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The Crystal Structure of $UMoC_2$*

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The structure of $UMoC_2$ has been determined from single-crystal X-ray data. The orthorhombic unit cell has the dimensions $a=5{\cdot}625$, $b=3{\cdot}249$ and $c=10{\cdot}980$ Å. There are four formula units per unit cell and all atoms are on the mirror planes in set 4(*c*) of space group *Pnma*. 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. The correction of Fourier coefficients for structures with anomalous scatters is discussed. There are no short C–C distances and this compound is not an acetylene type carbide.

Introduction

A specimen of $UMoC_2$ was given to us by Dr John Farr of this laboratory. Although the crystal structure of this compound was presumably known (Nowotny, Kieffer, Benesovsky & Laube, 1958), we decided to collect intensity data and refine the structure in the hope that more accurate carbon positions could be obtained. It was found that the structure given in the literature is in error. We find that the molybdenum atom and one of the carbon atoms are in quite different positions from those previously reported. The refinement of this structure was also of particular interest because, in order to obtain reasonable thermal parameters, it was desirable to add a secondary extinction parameter in the least-squares refinement and also to include in the calculated structure factors the imaginary portion of the anomalous dispersion correction to the form factors.

Crystallographic data

$UMoC_2$ is orthorhombic, space group *Pnma* as shown by the systematic extinctions and the structure determination. Lattice constants were measured on a carefully aligned General Electric Co. single-crystal orienter with Mo radiation ($\lambda\, K\alpha_1=0{\cdot}70926$ Å) and found to be $a=5{\cdot}625\pm0{\cdot}004$, $b=3{\cdot}249\pm0{\cdot}004$ and $c=10{\cdot}980\pm0{\cdot}006$ Å in good agreement with the values given by Nowotny *et al.* (1958). The calculated density with $Z=4$ is 11·85 g.cm^{-3}. All atoms lie on the mirror planes of *Pnma* in set 4(*c*), $x, \frac{1}{4}, z$.

Experimental

Intensities were measured with the single-crystal orienter and Mo $K\alpha$ radiation by using the stationary crystal and counter technique. The intensities and background corrections were measured with balanced filters, one filter consisting of zirconium foil and the other consisting of yttrium foil plus a small amount of aluminum foil. In addition a background dependent on 2θ was also subtracted. This background, also measured with the balanced filters, arises because of the small amount of $K\alpha$ radiation scattered by air and by the glass fiber on which the crystal is mounted and also, perhaps, from slight unbalance of the filter pair.

The crystal used was quite small with a maximum dimension of about 0·020 mm and was mounted on the *a* axis. Initially, intensities for reflections with $2\theta \le 45°$ were measured. Only the asymmetric quadrant of the reciprocal lattice was investigated and 123 reflections were observed out of a possible 156. After difficulties arose in the refinement the intensities were remeasured. The entire hemisphere of the reciprocal lattice with $2\theta \le 55°$ was investigated. There were 191 non-equivalent reflections observed out of 271 possible. Absorption corrections were applied to both data sets by the Busing & Levy (1957) method. 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 program for the IBM 7090. The crystal fragment did not have well defined boundary planes but its shape was approximated by a set of 13 planes. One's ability to measure and define the shape of a crystal by a small number of planes is the limiting factor in making proper absorption corrections. Transmission factors for this crystal varied from 0·20 to 0·27.

An R index formed by comparing equivalent observed reflections was 13·1% based on F^2 and 6·8% based on F. In this R index the numerator was the sum of the individual deviations from the mean of the observed equivalent values of F or F^2 and the denominator the sum of the observed values. It may be argued that our final R index, which is less than 6·8%, is meaningless. Nevertheless, we have refined to an R of about 4% and present the results.

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Table 1. *Coefficients of form factor functions*

Atom	*A*	*B*	*C*	*D*	*E*	Reference
U	44·51	2·316	17·14	22·78	15·05	Coefficients calculated from tables in *International Tables for X-ray Crystallography* (1962)
Mo	18·97	1·854	13·65	19·89	7·203	Forsyth & Wells (1959)
C	1·455	1·462	3·775	22·49	0·724	Forsyth & Wells (1959)

Determination of the structure

In all least-squares calculations, the function minimized was $\Sigma w(\Delta F)^2$. Form factors were used in functional form as follows:

$$f = A \exp(-Bs^2) + C \exp(-Ds^2) + E\,,$$

where $s = \sin\theta/\lambda$. The coefficients are given in Table 1. The real part of the anomalous dispersion was applied by changing the value of E. Zero weight was given to unobserved reflections. When other than unit weights were used, weights were determined by the counting statistics according to the method derived by Evans (1961). All R indices quoted include only observed reflections.

Table 2. *Atom positions for* $\mathrm{UMoC_2}$ *given by Nowotny et al.* (1958)

Atom	*x*	*y*	*z*
U	0·083	¼	0·143
Mo	0·350	¼	0·860
C(1)	0·50	¼	0·04
C(2)	0·72	¼	0·00

A least-squares refinement with unit weights was made with the first set of data by using the starting parameters given in Table 2. The uranium atom appeared to be properly located, but the molybdenum atom moved about 0·6 Å. The carbon atoms did not converge at all. A three-dimensional Patterson function was then computed and the approximate positions of all atoms, including the carbon atoms, were readily found. These positions were used as starting parameters in a second least-square refinement with unit weights and the atom positions converged to about the same values as were later obtained after more extensive calculations.

Although the position parameters converged, and the agreement between calculated and observed structure factors was reasonably good, ($R = 10\%$), the temperature factors of some or all of the atoms tended to become negative, in spite of the fact that values of $\Delta f'_{\mathrm{Mo}} = -1{\cdot}7$ electrons and of $\Delta f'_{\mathrm{U}}$ ranging from -8 to $-19{\cdot}5$ electrons were used. Negative temperature factors represent a physically impossible situation. Data strongly affected by absorption might result in negative temperature factors but these intensities had been corrected as well as possible for absorption.

At this point the second, more extensive, set of intensities was measured and the least-squares calculations continued. Again, some or all of the temperature factors tended to become negative regardless of the value of $\Delta f'_{\mathrm{U}}$ that was used. If $\Delta f'_{\mathrm{U}}$ were made small enough for B_{U} to remain positive, other B's became negative.

Two changes were then made in the least-squares program. One was the addition of a secondary extinction correction, g, as a least-squares parameter, and the other was the inclusion of $\Delta f''$, the imaginary portion of the anomalous dispersion correction in the calculation of the structure factors. Later, a further modification was made so that $\Delta f'$ and $\Delta f''$ could be included as least-squares parameters. The observation equations were of the form

$$\Delta F = |F_o| - \frac{K|F_c|}{\sqrt{(1 + gLp|F_c|^2)}} \tag{1}$$

where

K = scale factor
g = secondary extinction parameter
Lp = Lorentz-polarization factor

$$|F_c| = \sqrt{\{[\Sigma(f_i + \Delta f'_i)T_i \cos\varphi_i]^2 + [\Sigma\Delta f''_i T_i \cos\varphi_i]^2\}}$$
$$T_i = \exp(-B_i \sin^2\theta/\lambda^2)$$
$$\varphi_i = 2\pi(hx_i + ky_i + lz_i)$$

and the other terms have the usual meanings.

Except for the final calculations, in which the dispersion terms were treated as parameters, values used were $\Delta f''_{\mathrm{U}} = 13{\cdot}0$ (Roof, 1961), $\Delta f''_{\mathrm{Mo}} = 0{\cdot}9$ and $\Delta f'_{\mathrm{Mo}} = -1{\cdot}7$ (Dauben & Templeton, 1955).

Table 3. *Final least-squares parameters for* $\mathrm{UMoC_2}$

The dispersion terms were held constant

Atom	*x*	*z*	*B*	$\Delta f'$	$\Delta f''$
U	0·0819 ± 0·0003	0·1421 ± 0·0001	0·20 ± 0·03 Å^2	−15·0	13·0
Mo	0·4191 ± 0·0007	0·8986 ± 0·0002	0·39 ± 0·05	−1·7	0·9
C(1)	0·153 ± 0·006	0·752 ± 0·003	0·61 ± 0·47		
C(2)	0·751 ± 0·005	0·005 ± 0·002	0·00 ± 0·42		

$g = 7{\cdot}36 \pm 0{\cdot}20 \times 10^{-7}$

It was found that if the secondary extinction parameter were used, convergence with all temperature factors positive could be achieved with values of $\Delta f'_{\mathrm{U}}$ ranging at least from $-8\cdot0$ to $-19\cdot5$ electrons. Calculations were made both with unit weights and with Evans's weights. Without g as a parameter all positive temperature factors could not be obtained with $\Delta f''$ included for any value of $\Delta f'_{\mathrm{U}}$. Using the value of the standard deviation of the x parameter of uranium as a somewhat arbitrary criterion we concluded that the best results were obtained with $\Delta f'_{\mathrm{U}} = -15\cdot0$ electrons and with Evans's weights. These weights gave slightly lower standard deviations than did unit weights although the improvement was hardly significant. The final parameters obtained in this way are given in Table 3. The final changes as fractions of their standard deviations were $<10^{-3}$ for position parameters, $<10^{-2}$ for temperature factors and $0\cdot6$ for g. Observed and calculated structure factors, for which $R=4\cdot1\%$, are given in Table 4.

The $y=\frac{1}{4}$ section of the difference Fourier synthesis, with the uranium and molybdenum removed by using the parameters of Table 3, is shown in Fig. 1. The carbon atoms show up clearly. The molybdenum atom has disappeared nicely but a peak somewhat bigger than the carbon atom remains at the uranium position. Clearly the uranium temperature factor or the uranium dispersion terms in Table 3 are not correct.

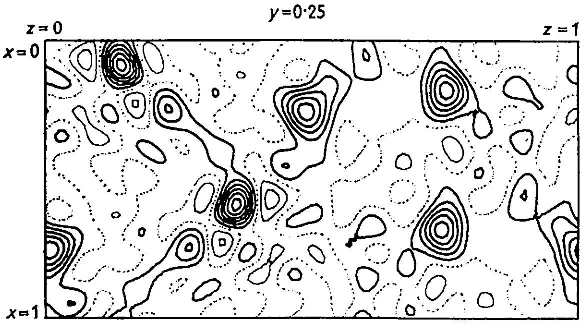

Fig. 1. Carbon-only difference Fourier synthesis with U and Mo subtracted, using the parameters given in Table 3. The contour interval is $2\cdot0$ e.Å^{-3}. The dotted line is the zero contour and the lighter lines are negative.

Some comments on the calculation of Fig. 1 are in order.* In the computation of a Fourier series for a crystal containing anomalous scatterers the observed coefficients must be corrected for effects of these anomalous scatterers, because what is usually desired is the true electron density and not the electron density as seen by the X-rays. For the centric case, as we have at present, let

Table 4. *Observed and calc. structure factors for* UMoC$_2$

If $|F_o|$ is negative the minus sign means 'less than'.
The columns headed A and B are respectively $(A+A_a)$ and B_a as explained in the text

h	k	l	$\|F_o\|$	$\|F_c\|$	A	B
0	0	2	-26	21	-18	-10
0	0	4	278	311	-307	-50
0	0	6	56	58	51	28
0	0	8	181	176	172	34
0	0	10	77	80	-69	-41
0	0	12	-40	19	-14	-13
0	0	14	71	85	72	45
0	1	1	121	118	-111	-38
0	1	3	-26	23	-11	-20
0	1	5	215	221	216	49
0	1	7	93	90	-90	-2
0	1	9	209	208	-201	-51
0	1	11	99	95	93	21
0	1	13	171	163	157	42
0	2	0	346	328	-323	-54
0	2	2	-29	18	15	10
0	2	4	241	236	231	49
0	2	6	54	52	-44	-28
0	2	8	153	147	-144	-34
0	2	10	68	70	58	40
0	2	12	-38	17	12	13
0	3	1	90	84	76	37
0	3	3	-32	21	9	19
0	3	5	155	153	-146	-48
0	3	7	64	63	63	1
0	3	9	163	156	148	49
0	4	0	210	199	193	51
0	4	2	-39	13	-8	-9
0	4	4	159	149	-142	-46
1	0	1	64	60	54	26
1	0	2	74	70	-66	-23
1	0	3	175	172	-167	-39
1	0	4	81	86	85	12
1	0	5	43	49	48	-8
1	0	6	58	59	56	19
1	0	7	199	199	193	45
1	0	8	108	108	-107	-20
1	0	9	85	87	-86	-10
1	0	10	39	34	-32	-12
1	0	11	170	171	-166	-42
1	0	12	100	101	98	25
1	0	13	97	90	86	25
1	0	14	-41	20	20	2
1	1	1	113	114	-113	-17
1	1	2	333	316	-313	-47
1	1	3	144	139	137	23
1	1	4	34	33	29	17
1	1	5	83	85	85	8
1	1	6	196	195	192	37
1	1	7	80	78	-74	-24
1	1	8	58	60	-51	-30
1	1	9	-30	11	-10	3
1	1	10	72	72	-69	-21
1	1	11	50	53	48	21
1	1	12	-48	70	59	38
1	1	13	-39	22	-18	-13
1	2	1	49	51	-44	-25
1	2	2	53	57	52	23
1	2	3	134	131	125	39
1	2	4	64	64	-63	-11
1	2	5	42	35	-34	8
1	2	6	52	49	-46	-19
1	2	7	174	165	-159	-44
1	2	8	93	91	89	20
1	2	9	76	74	73	10
1	2	10	43	29	27	11
1	2	11	153	148	143	41
1	2	12	89	88	-85	-24
1	3	1	70	72	71	17
1	3	2	200	199	194	45
1	3	3	92	90	-87	-22
1	3	4	-34	26	-21	-16
1	3	5	57	57	-57	-8
1	3	6	138	139	-134	-36
1	3	7	-46	57	52	24
1	3	8	50	47	37	29
1	3	9	-36	8	7	-3
1	4	1	-39	36	27	24
1	4	2	-40	38	-32	-22
1	4	3	77	85	-77	-36
1	4	4	-41	41	39	11
2	0	0	178	181	179	29
2	0	1	210	223	-220	-36
2	0	2	-25	19	-18	-5
2	0	3	193	197	-196	-23
2	0	4	170	171	-169	-26
2	0	5	193	195	190	43
2	0	6	32	23	18	14
2	0	7	67	70	70	4
2	0	8	72	68	66	18
2	0	9	109	108	-100	-41
2	0	10	40	43	-38	-21
2	0	11	-34	15	5	14
2	0	12	-43	21	-20	-7
2	0	13	54	54	47	31
2	1	0	124	122	-115	-41
2	1	1	68	65	-62	-20
2	1	2	80	80	79	10
2	1	3	-26	12	6	-10
2	1	4	94	93	85	37
2	1	5	103	100	97	25
2	1	6	151	151	-149	-28
2	1	7	37	35	-35	-1
2	1	8	83	81	-76	-27
2	1	9	102	104	-101	-26
2	1	10	183	180	176	40
2	1	11	59	55	54	11
2	1	12	-39	38	36	12
2	1	13	83	81	78	22
2	2	0	134	137	-134	-28
2	2	1	170	168	165	36
2	2	2	-29	14	13	5
2	2	3	146	147	146	22
2	2	4	133	133	130	25
2	2	5	164	159	-153	-42
2	2	6	-30	21	-15	-14
2	2	7	65	58	-58	-4
2	2	8	63	58	-55	-17
2	2	9	89	94	85	40
2	2	10	-42	38	33	20
2	2	11	-35	15	-4	-14
2	3	0	83	87	77	40
2	3	1	48	45	41	19
2	3	2	45	52	-51	-10
2	3	3	-33	10	-2	10
2	3	4	72	71	-61	-36
2	3	5	76	72	-68	-24
2	3	6	106	110	106	27
2	3	7	-38	25	25	1
2	3	8	56	62	56	26
2	3	9	82	79	75	25
2	4	0	88	86	82	26
2	4	1	104	107	-102	-33
2	4	2	-38	10	-9	-5
3	0	1	-26	1	-0	1
3	0	2	122	123	-114	-47
3	0	3	-26	4	-4	-1
3	0	4	134	137	135	23
3	0	5	-28	2	2	-0
3	0	6	103	100	92	38
3	0	7	-30	6	6	1
3	0	8	194	201	-197	-41
3	0	9	31	4	-4	-0
3	0	10	70	69	-65	-23
3	0	11	-40	5	-5	-1
3	0	12	183	182	175	49
3	1	1	208	219	-216	-35
3	1	2	-27	10	-10	-2
3	1	3	209	204	199	47
3	1	4	-26	1	0	0
3	1	5	127	122	121	16
3	1	6	-27	6	6	1
3	1	7	165	163	-155	-49
3	1	8	-31	1	0	-1
3	1	9	-34	39	-38	6
3	1	10	-32	3	-3	-1
3	1	11	79	81	70	42
3	1	12	-37	2	1	1
3	2	1	-28	1	0	-1
3	2	2	104	105	94	46
3	2	3	-29	3	3	1
3	2	4	111	113	-111	-23
3	2	5	-29	2	-2	0
3	2	6	83	86	-78	-37
3	2	7	-34	5	-5	-1
3	2	8	172	173	168	40
3	2	9	-40	4	4	0
3	2	10	58	61	56	23
3	2	11	-36	5	4	1
3	3	1	151	153	149	33
3	3	2	-33	7	7	1
3	3	3	142	147	-140	-45
3	3	4	-37	1	-0	-0
3	3	5	86	88	-87	-15
3	3	6	-36	4	-4	-1
3	3	7	122	124	115	47
3	3	8	-36	1	-0	1
4	0	0	130	129	-127	-25
4	0	1	182	187	-184	-37
4	0	2	-31	22	22	5
4	0	3	134	141	-140	-23
4	0	4	112	111	109	23
4	0	5	153	153	147	43
4	0	6	38	15	-8	-13
4	0	7	76	72	71	4
4	0	8	49	57	-55	-16
4	0	9	106	105	-96	-41
4	0	10	-42	42	38	19
4	0	11	-35	19	12	15
4	1	0	91	91	-82	-42
4	1	1	49	42	38	17
4	1	2	55	52	50	10
4	1	3	-27	12	7	9
4	1	4	94	92	84	38
4	1	5	85	83	-80	-23
4	1	6	142	142	-139	-29
4	1	7	41	31	31	1
4	1	8	69	63	-57	-27
4	1	9	69	75	71	23
4	1	10	155	154	149	40
4	1	11	47	38	-37	-10
4	2	0	103	108	105	25
4	2	1	152	157	153	36
4	2	2	-32	19	-18	-5
4	2	3	116	119	117	22
4	2	4	97	95	-92	-22
4	2	5	128	131	-124	-42
4	2	6	-33	14	6	13
4	2	7	-46	62	-61	-4
4	2	8	50	49	47	15
4	2	9	91	92	83	40
4	3	0	58	71	59	40
4	3	1	-37	32	-28	-17
4	3	2	-38	38	-37	-10
4	3	3	-34	10	-5	-9
4	3	4	64	71	-61	-36
4	3	5	64	63	59	22
4	3	6	104	107	104	27
5	0	1	39	44	-37	-24
5	0	2	52	52	-46	-24
5	0	3	105	108	101	37
5	0	4	65	61	59	12
5	0	5	-33	27	-26	8
5	0	6	49	45	40	20
5	0	7	138	138	-131	-42
5	0	8	62	87	-85	-22
5	0	9	70	61	61	10
5	0	10	46	29	-27	-12
5	1	1	78	82	-80	-18
5	1	2	192	192	187	43
5	1	3	97	98	95	25
5	1	4	-34	26	-21	-16
5	1	5	61	65	64	8
5	1	6	135	133	-129	-35
5	1	7	-47	64	-58	-26
5	1	8	51	46	37	28
5	1	9	-36	9	-9	3
5	2	1	42	39	31	24
5	2	2	-38	46	39	24
5	2	3	90	94	-87	-36
5	2	4	-45	52	-51	-12
5	2	5	-37	24	22	-7
5	2	6	48	40	-35	-20
5	2	7	124	121	114	41
5	3	1	61	61	59	18
5	3	2	145	145	-139	-42
6	0	0	207	217	-211	-52
6	0	1	-33	13	-13	-2
6	0	2	-35	9	-0	9
6	0	3	-32	7	-6	-1
6	0	4	174	180	174	47
6	0	5	-36	6	5	3
6	0	6	-38	50	-42	-27
6	0	7	-38	8	8	0
6	0	8	108	104	-99	-32
6	1	0	-32	3	1	-2
6	1	1	82	83	75	36
6	1	2	-33	1	1	1
6	1	3	-43	19	-2	19
6	1	4	-36	5	5	2
6	1	5	127	126	-116	-47
6	1	6	-36	11	-10	-2
6	1	7	45	46	46	1
6	2	0	184	190	183	51
6	2	1	-36	11	11	2
6	2	2	-36	9	1	-9
6	2	3	-37	6	6	1
6	2	4	158	157	-151	-46
7	0	1	-40	37	-27	-25
7	0	2	46	36	31	20
7	0	3	83	87	78	37
7	0	4	47	36	-35	-9
7	1	1	51	47	44	14
7	1	2	147	156	150	44
0	0	0	0	517		

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* We have been guided in our thoughts on this subject by Dr A. L. Patterson who kindly sent to us a preprint of a paper on the correction of Fourier coefficients for anomalous dispersion.

Table 5. *Least-squares parameters for* $UMoC_2$ *without* $\Delta f''$ *terms*

Atom	x	z	B	$\Delta f'$
U	$0{\cdot}0819 \pm 0{\cdot}0003$	$0{\cdot}1421 \pm 0{\cdot}0001$	$0{\cdot}04 \pm 0{\cdot}03$ Å^2	$-15{\cdot}0$
Mo	$0{\cdot}4195 \pm 0{\cdot}0007$	$0{\cdot}8986 \pm 0{\cdot}0006$	$0{\cdot}61 \pm 0{\cdot}05$	$-1{\cdot}7$
C(1)	$0{\cdot}156 \pm 0{\cdot}006$	$0{\cdot}752 \pm 0{\cdot}003$	$1{\cdot}05 \pm 0{\cdot}52$	
C(2)	$0{\cdot}755 \pm 0{\cdot}006$	$0{\cdot}006 \pm 0{\cdot}003$	$0{\cdot}38 \pm 0{\cdot}47$	

$g = 7{\cdot}58 \pm 0{\cdot}22 \times 10^{-7}$

$$A = \Sigma f_i \cos \varphi_i$$
$$A_a = \Sigma \Delta f_i' \cos \varphi_i$$
$$B_a = \Sigma \Delta f_i'' \cos \varphi_i$$

where f is the normal scattering factor uncorrected for the dispersion terms $\Delta f'$ and $\Delta f''$. Then

$$|F_o|^2 = [(A + A_a)^2 + B_a^2] \,. \quad (2)$$

The coefficient that one should use in a Fourier series to obtain the true electron density is

$$A_o = (\text{Sign of } A_c)\sqrt{[|F_o|^2 - 2AA_a - A_a^2 - B_a^2]} \,. \quad (3)$$

A Fourier synthesis calculated with uncorrected coefficients will usually have smaller peaks than one computed with coefficients given by equation (3), because $\Delta f'$ is usually negative.

For a difference Fourier synthesis in which the contributions of the anomalous scatters are to be removed, as in Fig. 1, it follows from (2) that the coefficients are

$$C = -A - A_a + (\text{Sign of } A)\sqrt{\{|F_o|^2 - B_a^2\}} \,, \quad (4)$$

where A, A_a and B_a contain only contributions from the anomalous scatterers, uranium and molybdenum in the present case.

Table 5 gives the results from a least-square calculation without any $\Delta f''$ terms but with $\Delta f_U' = -15{\cdot}0$ and $\Delta f_{Mo}' = -1{\cdot}7$ electrons and with an extinction parameter. For this calculation $R = 4{\cdot}3\%$ and the standard deviations are all about 5% greater than those in Table 3. Fig. 2 shows a difference Fourier synthesis with uranium and molybdenum removed. Again the carbon atoms show up well. There are no peaks remaining at the uranium and molybdenum positions, indicating that these atoms have been more accurately accounted for than in Fig. 1.

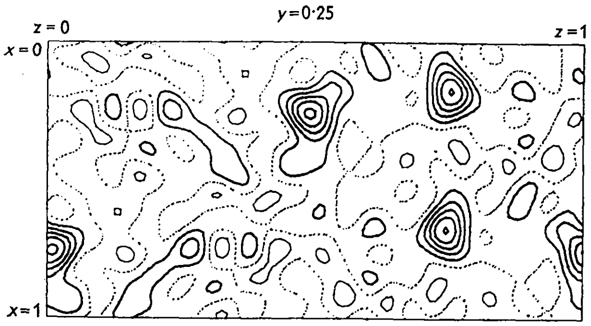

Fig. 2. Carbon-only difference Fourier synthesis with U and Mo subtracted, using the parameters given in Table 5. Contours as in Fig. 1.

Finally, an attempt was made to least-square with the dispersion terms as parameters. When the molybdenum terms were held constant at $\Delta f' = -1{\cdot}7$ and $\Delta f'' = 0{\cdot}9$, $\Delta f_U'$ converged to $-10{\cdot}6$ and $\Delta f_U''$ converged to zero, a value completely contrary to theory and to Roof's (1961) experimental results but in agreement with the difference Fourier synthesis of Fig. 2. When all four dispersion terms were allowed to vary, the calculations did not converge at all. It might be pointed out that the program was tested with synthetic data and found to work perfectly so that even though some correlation terms are large, with accurate enough data these parameters can be refined by least-squares.

It is concluded that our data are not accurate enough to determine dispersion corrections experimentally and that very accurate data indeed are required for this purpose. Further, for meaningful results it is probably necessary to obtain data on an absolute scale because of the high correlation between scale factor, temperature factor and dispersion corrections.

In any event, except for the uranium and molybdenum temperature factors, parameter differences were at most about one-half a standard deviation so that there is no doubt about the determination of the structure itself, which was the main objective of the work.

Discussion of the structure

The interatomic distances between neighbors are given in Table 6. Two atoms are defined as neighbors if the midpoint between them is closer to those two atoms than to any other atom. This definition is similar to but not necessarily the same as that given by Frank & Kasper (1958). The two definitions are the same if the line between two atoms which are neighbors passes through the common domain surface.*

The standard deviations in Table 6 have been computed with all correlation terms included, but neglecting errors in unit-cell dimensions. The inclusion of correlation terms can be quite important though usually it is not. The extreme cases are the C(1)–C(1) distances of $2{\cdot}813 \pm 0{\cdot}001$ Å with correlation terms and $\pm 0{\cdot}047$ Å without, and the C(2)–C(2) distance

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* In many previous papers on intermetallic structures we have stated that the atoms listed as neighbors satisfy the Frank & Kasper definition when in fact the present definition was the one that was satisfied.

Table 6. *Interatomic distances in* $UMoC_2$

U–2 C(1)	2·40 ±0·025 Å	Mo–C(1)	2·11 ±0·034 Å
–2 C(1)	2·51 ±0·026	–C(1)	2·20 ±0·034
–C(2)	2·39 ±0·029	–2 C(2)	2·16 ±0·019
–2 C(2)	2·48 ±0·020	–C(2)	2·20 ±0·029
–2 Mo	3·274 ±0·004	–2 Mo	2·903 ±0·004
–Mo	3·279 ±0·003	–2 U	3·274 ±0·004
–2 U	3·249 ±0·005	–U	3·279 ±0·003
C(1)–2 C(1)	2·813 ±0·001	C(2)–C(1)	2·88 ±0·04
–2 C(1)	3·249 ±0·005	–2 C(2)	3·24 ±0·05
–C(2)	2·87 ±0·04	–2 Mo	2·16 ±0·018
–Mo	2·11 ±0·034	–Mo	2·20 ±0·029
–Mo	2·20 ±0·034	–U	2·39 ±0·029
–2 U	2·40 ±0·025	–2 U	2·48 ±0·020
–2 U	2·51 ±0·026		

Additional distances < 3·5 Å

U–2 Mo	3·251 Å	C(1)–2 C(2)	3·17 Å
–2 Mo	3·283		
		C(2)–2 C(1)	3·17
Mo–2 U	3·251	–2 C(2)	3·249
–2 U	3·283	–2 C(2)	3·26
–2 Mo	3·249		

of 3·24 ± 0·053 Å with correlation terms and ± 0·037 Å without.

Fig. 3 shows the structure in projection down the *b* axis. The carbon atoms all lie in planes at $z \simeq 0$, $\frac{1}{4}$, $\frac{1}{2}$ and $\frac{3}{4}$ although they are not required to do so by symmetry. These planes result because $z_{C1} \simeq \frac{3}{4}$ and $z_{C2} \simeq 0$. In between these carbon atom planes are slightly puckered planes containing the U and Mo atoms.

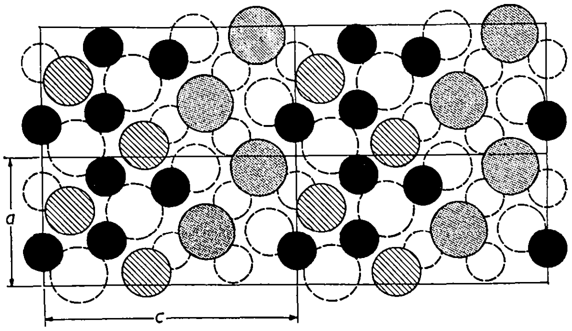

Fig. 3. Projection of $UMoC_2$ down the *b* axis. The large circles are U, the medium circles Mo and the small circles C atoms. The solid circles are at $y = \frac{3}{4}$ and the dashed circles at $y = \frac{1}{4}$.

An interesting view of the structure is shown in Fig. 4. The C(2) atoms at $z \simeq 0$ form a hexagonal network and the C(1) atoms at $z \simeq \frac{1}{4}$ form a nearly square network. The U atoms at $z = 0{\cdot}142$ lie above the center of a triangle of C(2) atoms and below the center of a square formed by C(1) atoms. The Mo atoms at $z = 0{\cdot}101$ lie above the center of a triangle of C(2) atoms and beneath the midpoint of a pair of C(1) atoms. The U and Mo atoms together form a slightly puckered hexagonal array and all the C atoms are either above or below the approximate centers of triangles of this hexagonal array.

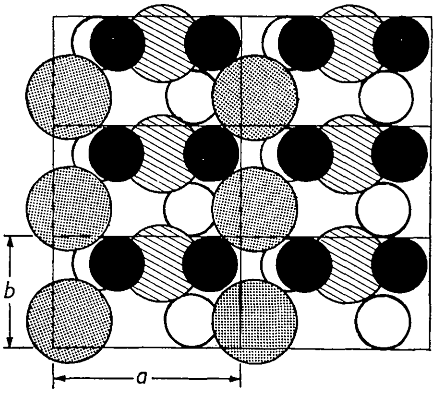

Fig. 4. A portion of $UMoC_2$ projected down the *c* axis. Atoms lying between $z = 0$ and $\frac{1}{4}$ are shown. The solid small circles are C atoms at $z \simeq \frac{1}{4}$ and the small open circles C atoms at $z \simeq 0$. The large circles are U atoms at $z = 0{\cdot}142$ and the medium circles are Mo atoms at $z = 0{\cdot}101$.

The principal difference between the present results and the structure proposed by Nowotny *et al.* is in the location of C(1). There now is no very short C–C distance of 1·31 Å and this compound cannot be an acetylene type carbide. The same is probably true for $UCrC_2$ and UWC_2.

All computations were made with an IBM 7090 using programs written by the authors. Figs. 1 and 2 were plotted with an SC 4020 cathode ray plotter using a magnetic tape input prepared on the 7090.

Note added in proof.— The paper by Dr A. L. Patterson referred to in a footnote has since been published (Patterson, 1963).

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