comparisons to be made of detectability. For example, we assume that the X-ray data go out to the copper limit ($s_0 = 8{\cdot}2$ Å^{-1}) and that the electron diffraction data go out to a typical value of 10 Å^{-1}. We assume that the W temperature factor is 0·5 Å^2, the C 1 Å^2, and the H 3 Å^2. Then we obtain for the ratios of peak heights*

three-dimensions	X-rays	H : C : W	= 1 : 20 : ~480
	electrons		= 1 : 7 : 58
two-dimensions	X-rays		= 1 : 14 : 340
	electrons		= 1 : 6 : 43

* Our calculations on H, C, and W have verified that Vainshtein's (1956) semi-empirical method of computing central quantities such as peak heights and curvatures is reliable to within 25%.

From these ratios we conclude that the advantage of using electrons rather than X-rays for the detection of light atoms in the presence of heavy atoms is striking. These ratios of peak heights seem more in keeping with experience than do the ratios of peak volumes.

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The crystal structure of the lanthanide oxyiodides, SmOI, TmOI and YbOI.*

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In a program of investigation of unusual valence states of lanthanide compounds, TmOI was obtained during preparation of TmI_2 (Asprey & Kruse, 1960). Pure samples of anhydrous SmOI, TmOI, and YbOI have been prepared for purposes of identification. Subsequently, analysis of their crystal structures was carried out.

The oxyiodides are prepared by evaporation of the triiodide solution and heating the residue as described by Asprey & Kruse (1960). In a slightly different preparation, a solution of lanthanide triiodide was saturated with NH_4I and evaporated to dryness. The resultant residue was dried and annealed under vacuum in a quartz capillary at 550 °C. over night to remove NH_4I and residual lanthanide triiodide. The X-ray powder shots were made using a standard 114·5 mm. Norelco camera and Cu $K\alpha$ radiation.

These lanthanide oxyiodides crystallize in the tetragonal PbFCl structure type, as do a number of other lanthanide and actinide oxyhalides (Wyckoff, 1960). The unit cell dimensions for the three oxyiodides are given in Table 1.

Table 1. *Unit-cell dimensions of lanthanide oxyiodides*

Structure type: PbFCl
Tetragonal space group, $P4/nmm$–D_{4h}^7

	a_0	c_0
SmOI	4·008 ± 0·005 Å	9·192 ± 0·008 Å
TmOI	3·887 ± 0·001	9·166 ± 0·002
YbOI	3·870 ± 0·006	9·161 ± 0·008

Previously reported oxyiodides (Wyckoff, 1960)

BiOI	3·985 Å	9·129 Å
LaOI	4·144	9·126
PuOI	4·042	9·169

The sample of TmOI was of more immediate concern and gave the best powder patterns, consequently parameter values were determined to compare calculated with observed intensities. The final parameters obtained for TmOI are given in Table 2 along with parameters reported for LaOI, PuOI and BiOI. Table 3 presents the pertinent interatomic distances for TmOI. The distances all fall within ranges anticipated for these ions except for the relatively short I–I distance of 3·89 Å. However, the other isostructural oxyhalides show this same shortening of the halogen–halogen distances between adjacent halogen layers.

Table 2. *Atomic position parameters for* TmOI *and previously reported* MOI *structures*

Space group positions: O (a): 0, 0, 0; ½, ½, 0
I (c): 0, ½, u; ½, 0, $\bar{u}$
M (c): 0, ½, u; ½, 0, $\bar{u}$

TmOI:	$U_I = 0{\cdot}680$	$U_{Tm} = 0{\cdot}125$
LaOI:	$U_I = 0{\cdot}660$	$U_{La} = 0{\cdot}135$
PuOI:	$U_I = 0{\cdot}67$	$U_{Pu} = 0{\cdot}13$
BiOI:	$U_I = 0{\cdot}668$	$U_{Bi} = 0{\cdot}132$

Table 3. *Interatomic distances in* TmOI

(In Å, all ±0·02)

Tm–Tm	3·58; 3·89	I–I	3·89; 4·29
Tm–I	3·28	I–O	3·52
Tm–O	2·26	O–O	2·75; 3·89

A tabulation of the partial powder X-ray diffraction patterns of SmOI, TmOI, and YbOI is given in Table 4. The relative peak intensities are essentially the same for all three samples. The I_o has been corrected for absorption by a cylindrical powder specimen with $\mu r = 20{\cdot}0$. An isothermal overall temperature factor correction with $\beta = 2{\cdot}0$ was included in the I_c.

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Table 4. *Partial powder X-ray diffraction patterns of* TmOI, SmOI, *and* YbOI

	TmOI				SmOI		YbOI	
hkl	I_c*	I_o†	d_c	d_o	d_c	d_o	d_c	d_o
001	15	17	9·166 Å	9·149 Å	9·192 Å	9·180 Å		
002	2	2	4·583	4·583	4·596	4·545		
101	<1	2	3·579	3·602	3·674	—		
003	<1	—	3·005	—	3·064	—		
102	100	100	2·964	2·946	3·021	3·006	2·956 Å	2·963 Å
110	59	54	2·748	2·732	2·834	2·823	2·737	2·737
111	3	2	2·633	2·614	2·708	2·575	2·622	2·625
103	24	26	2·402	2·387	2·434	2·421	2·397	2·409
112	10	6	2·357	2·346	2·412	2·418	2·349	—
004	11	5	2·291	2·282	2·298	2·294	2·290	2·250
113	<1	—	2·043	—	2·081	—	2·038	—
104	11	6	1·974	1·964	1·994	2·001	1·971	—
200	34	38	1·943	1·936	2·004	2·056	1·935	1·938
201	5	6	1·901	1·894	1·958	—	1·893	1·896
005	8	7	1·833	1·828	1·838	1·838	1·832	1·854
202	3	—	1·789	—	1·837	—	1·782	—
114	25	20	1·760	1·754	1·785	1·781	1·756	1·764
211	<1	—	1·708	—	1·759	—	1·701	—
105	2	—	1·658	—	1·671	—	1·656	—
203	<1	—	1·640	—	1·677	—	1·634	—
212	66	66	1·625	1·621	1·670	1·667	1·619	1·622
006	2	—	1·528	—	1·532	—	1·527	1·529
115	22	24	1·525	1·522	1·542	1·541	1·522	1·529
213	19	19	1·511	1·508	1·547	1·549	1·506	1·510
204	11	9	1·482	1·479	1·510	1·507	1·478	1·485
106	4	5	1·422	1·419	1·431	1·427	1·420	—
214	10	7	1·385	1·385	1·413	1·416	1·381	1·372
220	14	23	1·374	1·372	1·417		1·368	
221	2	4	1·359	1·386	1·400	—	1·353	—
116	3	—	1·335	—	1·348	—	1·333	—
205	15	14	1·334	1·332	1·355	1·353	1·330	1·338
222	2	—	1·316	—	1·354	—	1·311	—
007	2	—	1·309	—	1·313	—	1·309	—
301	<1	—	1·283	—	1·322	—	1·277	—
215	1	—	1·261	—	1·283	—	1·258	—
223	<1	—	1·253	—	1·286	—	1·249	—
302	17	18	1·247	1·246	1·283	1·284	1·242	1·246
107	13	13	1·241	1·239	1·248	1·246	1·240	
310	18	17	1·229	1·229	1·267	1·268	1·224	1·227
311	3	2	1·218	1·225	1·256	—	1·213	—
206	3	—	1·201	—	1·217	—	1·199	1·198
303	5	8	1·193	1·207	1·225	1·224	1·188	—
312	4	—	1·187	—	1·222	—	1·182	—
117	3	—	1·182	—	1·191	—	1·181	—
224	7	7	1·178	1·177	1·206	1·206	1·175	—
216	4	2	1·147	1·146	1·165	1·165	1·145	—
008	<1	—	1·145	—	1·490	—	1·145	—
313	<1	—	1·140	—	1·171	—	1·136	—
304	2	2	1·128	1·127	1·155	1·156	1·124	—
225	8	10	1·100	1·099	1·122	1·123	1·096	—
108	<1	—	1·099	—	1·104	—	1·098	—
207	3	—	1·086	—	1·098	1·081	1·084	1·083
314	13	14	1·083	1·083	1·110	1·111	1·079	
321	<1	—	1·071	—	1·104	—	1·066	—
305	<1	—	1·058	—	1·081	(322)	1·055	—
118	1	—	1·057	—	1·065	—	1·056	—
322	21	22	1·049	1·049	1·080	1·081	1·045	1·048
217	18	26	1·046	1·046	1·059	1·059	1·044	
226	2	—	1·022	—	1·040	(323)	1·019	
315	14	18	1·021	1·021	1·043	(323)	1·018	1·019
009	2	—	1·018	—	1·021	—	1·018	
323	7	10	1·017	1·017	1·045	1·044	1·013	—
306	2	—	0·988	—	1·007	—	0·985	—

* Calculated intensities normalized to yield strongest I = 100.

† Relative peak intensities above background from densitometer measurements. Very, very weak observed lines have been given a relative value of 2 on this scale.