symmetrical interactions at 95 °K than at 300 °K, a feature which will be of interest in relation to the crystal structures of the aromatic hydrocarbons (Mason, 1961). It also affords an explanation of the temperature dependence of the crystal susceptibilities; the calculated *molecular* susceptibilities are found, as could be intuitively expected, to be temperature independent (Leela, 1962).

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The Crystal Structure of UF_4*

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The crystal structure of UF_4 has been determined from single-crystal X-ray data. The monoclinic unit cell has the dimensions $a = 12{\cdot}73$, $b = 10{\cdot}75$, $c = 8{\cdot}43$ Å and $\beta = 126°\ 20'$; space group $C2/c$. It contains twelve formula units per unit cell. These cell dimensions are identical with those of Shankar, Khubchandani & Padmanabhan (1957). In the least-squares refinement of the structure a secondary extinction parameter and the real and imaginary portions of the anomalous dispersion corrections were used. Normal interatomic distances were observed. Uranium atoms have as neighbors eight fluorine atoms arranged in a slightly distorted antiprism configuration.

Introduction

Two items have renewed our interest in the structure of UF_4; first, the determination of the crystal structure of ZrF_4 by Burbank & Bensey (1956) in which fluorine atom positions are given and, second, a single crystal fragment of UF_4 given to us by W. P. Ellis of this Laboratory for structure analysis. The fragment selected for structure analysis yielded the best optical extinction figure of several score examined and therefore was the most strain-free sample available.

Crystallographic data

The crystal structure of UF_4 was first described by Zachariasen (1949). A monoclinic unit cell containing twelve formula units, isostructural with ZrF_4 and HfF_4, was proposed. Only the uranium atom positions were given and these only approximately (see Table 1). Shankar, Khubchandani & Padmanabhan (1957) used

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Table 1. *Uranium atom positions in* UF_4

Atom	Position set	Zachariasen	Present work
U(1)	*e*	$x = 0.000$	$x = 0.0000$
		$y = 0.200$	$y = 0.2126 \pm 0.0002$
		$z = 0.250$	$z = 0.2500$
U(2)	*f*	$x = 0.208$	$x = 0.2042 \pm 0.0002$
		$y = 0.437$	$y = 0.4281 \pm 0.0002$
		$z \simeq -0.17$	$z = 0.8307 \pm 0.0003$

more accurate measurements and found for UF_4: monoclinic,

$$a = 12.73,\ b = 10.75,\ c = 8.43\ \text{Å};\ \beta = 126°\ 20',$$

$Z = 12$, density 6.72 g.cm^{-3} and space group No. 15, $C2/c$. Neither of these references propose any positional parameters for the fluorine atoms.

Experimental

Intensity measurements for reflections with $\theta \leq 20.0°$ were made with a single-crystal orienter on an XRD 5 apparatus, Mo $K\alpha$ radiation and balanced filters being used. The entire hemisphere of the reciprocal lattice was investigated so that most reflections were measured twice. Lorentz-polarization corrections were made in the usual manner. The intensities were also corrected for the effects of absorption. A program to calculate these corrections, which had been written by Burnham (1962) for Weissenberg geometry, was modified for single-crystal orienter geometry and incorporated into our data processing programs. After correction for absorption, equivalent reflections were averaged. An R index formed by comparing individual values of equivalent reflections with their mean values was 3·0% based on F and 5·9% based on F^2. There were 362 non-equivalent reflections observed out of a possible 435.

Determination of the structure

The initial structure was obtained by combining the uranium atom positions of Zachariasen (1949) with the fluorine atom positions of Burbank & Bensey (1956). This structure refined readily by the least-squares technique. Atomic form factors were used in the functional form given by Forsyth & Wells (1959). In all least-squares calculations, the function minimized was $\Sigma w(\Delta F)^2$ and unit weights were used.

In addition to the usual positional and thermal parameters, a secondary extinction correction was included (Cromer, Larson & Roof, 1964). The least-squares program was further altered so that $\Delta f''$, the imaginary portion of the anomalous dispersion correction, could be included in the calculated structure factors.

Table 2. *Variation in sum of residuals squared as a function of* $\Delta f'$

$\Delta f'$	Σ
− 5·0	4.210×10^3
−10·0	4.187×10^3
−15·0	4.191×10^3
−20·0	4.236×10^3

A value of $\Delta f'' = +13.0$ electrons (Roof, 1961), was used throughout the least-squares analysis. As a function of $\Delta f'$ the sum of residuals squared varies as shown in Table 2, indicating that the 'best' solution would occur at approximately $\Delta f' = -12.5$. Positive thermal parameters occur in the range $\Delta f' = -10$ to -20. Negative thermal parameters occur outside this range. The very shallow minimum in Σ as given in Table 2, and the wide range in $\Delta f'$ in which positive thermal parameters occur indicates that this structure is not sensitive to the value of $\Delta f'$.

The final least-squares parameters for $\Delta f' = -15.0$ are given in Table 3. The final changes as fractions of their standard deviations were $< 1 \times 10^{-3}$ for position parameters, $< 1.5 \times 10^{-3}$ for temperature factors and $< 1.5 \times 10^{-2}$ for g. Observed and calculated structure factors, for which $R = 6.6\%$, are given in Table 4.

Discussion of the structure

A view of the structure of UF_4 down the positive b axis is given in Fig. 1. The interatomic distances are listed in Table 5. The standard deviations given in this table have been computed with all correlation terms obtained from the least-squares matrix included. According to the definition of neighbor given by Cromer, Larson and Roof (1964), each atom with its neighbors forms a polyhedron as described in Table 6.

Table 3. *Final least-squares parameters for* UF_4

The uranium atoms are corrected for the effects of anomalous dispersion with $\Delta f' = -15.0$ and $\Delta f'' = +13.0$.
The secondary extinction coefficient $g = (2.63 \pm 0.07) \times 10^{-7}$

Atom	Position set	x	y	z	B
U(1)	*e*	0·0000	0·2126 ± 0·0002	0·2500	0·33 ± 0·08 Å^2
U(2)	*f*	0·2042 ± 0·0002	0·4281 ± 0·0002	0·8307 ± 0·0003	0·30 ± 0·07
F(1)	*c*	0·2500	0·2500	0·0000	2·41 ± 0·78
F(2)	*e*	0·0000	0·5921 ± 0·0032	0·2500	1·52 ± 0·68
F(3)	*f*	0·8843 ± 0·0026	0·2973 ± 0·0027	0·9309 ± 0·0039	2·92 ± 0·59
F(4)	*f*	0·8786 ± 0·0023	0·0525 ± 0·0024	0·0459 ± 0·0034	1·98 ± 0·51
F(5)	*f*	0·7894 ± 0·0023	0·5298 ± 0·0022	0·8940 ± 0·0034	1·91 ± 0·51
F(6)	*f*	0·6192 ± 0·0024	0·1178 ± 0·0023	0·7834 ± 0·0037	2·30 ± 0·54
F(7)	*f*	0·6287 ± 0·0022	0·3491 ± 0·0023	0·6633 ± 0·0033	1·68 ± 0·49

Table 4. *Observed and calculated structure factors for* UF_4

If $|F_o|$ is negative the minus sign means 'less than'. The terms A and B are as defined in Cromer, Larson & Roof (1964)

h	k	l	$\|F_o\|$	$\|F_c\|$	A	B
0	0	2	678	538	-535	-53
0	0	4	-37	38	37	3
0	0	6	150	151	149	24
2	0	-6	582	553	-549	-69
2	0	-4	742	659	655	69
2	0	-2	279	292	-291	-27
2	0	0	220	242	-241	-18
2	0	2	96	94	91	21
2	0	4	190	167	166	19
4	0	-6	-40	6	6	-0
4	0	-4	239	228	-226	-26
4	0	-2	-21	13	-12	5
4	0	0	331	340	337	47
4	0	2	644	592	-587	-75
4	0	4	415	585	581	56
6	0	-8	139	140	-138	-19
6	0	-6	151	159	-157	-22
6	0	-4	541	604	600	67
6	0	-2	668	701	-697	-73
6	0	0	247	259	257	33
6	0	2	54	61	59	13
8	0	-8	494	466	461	73
8	0	-6	556	578	-574	-54
8	0	-4	64	70	69	6
8	0	-2	154	169	168	25
8	0	0	-37	35	34	-8
10	0	-6	53	70	66	22
10	0	-4	99	104	102	15
10	0	-2	392	416	-411	-61
12	0	-6	427	457	-451	-72
12	0	-4	392	413	409	58
1	1	-6	88	68	-66	-14
1	1	-5	105	100	99	17
1	1	-4	367	326	-325	-28
1	1	-3	51	45	-45	-3
1	1	-2	499	430	429	39
1	1	-1	129	132	132	9
1	1	0	103	106	-105	-7
1	1	1	381	362	-361	-30
1	1	2	309	265	-262	-37
1	1	3	488	432	430	46
1	1	4	481	441	438	50
1	1	5	295	283	-280	-41
1	1	6	116	130	-128	-22
3	1	-7	-51	44	-44	-3
3	1	-6	178	153	151	25
3	1	-5	207	169	168	19
3	1	-4	94	74	72	17
3	1	-3	310	307	-305	-40
3	1	-2	419	495	-492	-50
3	1	-1	460	525	523	47
3	1	0	371	418	416	41
3	1	1	210	198	-195	-33
3	1	2	-34	19	-19	1
3	1	3	109	93	92	11
3	1	4	289	243	-240	-35
3	1	5	-46	17	-16	-2
5	1	-7	338	302	-299	-45
5	1	-6	376	352	-348	-50
5	1	-5	347	337	335	41
5	1	-4	252	257	256	21
5	1	-3	177	183	-182	-21
5	1	-2	160	174	172	23
5	1	-1	40	42	-42	4
5	1	0	406	422	-420	-40
5	1	1	56	55	-55	-7
5	1	2	96	94	93	13
5	1	3	141	133	130	26
7	1	-8	-41	15	-14	-4
7	1	-7	-39	10	-3	-10
7	1	-6	286	294	292	37
7	1	-5	-30	17	17	3
7	1	-4	239	248	-247	-30
7	1	-3	158	149	-149	-16
7	1	-2	55	58	-56	-11
7	1	-1	297	308	306	37
7	1	0	375	394	391	47
7	1	1	349	350	-347	-46
7	1	2	266	266	-263	-43
9	1	-7	198	197	-195	-27
9	1	-6	214	219	-216	-33
9	1	-5	286	293	289	44
9	1	-4	343	364	360	51
9	1	-3	319	333	-330	-42
9	1	-2	137	145	-143	-26
9	1	-1	170	169	167	23
9	1	0	135	137	-136	-18
11	1	-7	231	232	-230	-32
11	1	-6	-33	16	-16	-2
11	1	-5	81	95	94	12
11	1	-4	268	279	-277	-34
11	1	-3	-32	9	9	-2
11	1	-2	197	199	197	32
0	2	0	130	125	125	9
0	2	1	636	545	-543	-47
0	2	2	52	48	47	6
0	2	3	83	80	79	14
0	2	4	322	309	-307	-36
0	2	5	145	151	149	21
0	2	6	318	326	322	52
2	2	-7	221	215	-211	-32
2	2	-6	56	51	-51	-5
2	2	-5	431	386	382	51
2	2	-4	68	57	57	4
2	2	-3	246	227	-225	-32
2	2	-2	193	184	182	22
2	2	-1	73	73	-73	-7
2	2	0	528	542	-540	-50
2	2	1	237	233	231	29
2	2	2	547	508	505	51
2	2	3	-47	42	-40	-12
2	2	4	163	138	-135	-26
2	2	5	211	201	-200	-26
4	2	-7	100	98	-97	-11
4	2	-6	292	261	259	37
4	2	-5	163	148	-146	-23
4	2	-4	552	558	-556	-54
4	2	-3	125	124	122	24
4	2	-2	280	317	314	41
4	2	-1	64	70	70	8
4	2	0	77	73	-72	-10
4	2	1	394	396	-393	-44
4	2	2	60	66	-66	-9
4	2	3	433	408	405	48
4	2	4	-47	29	-29	2
6	2	-7	52	48	47	10
6	2	-6	197	191	190	24
6	2	-5	244	251	250	29
6	2	-4	98	104	104	3
6	2	-3	494	560	-558	-51
6	2	-2	57	46	46	-6
6	2	-1	334	369	367	36
6	2	0	124	123	-122	-18
6	2	1	-34	20	20	2
6	2	2	299	285	281	45
6	2	3	191	191	-190	-27
8	2	-7	319	311	-307	-46
8	2	-6	58	42	42	4
8	2	-5	121	135	134	16
8	2	-4	224	245	-243	-34
8	2	-3	188	198	197	19
8	2	-2	370	388	385	53
8	2	-1	170	180	-178	-26
8	2	0	307	321	-318	-42
8	2	1	40	36	-36	-3
10	2	-7	173	180	178	27
10	2	-6	311	320	316	50
10	2	-5	96	101	-100	-14
10	2	-4	200	211	-209	-28
10	2	-3	106	134	-132	-23
10	2	-2	33	10	-10	-1
10	2	-1	312	317	313	48
12	2	-5	302	319	315	47
12	2	-4	-35	15	-15	-1
1	3	-6	64	76	74	14
1	3	-5	232	206	-203	-34
1	3	-4	176	148	-146	-24
1	3	-3	715	695	692	68
1	3	-2	243	222	220	27
1	3	-1	499	526	-523	-56
1	3	0	165	173	-172	-20
1	3	1	67	65	65	9
1	3	2	188	168	167	9
1	3	3	260	225	224	28
1	3	4	-45	32	-32	-6
1	3	5	112	110	-108	-19
3	3	-7	454	406	401	64
3	3	-6	190	164	162	23
3	3	-5	314	286	-284	-32
3	3	-4	112	111	-110	-14
3	3	-3	179	169	-169	-15
3	3	-2	44	39	39	6
3	3	-1	199	208	206	30
3	3	0	63	69	-69	-8
3	3	1	81	89	89	2
3	3	2	147	130	129	18
3	3	3	415	382	-379	-49
3	3	4	256	225	-224	-26
5	3	-7	209	181	-179	-28
5	3	-6	101	95	95	6
5	3	-5	104	90	89	17
5	3	-4	134	143	-142	-13
5	3	-3	264	284	282	28
5	3	-2	190	195	194	23
5	3	-1	593	638	-634	-66
5	3	0	277	290	-289	-27
5	3	1	497	512	509	59
5	3	2	120	120	118	20
5	3	3	104	104	-103	-15
7	3	-7	381	372	368	50
7	3	-6	164	164	162	26
7	3	-5	491	546	-542	-67
7	3	-4	219	230	-228	-25
7	3	-3	267	305	303	38
7	3	-2	138	152	152	15
7	3	-1	52	53	53	10
7	3	0	-33	25	-24	-6
7	3	1	222	223	-221	-29
7	3	2	-42	50	49	7
9	3	-7	84	89	88	12
9	3	-6	-33	34	33	9
9	3	-5	213	210	209	26
9	3	-4	-29	16	16	-5
9	3	-3	107	110	-108	-21
9	3	-2	70	81	80	11
9	3	-1	104	110	-108	-21
9	3	0	126	134	-132	-21
11	3	-6	97	119	118	16
11	3	-5	283	297	-294	-45
11	3	-4	169	172	-171	-25
11	3	-3	403	436	431	66
0	4	0	-33	16	16	3
0	4	1	229	181	-180	-23
0	4	2	-66	35	34	-9
0	4	3	116	118	-117	-18
0	4	4	127	137	135	20
0	4	5	407	393	388	59
0	4	6	176	172	-170	-26
2	4	-6	-48	11	-10	-4
2	4	-5	230	205	203	28
2	4	-4	-41	35	35	5
2	4	-3	-35	26	-26	-4
2	4	-2	145	142	-141	-15
2	4	-1	268	283	-280	-44
2	4	0	172	172	170	25
2	4	1	717	699	695	70
2	4	2	259	228	-226	-26
2	4	3	414	376	-373	-49
2	4	4	110	102	101	16
2	4	5	-48	2	-2	1
4	4	-7	124	122	121	20
4	4	-6	115	104	-102	-20
4	4	-5	485	472	-468	-62
4	4	-4	215	204	203	27
4	4	-3	501	552	548	65
4	4	-2	228	243	-242	-34
4	4	-1	190	195	-193	-25
4	4	0	151	151	150	10
4	4	1	186	191	-190	-19
4	4	2	-38	31	-31	-3
4	4	3	206	200	198	25
4	4	4	-52	48	47	7
6	4	-7	311	297	294	45
6	4	-6	149	141	-140	-15
6	4	-5	-31	11	11	1
6	4	-4	35	33	32	5
6	4	-3	236	260	-258	-29
6	4	-2	-27	15	-15	-4
6	4	-1	59	52	51	10
6	4	0	78	75	74	13
6	4	1	228	228	225	37
6	4	2	189	181	-180	-23
8	4	-7	148	153	-151	-24
8	4	-6	-34	45	-44	-8
8	4	-5	45	57	-55	-14
8	4	-4	142	147	146	19
8	4	-3	380	434	430	58
8	4	-2	155	163	-161	-26
8	4	-1	463	497	-492	-66
8	4	0	126	127	125	22
8	4	1	179	183	180	30
10	4	-6	157	163	-161	-25
10	4	-5	327	348	-345	-50
10	4	-4	88	89	87	17
10	4	-3	-32	16	15	5
10	4	-2	-35	31	-30	-6
1	5	-6	-61	111	-110	-16
1	5	-5	-50	10	10	-2
1	5	-4	401	372	369	46
1	5	-3	287	258	257	28
1	5	-2	650	582	-580	-55
1	5	-1	203	203	-202	-18
1	5	0	302	307	305	33
1	5	1	158	135	-134	-18
1	5	2	-43	28	-28	-2
1	5	3	301	325	322	46
1	5	4	-48	29	-28	-8
1	5	5	251	264	-261	-39
3	5	-6	355	338	-336	-44
3	5	-5	-44	31	-31	-0
3	5	-4	125	113	112	15
3	5	-3	333	330	-328	-37
3	5	-2	63	68	67	7
3	5	-1	479	513	511	48
3	5	0	-27	24	24	-1
3	5	1	147	140	-138	-23
3	5	2	188	195	-193	-28
3	5	3	79	73	-72	-14
3	5	4	368	332	328	51
5	5	-6	61	57	56	8
5	5	-5	263	242	239	38
5	5	-4	103	112	111	23
5	5	-3	44	26	-26	-3
5	5	-2	309	333	-330	-44
5	5	-1	213	234	-232	-27
5	5	0	409	433	430	55
5	5	1	85	95	92	21
5	5	2	249	243	-241	-33
5	5	3	65	79	78	12
7	5	-7	122	112	111	13
7	5	-6	346	351	-347	-52
7	5	-5	159	165	-162	-28
7	5	-4	351	368	365	48
7	5	-3	-29	47	47	5
7	5	-2	144	152	-151	-19
7	5	-1	187	188	185	32
7	5	0	-34	17	-16	-6
7	5	1	302	303	-299	-47
9	5	-6	-35	30	-30	4
9	5	-5	295	304	300	44
9	5	-4	-32	27	-26	-9
9	5	-3	264	274	-271	-41
9	5	-2	86	91	-90	-9
9	5	-1	57	57	57	8
0	6	0	452	434	-431	-50
0	6	1	370	377	-374	-43
0	6	2	216	221	219	28
0	6	3	194	193	191	26
0	6	4	-73	69	67	16
0	6	5	75	88	87	-7
2	6	-5	343	328	325	45
2	6	-4	347	318	-315	-43
2	6	-3	297	277	-275	-35
2	6	-2	106	114	114	3
2	6	-1	161	172	171	15
2	6	0	275	273	271	35
2	6	1	-35	17	-17	4
2	6	2	317	297	-295	-37
2	6	3	52	49	47	12
2	6	4	-49	18	18	1
4	6	-6	152	129	-128	-18
4	6	-5	-40	14	12	7
4	6	-4	315	301	299	41
4	6	-3	65	67	-67	-6
4	6	-2	162	171	-169	-22
4	6	-1	111	120	118	23
4	6	0	208	207	-206	-23
4	6	1	282	289	-286	-41
4	6	2	366	358	355	48
4	6	3	315	302	299	43
6	6	-6	-47	13	13	1
6	6	-5	170	175	172	33
6	6	-4	280	288	-285	-41
6	6	-3	312	331	-328	-45
6	6	-2	312	347	344	46
6	6	-1	251	265	263	37
6	6	0	84	76	-75	-11
6	6	1	100	105	-104	-17
8	6	-6	218	213	211	30
8	6	-5	220	226	224	27
8	6	-4	52	51	49	13
8	6	-3	39	28	-27	-8
8	6	-2	290	292	-289	-40
8	6	-1	-36	39	39	3
8	6	0	150	154	151	26
10	6	-4	-34	20	20	3
1	7	-5	-54	27	27	2
1	7	-4	-51	73	72	12
1	7	-3	42	31	31	-3
1	7	-2	178	161	-160	-23
1	7	-1	-35	32	32	3
1	7	0	76	65	-64	-11
1	7	1	-42	11	-11	-2
1	7	2	400	396	392	58
1	7	3	-49	34	34	1
1	7	4	525	484	-479	-72
3	7	-5	-44	7	-6	2
3	7	-4	252	234	-231	-37
3	7	-3	45	39	-39	-1
3	7	-2	555	597	593	73
3	7	-1	32	31	31	1
3	7	0	450	478	-474	-63
3	7	1	-36	2	-1	-1
3	7	2	81	86	84	17
3	7	3	-47	47	47	2
5	7	-5	-44	40	40	1
5	7	-4	257	256	-253	-40
5	7	-3	45	27	-27	-2
5	7	-2	85	92	-92	-7
5	7	-1	57	50	50	3
5	7	0	149	169	167	25
5	7	1	-40	47	-47	-3
5	7	2	-45	41	41	4
7	7	-5	-38	55	54	3
7	7	-4	64	77	75	14
7	7	-3	63	58	-58	-2
7	7	-2	164	168	166	30
7	7	-1	-33	18	-18	1
7	7	0	416	427	-422	-68
9	7	-4	451	473	-468	-72
9	7	-3	-34	24	24	-1
0	8	0	396	384	-380	-52
0	8	1	303	323	320	43
0	8	2	187	189	187	31
0	8	3	171	153	-151	-24
0	8	4	107	84	83	14
2	8	-4	314	297	-293	-45
2	8	-3	322	290	288	35
2	8	-2	-38	47	46	8
2	8	-1	75	75	-74	-13
2	8	0	207	203	201	30
2	8	1	-43	26	26	1
2	8	2	255	230	-228	-32
2	8	3	-56	68	-68	-10
4	8	-5	-43	9	-8	-4
4	8	-4	277	250	247	36
4	8	-3	44	37	37	3
4	8	-2	73	75	-73	-17
4	8	-1	193	201	-200	-21
4	8	0	158	163	-161	-25
4	8	1	294	303	300	41
6	8	-4	299	305	-302	-43
6	8	-3	280	293	289	45
6	8	-2	297	325	322	48
6	8	-1	247	248	-245	-37
6	8	0	90	96	-95	-14
1	9	-3	132	158	-156	-25
1	9	-2	358	330	-326	-49
1	9	-1	103	104	103	15
1	9	0	151	161	158	29
1	9	1	84	84	81	21
1	9	2	-49	5	-5	-1
3	9	-3	263	245	242	39
3	9	-2	51	53	52	7
3	9	-1	341	358	-355	-51
3	9	0	-37	17	17	-2
3	9	1	198	192	190	26
5	9	-3	-36	21	20	5
5	9	-2	237	253	-250	-39
5	9	-1	140	153	151	24
0	10	0	-67	32	32	8
0	10	1	165	186	184	25
2	10	-2	113	109	-108	-17
2	10	-1	253	259	256	40
2	10	0	177	180	179	25

Table 5. *Interatomic distances in* UF_4

	(Å)
U(1)–2 F(3)	$2 \cdot 354 \pm 0 \cdot 027$
–2 F(4)	$2 \cdot 272 \pm 0 \cdot 025$
–2 F(6)	$2 \cdot 280 \pm 0 \cdot 025$
–2 F(7)	$2 \cdot 253 \pm 0 \cdot 023$
U(2)–F(1)	$2 \cdot 249 \pm 0 \cdot 002$
–F(2)	$2 \cdot 274 \pm 0 \cdot 004$
–F(3)	$2 \cdot 273 \pm 0 \cdot 028$
–F(4)	$2 \cdot 288 \pm 0 \cdot 024$
–F(5)	$2 \cdot 230 \pm 0 \cdot 023$
–F(5)	$2 \cdot 318 \pm 0 \cdot 023$
–F(6)	$2 \cdot 230 \pm 0 \cdot 025$
–F(7)	$2 \cdot 263 \pm 0 \cdot 024$
F(1)–2 F(2)	$3 \cdot 083 \pm 0 \cdot 019$
–2 F(3)	$3 \cdot 003 \pm 0 \cdot 027$
–2 F(5)	$2 \cdot 681 \pm 0 \cdot 024$
–2 F(7)	$2 \cdot 817 \pm 0 \cdot 023$
–2 U(2)	$2 \cdot 249 \pm 0 \cdot 002$
F(2)–2 F(1)	$3 \cdot 083 \pm 0 \cdot 019$
–2 F(3)	$2 \cdot 927 \pm 0 \cdot 032$
–2 F(5)	$2 \cdot 667 \pm 0 \cdot 025$
–2 F(6)	$2 \cdot 640 \pm 0 \cdot 039$
–2 F(7)	$3 \cdot 961 \pm 0 \cdot 034$
–2 U(2)	$2 \cdot 274 \pm 0 \cdot 004$
F(3)–F(1)	$3 \cdot 003 \pm 0 \cdot 027$
–F(2)	$2 \cdot 927 \pm 0 \cdot 032$
–F(4)	$2 \cdot 820 \pm 0 \cdot 038$
–F(5)	$2 \cdot 712 \pm 0 \cdot 036$
–F(6)	$2 \cdot 601 \pm 0 \cdot 036$
–F(6)	$2 \cdot 842 \pm 0 \cdot 037$
–F(6)	$3 \cdot 419 \pm 0 \cdot 036$
–F(7)	$2 \cdot 700 \pm 0 \cdot 034$
–F(7)	$2 \cdot 962 \pm 0 \cdot 036$
–U(1)	$2 \cdot 354 \pm 0 \cdot 027$
–U(2)	$2 \cdot 273 \pm 0 \cdot 028$
F(4)–F(3)	$2 \cdot 820 \pm 0 \cdot 038$
–F(4)	$2 \cdot 965 \pm 0 \cdot 046$
–F(4)	$3 \cdot 776 \pm 0 \cdot 044$
–F(5)	$2 \cdot 626 \pm 0 \cdot 032$
–F(5)	$2 \cdot 998 \pm 0 \cdot 033$
–F(6)	$2 \cdot 763 \pm 0 \cdot 031$

	(Å)
F(4)–F(7)	$2 \cdot 722 \pm 0 \cdot 031$
–F(7)	$2 \cdot 776 \pm 0 \cdot 035$
–F(7)	$2 \cdot 916 \pm 0 \cdot 033$
–U(1)	$2 \cdot 272 \pm 0 \cdot 025$
–U(2)	$2 \cdot 288 \pm 0 \cdot 024$
F(5)–F(1)	$2 \cdot 681 \pm 0 \cdot 024$
–F(2)	$2 \cdot 667 \pm 0 \cdot 025$
–F(3)	$2 \cdot 712 \pm 0 \cdot 036$
–F(3)	$3 \cdot 673 \pm 0 \cdot 034$
–F(4)	$2 \cdot 626 \pm 0 \cdot 032$
–F(4)	$2 \cdot 998 \pm 0 \cdot 033$
–F(5)	$4 \cdot 582 \pm 0 \cdot 046$
–F(6)	$2 \cdot 558 \pm 0 \cdot 034$
–F(6)	$2 \cdot 741 \pm 0 \cdot 033$
–F(7)	$2 \cdot 650 \pm 0 \cdot 033$
–F(7)	$3 \cdot 702 \pm 0 \cdot 034$
–U(2)	$2 \cdot 230 \pm 0 \cdot 023$
–U(2)	$2 \cdot 318 \pm 0 \cdot 023$
F(6)–F(2)	$2 \cdot 640 \pm 0 \cdot 039$
–F(3)	$2 \cdot 601 \pm 0 \cdot 036$
–F(3)	$2 \cdot 842 \pm 0 \cdot 037$
–F(3)	$3 \cdot 419 \pm 0 \cdot 036$
–F(4)	$2 \cdot 763 \pm 0 \cdot 034$
–F(5)	$2 \cdot 559 \pm 0 \cdot 034$
–F(5)	$2 \cdot 742 \pm 0 \cdot 033$
–F(6)	$2 \cdot 739 \pm 0 \cdot 047$
–F(6)	$4 \cdot 254 \pm 0 \cdot 050$
–F(7)	$2 \cdot 714 \pm 0 \cdot 035$
–U(1)	$2 \cdot 280 \pm 0 \cdot 025$
–U(2)	$2 \cdot 231 \pm 0 \cdot 025$
F(7)–F(1)	$2 \cdot 817 \pm 0 \cdot 023$
–F(2)	$3 \cdot 961 \pm 0 \cdot 034$
–F(3)	$2 \cdot 670 \pm 0 \cdot 034$
–F(3)	$2 \cdot 962 \pm 0 \cdot 036$
–F(4)	$2 \cdot 722 \pm 0 \cdot 031$
–F(4)	$2 \cdot 776 \pm 0 \cdot 035$
–F(4)	$2 \cdot 916 \pm 0 \cdot 033$
–F(5)	$2 \cdot 650 \pm 0 \cdot 033$
–F(5)	$3 \cdot 702 \pm 0 \cdot 034$
–F(6)	$2 \cdot 714 \pm 0 \cdot 035$
–U(1)	$2 \cdot 253 \pm 0 \cdot 023$
–U(2)	$2 \cdot 263 \pm 0 \cdot 024$

Table 6. *Description of polyhedra in* UF_4

Atom	Neighboring atoms	Polyhedron description
U(1)	8 F	8 three-sided and 2 four-sided faces
U(2)	8 F	10 three-sided faces and 1 four-sided face
F(1)	8 F and 2 U	12 three-sided and 2 four-sided faces
F(2)	10 F and 2 U	20 three-sided faces
F(3)	10 F and 2 U	16 three-sided and 2 four-sided faces
F(4)	9 F and 2 U	18 three-sided faces
F(5)	11 F and 2 U	18 three-sided and 2 four-sided faces
F(6)	10 F and 2 U	20 three-sided faces
F(7)	10 F and 2 U	16 three-sided and 2 four-sided faces

There exists a basic repeating unit consisting of five uranium atoms arranged in a distorted pyramid with

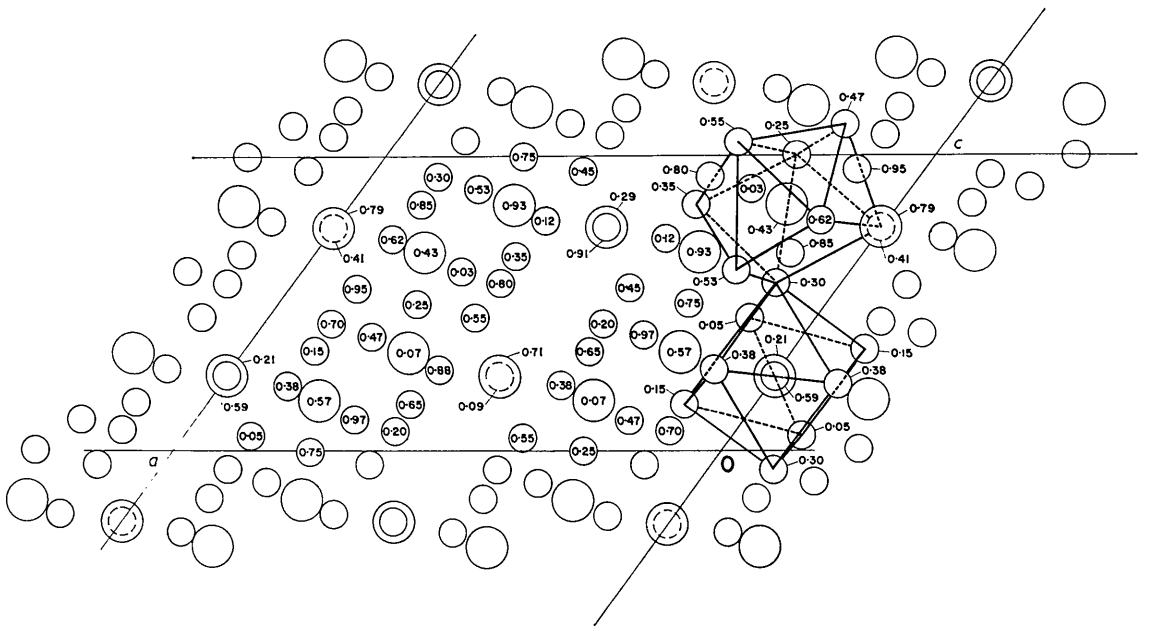

Fig. 1. The structure of UF_4 viewed down the positive b axis. Large circles are uranium atoms, small circles are fluorine atoms. Numbers represent the positional parameter y as a fraction of the unit-cell edge. The slightly distorted antiprisms about U(1) ($y=0{\cdot}21$) and about U(2) ($y=0{\cdot}43$) are also shown.

four atoms forming a rhomb-shaped base and the fifth comprising the apex of the pyramid. On approximately each edge of this pyramid there is a fluorine atom. Also, the eight fluorine atoms which are neighbors to U(1) (and the eight fluorine atoms which are neighbors to U(2)) are arranged in a slightly distorted antiprism configuration.

There is no significant difference between the structure of UF_4 refined in this paper and the structure of ZrF_4 given by Burbank & Bensey; this leads to the conclusion that these materials are isostructural.

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