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Peak heights of electron density and Patterson function in the crystal.

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Peak heights of atoms in a Fourier map and the corresponding Patterson functions are tabulated in a practically useful form, for various atoms with various temperature factors.

Peak heights of the electron density in a Fourier map and the Patterson function can be calculated by integrations of atomic form factors:

$$\varrho_i(0) = \int f_i d\tau$$

$$P_{ij}(0) = \int f_i f_j d\tau \,, \qquad (1)$$

where f_i is the ith atomic form factor including the temperature factor, and $d\tau$ is a volume element in reciprocal space. The knowledge of the values of ϱ_i and P_{ij} including the effect due to the temperature factors gives a useful guide for the identification of atomic species in the course of the structure analysis. Such values have not been published in any convenient tabulated form so far as the author is aware.

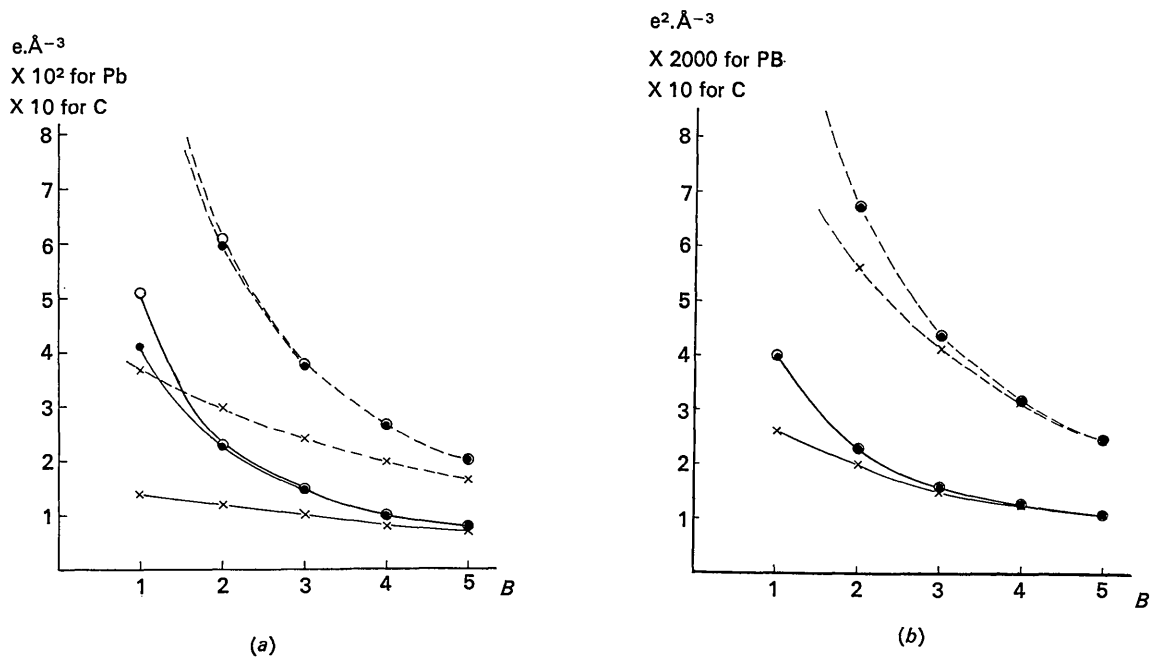

Fig. 1. Variation of peak heights with temperature factor. (*a*) $\varrho(0)$, (*b*) $P_{ii}(0)$. Range of integration: open circles, infinite range; solid circles, Mo $K\alpha$ range; crosses, Cu $K\alpha$ range. Full lines, carbon; dashed lines, lead.

Table 1. *Atomic peak height* $\varrho(0)$ (e.Å^{-3}) *and Patterson peak height* $P(0)$ (e.^{2}Å^{-3}). *Infinite range*

		Atomic Peak					Patterson Peak				
ATOM	Z	B=1	B=2	B=3	B=4	B=5	B=1	B=2	B=3	B=4	B=5
H	1	1.	1.	1.	1.	1.	.	.	.	.	.
HE	2	3.	5.	4.	3.	3.	3.	3.	2.	2.	2.
LI	3	20.	11.	7.	6.	4.	11.	7.	5.	4.	3.
BE	4	31.	16.	10.	7.	6.	19.	11.	7.	6.	4.
B	5	41.	20.	12.	9.	7.	28.	16.	11.	8.	7.
C	6	52.	23.	15.	10.	8.	40.	23.	16.	13.	11.
N	7	63.	27.	17.	12.	10.	57.	34.	25.	20.	17.
O	8	71.	32.	20.	15.	12.	81.	50.	37.	30.	25.
F	9	80.	37.	24.	18.	14.	114.	72.	54.	44.	37.
NE	10	91.	43.	29.	21.	17.	159.	102.	77.	61.	51.
NA	11	104.	50.	33.	25.	20.	210.	133.	98.	76.	62.
MG	12	117.	57.	38.	28.	22.	265.	164.	118.	91.	73.
AL	13	130.	64.	42.	31.	24.	324.	195.	138.	105.	84.
SI	14	144.	71.	46.	34.	26.	388.	227.	158.	119.	95.
P	15	158.	77.	50.	36.	28.	455.	260.	179.	134.	107.
S	16	172.	84.	54.	39.	30.	525.	295.	201.	151.	121.
CL	17	187.	90.	57.	41.	31.	599.	332.	226.	171.	136.
A	18	202.	96.	61.	43.	33.	677.	372.	255.	193.	155.
K	19	220.	102.	64.	46.	35.	758.	414.	284.	215.	173.
CA	20	242.	108.	68.	48.	37.	843.	457.	313.	237.	191.
SC	21	260.	114.	71.	51.	39.	935.	508.	349.	266.	213.
TI	22	276.	120.	75.	53.	41.	1035.	565.	391.	298.	239.
V	23	291.	126.	78.	56.	43.	1144.	630.	437.	334.	269.
CR	24	302.	132.	83.	59.	46.	1269.	708.	495.	380.	307.
MN	25	318.	138.	87.	62.	48.	1399.	783.	547.	419.	337.
FE	26	331.	145.	91.	66.	51.	1545.	872.	611.	467.	375.
CO	27	344.	152.	96.	69.	54.	1709.	971.	680.	520.	418.
NI	28	358.	159.	101.	73.	57.	1889.	1079.	756.	577.	463.
CU	29	371.	167.	106.	77.	60.	2098.	1209.	850.	649.	521.
ZN	30	386.	175.	112.	81.	63.	2307.	1327.	928.	706.	564.
GA	31	402.	183.	117.	85.	66.	2523.	1445.	1005.	760.	605.
GE	32	417.	192.	122.	89.	68.	2746.	1564.	1081.	814.	646.
AS	33	432.	200.	128.	92.	71.	2976.	1684.	1156.	868.	686.
SE	34	448.	208.	133.	96.	74.	3214.	1805.	1233.	922.	728.
BR	35	464.	216.	138.	99.	75.	3456.	1926.	1309.	977.	770.
KR	36	480.	225.	143.	102.	78.	3706.	2049.	1388.	1033.	815.
RB	37	498.	233.	148.	106.	81.	3962.	2174.	1466.	1089.	857.
SR	38	518.	241.	152.	109.	83.	4219.	2296.	1542.	1143.	898.
Y	39	537.	248.	157.	112.	85.	4480.	2420.	1620.	1199.	942.
ZR	40	557.	257.	161.	115.	88.	4747.	2547.	1701.	1258.	988.
CB	41	574.	265.	166.	118.	90.	5018.	2678.	1788.	1323.	1041.
MO	42	593.	273.	170.	121.	92.	5295.	2813.	1877.	1390.	1094.
TC	43	616.	281.	175.	124.	94.	5580.	2951.	1966.	1456.	1146.
RU	44	633.	288.	179.	127.	95.	5869.	3099.	2069.	1536.	1211.
RH	45	653.	295.	183.	130.	99.	6166.	3251.	2174.	1615.	1275.
PD	46	671.	303.	188.	133.	101.	6472.	3413.	2288.	1704.	1348.
AG	47	694.	310.	192.	136.	104.	6791.	3578.	2400.	1789.	1415.
CD	48	719.	318.	197.	139.	105.	7121.	3746.	2513.	1873.	1481.
IN	49	744.	326.	201.	142.	108.	7457.	3917.	2627.	1955.	1545.
SN	50	769.	333.	206.	145.	111.	7797.	4089.	2740.	2037.	1607.
SB	51	791.	341.	210.	149.	113.	8143.	4265.	2854.	2119.	1669.
TE	52	810.	348.	214.	152.	116.	8487.	4441.	2969.	2201.	1731.
I	53	827.	355.	219.	155.	118.	8839.	4622.	3086.	2286.	1796.
XE	54	842.	362.	223.	158.	120.	9195.	4804.	3205.	2371.	1862.
CS	55	856.	369.	228.	161.	122.	9550.	4985.	3320.	2454.	1926.
BA	56	872.	376.	232.	164.	125.	9913.	5168.	3437.	2537.	1989.
LA	57	887.	384.	236.	167.	127.	10287.	5354.	3555.	2621.	2053.
CE	58	903.	392.	242.	171.	130.	10754.	5627.	3747.	2768.	2171.
PR	59	918.	399.	247.	175.	133.	11202.	5874.	3914.	2891.	2268.
ND	60	934.	407.	252.	178.	136.	11673.	6134.	4089.	3021.	2370.
PM	61	950.	416.	257.	182.	139.	12167.	6405.	4271.	3156.	2475.
SM	62	967.	424.	263.	186.	142.	12682.	6688.	4461.	3297.	2585.
EU	63	984.	433.	268.	190.	145.	13220.	6983.	4659.	3442.	2698.
GD	64	1001.	441.	274.	194.	148.	13729.	7242.	4824.	3560.	2788.
TB	65	1018.	451.	280.	199.	151.	14367.	7609.	5076.	3748.	2936.
DY	66	1036.	460.	286.	203.	155.	14977.	7940.	5296.	3909.	3061.
HO	67	1055.	469.	292.	207.	158.	15620.	8287.	5525.	4076.	3190.
ER	68	1074.	479.	298.	212.	161.	16279.	8642.	5759.	4246.	3322.
TM	69	1093.	489.	305.	216.	165.	16978.	9015.	6003.	4423.	3458.
YB	70	1113.	499.	311.	221.	168.	17678.	9389.	6249.	4601.	3596.
LU	71	1133.	508.	317.	225.	171.	18344.	9719.	6456.	4747.	3705.
HF	72	1155.	518.	323.	229.	174.	19027.	10053.	6664.	4893.	3815.
TA	73	1175.	528.	329.	233.	177.	19708.	10384.	6870.	5038.	3926.
W	74	1196.	537.	334.	237.	180.	20399.	10716.	7078.	5186.	4039.
RE	75	1216.	547.	340.	240.	183.	21087.	11047.	7286.	5334.	4153.
OS	76	1237.	556.	345.	244.	185.	21787.	11382.	7497.	5486.	4270.
IR	77	1258.	566.	351.	248.	188.	22495.	11721.	7712.	5641.	4390.
PT	78	1276.	575.	356.	251.	191.	23195.	12063.	7936.	5808.	4523.
AU	79	1297.	584.	362.	255.	193.	23911.	12408.	8158.	5970.	4650.
HG	80	1322.	593.	367.	259.	196.	24650.	12756.	8377.	6126.	4769.
TL	81	1348.	603.	372.	262.	199.	25378.	13097.	8591.	6278.	4885.
PB	82	1376.	612.	378.	266.	201.	26128.	13444.	8807.	6430.	4999.
BI	83	1404.	622.	383.	269.	204.	26872.	13787.	9019.	6578.	5111.
PO	84	1432.	631.	388.	273.	206.	27627.	14133.	9233.	6727.	5222.
AT	85	1459.	640.	393.	276.	209.	28385.	14481.	9448.	6877.	5334.
RN	86	1434.	649.	398.	280.	211.	29137.	14826.	9660.	7025.	5446.
FR	87	1507.	658.	403.	283.	214.	29889.	15171.	9872.	7173.	5557.
RA	88	1530.	666.	408.	286.	216.	30643.	15516.	10084.	7320.	5667.
AC	89	1553.	675.	413.	290.	219.	31381.	15852.	10289.	7462.	5773.
TH	90	1575.	683.	418.	293.	221.	32138.	16195.	10498.	7607.	5882.
PA	91	1596.	692.	423.	296.	224.	32920.	16589.	10766.	7811.	6046.
U	92	1618.	700.	428.	300.	226.	33718.	16977.	11019.	7998.	6193.
NP	93	1639.	709.	433.	303.	229.	34528.	17374.	11279.	8189.	6343.
PU	94	1660.	717.	438.	307.	232.	35361.	17808.	11578.	8413.	6527.
AM	95	1681.	726.	443.	310.	234.	36192.	18226.	11855.	8623.	6689.
CM	96	1703.	734.	448.	314.	237.	37016.	18621.	12105.	8801.	6824.
FM	100	1787.	768.	469.	329.	248.	40576.	20454.	13327.	9704.	7532.

Table 2. *Atomic peak height* $\varrho(0)$ (e.Å^{-3}) *and Patterson peak height* $P(0)$ (e^2.Å^{-3}). Cu $K\alpha$ *range*

ATOM	Z	ϱ R=1	R=2	R=3	R=4	R=5	P R=1	R=2	R=3	R=4	R=5
H	1	1.	1.	1.	1.	1.	.	.	.	.	.
HE	2	5.	4.	3.	3.	2.	3.	3.	2.	2.	2.
LI	3	3.	7.	6.	5.	4.	6.	5.	5.	4.	3.
BE	4	10.	8.	7.	6.	5.	13.	9.	7.	5.	4.
B	5	12.	10.	8.	7.	6.	18.	13.	10.	8.	7.
C	6	14.	12.	10.	8.	7.	26.	20.	15.	13.	11.
N	7	17.	14.	12.	10.	8.	35.	30.	24.	20.	17.
O	8	21.	17.	14.	12.	10.	59.	45.	36.	30.	25.
F	9	25.	21.	17.	15.	12.	87.	66.	53.	43.	36.
NE	10	30.	25.	21.	18.	15.	124.	94.	74.	60.	50.
NA	11	36.	29.	24.	20.	17.	165.	122.	94.	75.	62.
MG	12	40.	33.	27.	23.	19.	204.	149.	113.	89.	73.
AL	13	45.	36.	30.	25.	21.	242.	174.	131.	103.	83.
SI	14	48.	39.	32.	27.	22.	279.	199.	149.	116.	94.
P	15	51.	41.	34.	28.	24.	315.	224.	168.	131.	105.
S	16	54.	44.	36.	30.	25.	353.	251.	188.	147.	119.
CL	17	57.	46.	38.	31.	26.	392.	280.	211.	165.	135.
A	18	60.	48.	40.	33.	28.	435.	313.	237.	187.	153.
K	19	63.	51.	42.	35.	29.	483.	349.	264.	209.	171.
CA	20	66.	54.	44.	37.	31.	536.	386.	292.	230.	188.
SC	21	70.	57.	46.	39.	33.	597.	431.	327.	258.	211.
TI	22	74.	60.	49.	41.	35.	667.	483.	366.	290.	237.
V	23	78.	63.	52.	43.	37.	747.	541.	411.	325.	265.
CR	24	82.	67.	55.	46.	39.	840.	612.	467.	370.	303.
MN	25	87.	71.	58.	49.	41.	938.	681.	517.	409.	333.
FE	26	92.	75.	62.	51.	43.	1049.	761.	578.	456.	372.
CO	27	93.	79.	65.	54.	45.	1172.	848.	644.	508.	413.
NI	28	103.	84.	69.	57.	48.	1307.	946.	716.	564.	458.
CU	29	109.	89.	73.	61.	51.	1466.	1062.	805.	635.	516.
ZN	30	115.	93.	77.	64.	54.	1615.	1165.	878.	690.	559.
GA	31	121.	98.	80.	67.	56.	1764.	1266.	950.	742.	599.
GE	32	126.	102.	84.	69.	58.	1910.	1364.	1020.	794.	639.
AS	33	131.	106.	87.	72.	60.	2052.	1460.	1088.	845.	678.
SE	34	136.	110.	90.	74.	62.	2192.	1555.	1157.	896.	719.
BR	35	140.	113.	92.	77.	64.	2330.	1650.	1225.	949.	761.
KR	36	144.	116.	95.	79.	66.	2468.	1745.	1295.	1003.	804.
RB	37	148.	120.	98.	81.	68.	2609.	1842.	1365.	1056.	846.
SR	38	153.	123.	100.	83.	70.	2749.	1937.	1434.	1107.	885.
Y	39	156.	126.	103.	85.	71.	2887.	2033.	1503.	1160.	928.
ZR	40	160.	129.	105.	87.	73.	3027.	2131.	1576.	1216.	973.
CB	41	164.	132.	108.	89.	75.	3167.	2233.	1654.	1279.	1025.
MO	42	167.	135.	110.	91.	77.	3315.	2340.	1735.	1343.	1078.
TC	43	171.	138.	113.	93.	78.	3472.	2451.	1817.	1407.	1128.
RU	44	175.	141.	115.	96.	80.	3633.	2572.	1913.	1485.	1193.
RH	45	179.	144.	118.	98.	82.	3806.	2699.	2010.	1562.	1257.
PD	46	133.	148.	121.	100.	84.	3988.	2836.	2117.	1649.	1329.
AG	47	187.	151.	124.	103.	86.	4184.	2976.	2223.	1731.	1395.
CD	48	192.	155.	127.	105.	88.	4387.	3120.	2329.	1812.	1460.
IN	49	196.	158.	130.	108.	90.	4598.	3266.	2435.	1893.	1523.
SN	50	201.	162.	133.	110.	92.	4816.	3414.	2541.	1972.	1584.
SB	51	206.	166.	136.	113.	94.	5040.	3566.	2648.	2051.	1645.
TE	52	211.	170.	139.	115.	96.	5260.	3716.	2755.	2131.	1707.
I	53	215.	174.	142.	117.	98.	5479.	3866.	2863.	2212.	1771.
XE	54	220.	177.	145.	120.	100.	5694.	4014.	2971.	2294.	1836.
CS	55	224.	180.	147.	122.	102.	5907.	4160.	3077.	2374.	1898.
BA	56	228.	184.	150.	124.	104.	6125.	4309.	3183.	2454.	1960.
LA	57	232.	187.	153.	126.	106.	6344.	4458.	3290.	2534.	2023.
CE	58	238.	192.	157.	130.	109.	6674.	4698.	3472.	2678.	2139.
PR	59	243.	196.	160.	132.	111.	6970.	4907.	3627.	2797.	2235.
ND	60	248.	200.	164.	135.	113.	7283.	5128.	3791.	2923.	2336.
PM	61	254.	205.	167.	138.	116.	7609.	5358.	3961.	3054.	2440.
SM	62	260.	209.	171.	141.	119.	7950.	5598.	4138.	3190.	2548.
EU	63	265.	214.	175.	145.	121.	8305.	5847.	4321.	3331.	2660.
GD	64	270.	218.	178.	147.	123.	8613.	6057.	4471.	3443.	2747.
TB	65	277.	223.	182.	151.	126.	9059.	6375.	4708.	3627.	2894.
DY	66	283.	228.	186.	154.	129.	9458.	6653.	4912.	3782.	3017.
HO	67	289.	233.	191.	158.	132.	9874.	6943.	5124.	3943.	3144.
ER	68	296.	238.	195.	161.	135.	10301.	7240.	5340.	4108.	3274.
TM	69	302.	244.	199.	164.	138.	10749.	7550.	5566.	4279.	3408.
YB	70	309.	249.	203.	168.	141.	11197.	7861.	5792.	4450.	3543.
LU	71	314.	253.	206.	171.	143.	11589.	8125.	5979.	4589.	3650.
HF	72	320.	257.	210.	174.	145.	11978.	8388.	6165.	4728.	3758.
TA	73	325.	261.	213.	176.	147.	12357.	8645.	6350.	4867.	3866.
W	74	330.	265.	217.	179.	150.	12734.	8903.	6536.	5007.	3976.
RE	75	335.	269.	220.	181.	152.	13106.	9160.	6722.	5148.	4088.
OS	76	340.	273.	223.	184.	154.	13481.	9420.	6912.	5293.	4203.
IR	77	344.	277.	226.	187.	156.	13858.	9682.	7104.	5441.	4321.
PT	78	349.	281.	229.	189.	158.	14228.	9950.	7307.	5601.	4451.
AU	79	353.	284.	232.	192.	160.	14612.	10221.	7508.	5757.	4575.
HG	80	358.	288.	235.	194.	162.	15011.	10494.	7706.	5906.	4692.
TL	81	363.	292.	238.	197.	165.	15405.	10764.	7899.	6051.	4806.
PB	82	368.	296.	241.	199.	167.	15809.	11037.	8093.	6196.	4918.
BI	83	373.	300.	244.	202.	169.	16214.	11309.	8285.	6338.	5027.
PO	84	378.	304.	247.	204.	171.	16624.	11582.	8478.	6479.	5136.
AT	85	383.	308.	251.	207.	173.	17035.	11858.	8671.	6622.	5246.
RN	86	387.	311.	253.	209.	175.	17438.	12128.	8862.	6763.	5355.
FR	87	392.	315.	256.	211.	177.	17835.	12395.	9052.	6904.	5463.
RA	88	396.	318.	259.	214.	179.	18236.	12664.	9241.	7044.	5571.
AC	89	401.	322.	262.	216.	180.	18628.	12926.	9425.	7179.	5675.
TH	90	405.	325.	265.	218.	182.	19022.	13190.	9611.	7316.	5781.
PA	91	410.	329.	268.	221.	184.	19457.	13510.	9858.	7514.	5943.
U	92	414.	333.	271.	223.	187.	19897.	13822.	10089.	7693.	6087.
NP	93	419.	336.	274.	226.	189.	20350.	14143.	10328.	7878.	6235.
PU	94	423.	340.	277.	229.	191.	20842.	14505.	10606.	8100.	6417.
AM	95	428.	344.	280.	231.	193.	21326.	14849.	10862.	8299.	6576.
CM	96	433.	348.	283.	234.	195.	21793.	15167.	11090.	8468.	6709.
FM	100	453.	365.	297.	245.	205.	23955.	16697.	12224.	9344.	7407.

The form factor f_0 for a stationary atom is approximated by a sum of the Gaussian functions (Forsyth & Wells, 1955)

$$f_{i0} = A_{i1}\exp(-a_{i1}s^2) + A_{i2}\exp(-a_{i2}s^2) + A_{i3}\exp(-a_{i3}s^2) \quad (2)$$

with $a_{i3}=0$, where $s=\sin\theta/\lambda$. Equation (1) is, then, easily integrated, and we obtain

$$\left.\begin{aligned}\varrho_i(0) &= 8\pi^{3/2}\sum_{k=1}^{3}\frac{A_{ik}}{(a_{ik}+B_i)^{3/2}}\\ P_{ij}(0) &= 8\pi^{3/2}\sum_{k=1}^{3}\sum_{k'=1}^{3}\frac{G_{kk'}}{(g_{kk'})^{3/2}}\end{aligned}\right\} \quad (3)$$

where

$$G_{kk'}=A_{ik}A_{jk'},\ g_{kk'}=a_{ik}+B_i+a_{jk'}+B_j$$

and B_i is the isotropic temperature factor of the ith atom. Although the relations (3) are not suitable at very low temperatures, they give sufficiently good approximations for most purposes. Parameters A_k and a_k in equation (2) were obtained by Moore (1963), and also by Hosoya & Satake (1965). Hosoya & Satake's parameters for the Mo range were used for calculation of the function $\varrho(0)$ and the self Patterson function $P_{ii}(0)$ of various atoms. The results are shown in Table 1.

Practically, however, observed values are in general considerably smaller than these values because of termination. In order to calculate $\varrho(0)$ and $P_{ii}(0)$ subjected to the termination effect, equations (1) were rewritten as

$$\left.\begin{aligned}\varrho_i(0) &= 32\pi\int_0^{1/\lambda} s^2 f_i\,ds\\ P_{ii}(0) &= 32\pi\int_0^{1/\lambda} s^2 f_i^2\,ds\end{aligned}\right\} \quad (4)$$

Substituting relation (2) into (4), values of $\varrho_i(0)$ and $P_{ii}(0)$ were obtained numerically for various wavelengths. Typical results are shown in Fig. 1. With Mo $K\alpha$, the termination is not very serious unless the temperature factor is too small, but with Cu $K\alpha$ the reduction of peak height is significant. Therefore, values for the Cu $K\alpha$ range are shown in Table 2. Tables 1 and 2 will be helpful for judging the atomic species, by reading through the column with a relevant B value.

The numerical calculations were carried out on OKITAC 5090H computer of this Institute. The author expresses his sincere thanks to Dr T. Ito of this Institute for his critical discussions.

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The crystal structure of $CsUF_6$*.

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$CsUF_6$ is rhombohedral, $a=5{\cdot}417$ Å, $\alpha=95°29{\cdot}5'$, space group $R\bar{3}$, with one formula unit per unit cell. The U atom has 6F neighbors at 2·057 Å which make an octahedron slightly compressed along the threefold axis. The Cs atom has 12 neighbors, 6 at 3·101 and 6 at 3·147 Å. The compound is isostructural with $KOsF_6$.

The preparation of cesium uranium(V) hexafluoride was first reported by Penneman, Sturgeon & Asprey (1964), who found a rhombohedral lattice with hexagonal cell dimensions of $a=8{\cdot}036\pm0{\cdot}003$, $c=8{\cdot}388\pm0{\cdot}004$ Å. These dimensions suggest that the compound is isostructural with $KOsF_6$ whose structure, based on powder diffraction data, was reported by Hepworth, Jack & Westland (1956). Optical properties, cleavage and twinning were reported by Sturgeon, Penneman, Kruse & Asprey (1965). A partial absorption spectrum was reported by Asprey & Penneman (1964) and a detailed analysis of the absorption spectrum was made by Reisfeld & Crosby (1965), who assumed the centric space group $R\bar{3}$. $CsPuF_6$ (Penneman, Sturgeon, Asprey & Kruse, 1965) and $CsNpF_6$ (Asprey, Keenan, Penneman & Sturgeon, 1966) are isostructural with $CsUF_6$. The present structure determination was undertaken as a means of confirming the centric nature of the structure, and of refining this structure type on the basis of single-crystal data.

Crystals of $CsUF_6$ for this study were prepared by R. A. Penneman by recrystallization from cold, aqueous hydrogen fluoride solution. The crystals thus formed are pale greenish-blue rhombohedra up to 2 mm in diameter. Cleavage and twinning as reported by Sturgeon *et al.* (1965) were not observed on these crystals.

Precession photographs show the crystals to be rhombohedral with no systematic extinctions. The space group is thus $R3$, $R\bar{3}$, $R32$, $R3m$, or $R\bar{3}m$. Lattice constants were obtained from measurement of 2θ for Mo $K\alpha_1$ radiation ($\lambda=0{\cdot}70926$ Å) for several high order reflections with a carefully aligned single-crystal orienter on a General Electric XRD-5 spectrogoniometer. The hexagonal cell constants are $a=8{\cdot}021\pm0{\cdot}003$, $c=8{\cdot}430\pm0{\cdot}003$ Å (the rhombohedral cell has $a=5{\cdot}417$ Å, $\alpha=95°29'{\cdot}5$). These values differ significantly from those previously reported. The assumption of one formula unit per rhombohedral unit cell gives a calculated density of 5·145 g.cm^{-3}. Intensities from an entire hemisphere were measured to $2\theta\simeq50°$ with Mo $K\alpha$ radiation with balanced Zr–Y filters and the fixed-counter,

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