for a pair of inverse reflections under these conditions. His formulae are

$$\mathrm{I}_H = (D/2k)^2|V_H|^2 + (D/2k)^3\,\mathrm{Im}\,\{V_H \sum_G{}' V_{-G} V_{G-H}\} - \ldots$$

$$\mathrm{I}_{\bar{H}} = (D/2k)^2|V_H|^2 - (D/2k)^3\,\mathrm{Im}\,\{V_H \sum_G{}' V_{-G} V_{G-H}\} - \ldots$$

where H stands for h, k, l, D = crystal thickness, $k = 2\pi/\lambda$, Im { } denotes the imaginary part of { } and the prime after the symbol Σ indicates the absence of terms with $G = 0$ or H. This difference arises because of the fact that though $|V_H| = |V_{\bar{H}}|$ the phases of V_H and $V_{\bar{H}}$ are different. Consequently, if V_H can be obtained from the structure, it should be possible to find the absolute configuration from the difference in intensity of inverse reflections using a thick crystal to accentuate the effect of dynamical interactions.

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The crystal structure of $MoTe_2$.*

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An investigation of the Mo–Te system has been undertaken to determine the thermoelectric properties of its constituent phases. Our work confirms the existence of $MoTe_2$ and Mo_2Te_3, the two phases previously reported by Morette (1942). This paper describes a refinement of the molybdenum ditelluride structure.

$MoTe_2$ was prepared from the elements, using 99·999% pure Te and Mo, further purified by heat treatment in H_2 at 850 °C., Stoichiometric quantities of the elements were sealed in vacuo in carbonized quartz ampules. The specimen was reacted and homogenized for several hours at 1100 °C. using R–F induction heating. Chemical analysis of the resultant product, a loosely sintered polycrystalline specimen, yielded 33·44 at.% Mo, 66·56% Te. The specimen was crushed and the specific gravity of the powder measured as $7{\cdot}8 \pm 0{\cdot}2$. $MoTe_2$ oxidizes slowly when exposed to air at room temperature; the powder pattern of finely divided $MoTe_2$ begins to show molybdenum dioxide lines after about a week in air.

The crystal structure of $MoTe_2$ was determined from its powder pattern, using a diffractometer and filtered Cu $K\alpha$ radiation. The diffraction spectra were easily indexed by comparison with the MoS_2 pattern and the lattice parameters were computed from several high-angle lines, using graphic extrapolation to $\theta = 90°$. $MoTe_2$ has a hexagonal unit cell, space group $P6_3/mmc$, with $a = 3{\cdot}519 \pm 0{\cdot}001$, $c = 13{\cdot}964 \pm 0{\cdot}004$ Å, and a calculated specific gravity of 7·78 g.cm.$^{-3}$. It is isomorphous with molybdenite, with Mo at $\pm(\frac{1}{3}, \frac{2}{3}, \frac{1}{4})$ and with Te at $\pm(\frac{1}{3}, \frac{2}{3}, z)$ and $\pm(\frac{2}{3}, \frac{1}{3}, z+\frac{1}{2})$, where $z \simeq \frac{5}{8}$. The positional parameter of tellurium, z, was determined from the powder-pattern intensities. Preferred orientation of the $MoTe_2$ powder parallel to the (00·1) cleavage face made accurate intensity determination difficult, but consistent results were obtained by sifting the powder ($< 44\mu$) onto a glass slide covered with glue. A comparison of the observed intensities for specimens with preferred and random orientations is given in Table 1.

The random-orientation intensities were compared with calculated structure factors to obtain the tellurium coordinate. The calculated structure factors were computed from

$$F_c(hkl) = 2[p(hkl)]^{\frac{1}{2}} \sum_i f_i \cos 2\pi(hx_i + ky_i + lz_i)\,,$$

where p is the multiplicity factor and the summation was carried out over one formula unit. The observed intensities were scaled to the F_o values to give an observed structure factor

$$F_o(hkl) = K(\theta)P(\theta)[I_0(hkl)]^{\frac{1}{2}},$$

where $P(\theta)$ is the Lorentz polarization correction and $K(\theta)$ a scaling factor which includes, among other things, the Mo and Te temperature factors. $K(\theta)$ was calculated by scaling the observed and calculated structure factors in zones. The structure factors were computed for various values of z; the best agreement between theory and experiment was obtained for $z = 0{\cdot}620$, as shown in Fig. 1. The lowest R factor is still quite large (17%), but much of the discrepancy can be attributed to preferred orientation or to anisotropic temperature factors, since the

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Table 1. *The powder pattern of* $MoTe_2$

$hk \cdot l$	d_c	d_o	Intensity (preferred)	Intensity (random)	F_o	F_c
00·2	6·98	6·99	80	15	79	−93
00·4	3·491	3·493	100	14	150	−153
10·0	3·047	3·048	9	36	291	−300
10·1	2·977	2·983	3	10	155	150
10·2	2·793	2·797	2	4	105	99
10·3	2·550	2·550	51	100	596	585
00·6	2·327	2·324	34	6	170	−133
10·4	2·296	2·295	4	6	170	167
10·5	2·059	2·060	35	35	458	−459
10·6	1·850	1·850	3	4	172	147
11·0	1·760	1·762	4	25	475	492
00·8	1·746	1·746	84	15	382	277
11·2	1·706	1·709	1	3	173	−161
10·7	1·669	1·669	4	4	212	−195
11·4	1·571	1·573	2	6	280	−283
20·0	1·524	1·525	1	3	212	−229
20·1	1·515	1·515	12	9	359	−119
10·8	1·515					−317
20·2	1·489	1·488	< 1	1	105	82
20·3	1·448	1·449	5	11	413	−458
11·6	1·404	1·403	2	3	243	−258
20·4	1·397	1·397	1	1	156	136
00·10	1·396					−14
10·9	1·383	1·382	1	< 1	< 86	37
20·5	1·338	1·340	2	6	348	368
20·6	1·275	1·274	1	1	139	124
10·10	1·269					17
11·8	1·239	1·240	9	13	574	571
20·7	1·211	1·211	1	1	161	164
10·11	1·172	1·173	17	11	568	456
00·12	1·164	1·165	2	1	158	−90
21·0	1·152	1·153	< ½	2	249	−280
21·1	1·148	1·149	2	3	322	147
20·8	1·148					−274
21·2	1·137	—	< ½	< ½	< 127	93
21·3	1·118	1·119	3	8	506	560
21·4	1·0938	1·0949	½	1	190	170
11·10	1·0938					−31
20·9	1·0871	1·0870	1	1	187	−32
10·12	1·0871					105
21·5	1·0648	1·0649	2	5	436	−461
21·6	1·0323	1·0320	½	½	150	153
20·10	1·0295	—	< ½	< ½	< 99	14
30·0	1·0158	1·0160	½	3	328	368
10·13	1·0131	1·0132	5	4	407	−246
30·2	1·0052	1·0054	< ½	½	102	167
21·7	0·9975	0·9977	2	2	283	−210
00·14	0·9925	—	< ½	< ½	< 144	124
30·4	0·9754	0·9755	4	6	504	−209
20·11	0·9753					−422
11·12	0·9706	0·9705	1	1	249	−201
21·8	0·9614	0·9616	1	2	340	−351
10·14	0·9480	0·9477	1	1	220	147
30·6	0·9310	0·9308	½	1	201	71
21·9	0·9248	0·9249	½	½	105	42
20·12	0·9248					96
10·15	0·8903	0·8904	2	1	254	−170
21·10	0·8885	—	< ½	< ½	< 136	20
22·0	0·8797	0·8799	½	1	252	336
30·8	0·8780	0·8781	4	7	583	467
20·13	0·8779					224
22·2	0·8728	0·8728	5	3	387	−111
00·16	0·8727					177
11·14	0·8677	0·8677	3	3	362	−277
22·4	0·8530	0·8530	4	8	605	−206
21·11	0·8530					537
31·0	0·8452	0·8452	½	1	201	−234
31·1	0·8437	0·8438	½	½	150	−125
31·2	0·8391	0·8390	4	2	325	76
10·16	0·8390					−209
20·14	0·8345	0·8344	½	½	184	136
31·3	0·8316	0·8318	2	4	424	−472
22·6	0·8229	0·8226	½	1	190	−189
31·4	0·8215	0·8215	< ½	½	150	141
30·10	0·8215					229
21·12	0·8186	0·8185	½	½	127	127
31·5	0·8090	0·8091	1	3	362	390
31·6	0·7945	0·7945	1	1	224	133
20·15	0·7944					150
10·17	0·7931	0·7930	½	½	96	−40
22·8	0·7856	0·7856	4	8	515	433
21·13	0·7856					−297
11·16	0·7818	0·7819	10	9	498	402
31·7	0·7782	0·7783	½	½	110	178

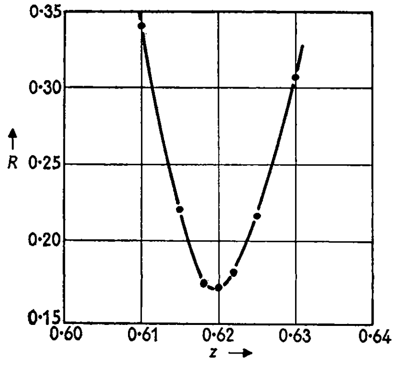

Fig. 1. Agreement between F_c and F_o for several values of the tellurium coordinate z. $R = \sum_{hkl} (F_o - |F_c|) / \sum_{hkl} F_o$.

calculated intensities of spectra with large l index are consistently low. The F_o and F_c values for $z = 0{\cdot}620$ are listed in Table 1.

In the $MoTe_2$ structure, each Mo is coordinated to a trigonal prism of six telluriums; the Mo–Te distance is 2·73 Å. Each Te is surrounded by ten other tellurium atoms: six in the close-packed (00·1) plane at 3·52 Å, one directly below it at 3·63 Å, and three above it at 3·92 Å across the cleavage plane. The Te–Mo–Te bond angles are 83·5° (3), 80·4° (6), and 133·9° (6), in good agreement with the d^4sp hybrid bonds proposed by Hultgren (1932).

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