the minimum considerably. It is a logical step to attempt to synthesize under pressure $MAlO_3$, where M is of smaller ionic radius than Lu^{3+}. We believe In^{3+} and possibly Sc^{3+} are likely M-cations and expect to proceed with these experiments in the near future.

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