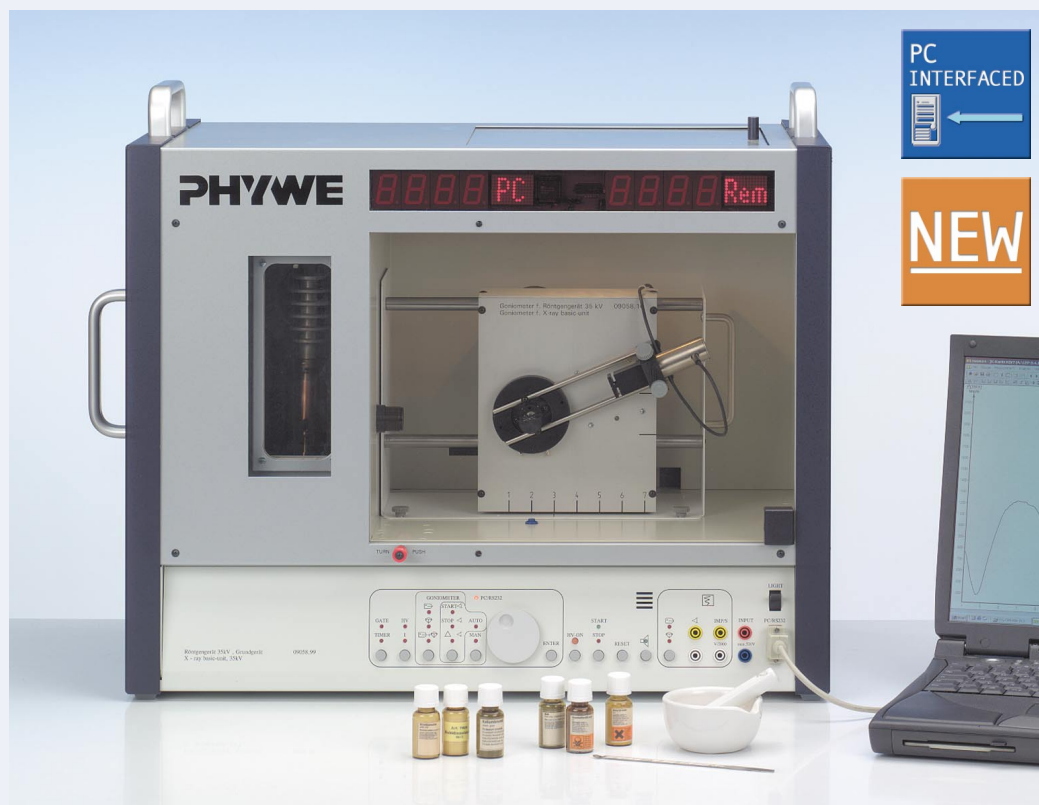


5.4.21-00 Diffractometric Debye-Scherrer patterns of powder samples with the three cubic Bravais lattices



What you can learn about ...

- Crystal lattices
- Crystal systems
- Bravais-lattice
- Reciprocal lattice
- Miller indices
- Structure factor
- Atomic scattering factor
- Bragg scattering
- Characteristic X-rays
- Monochromatization of X-rays

Principle:

Polycrystalline powder samples, which crystallize in the three cubic Bravais types, simple, face-centered and body-centered, are irradiated with the radiation from a X-ray tube with a copper anode. A swivelling Geiger-Mueller counter tube detects the radiation that is constructively reflected from the various lattice planes of the crystallites. The Bragg diagrams are automatically recorded. Their evaluation gives the assign-

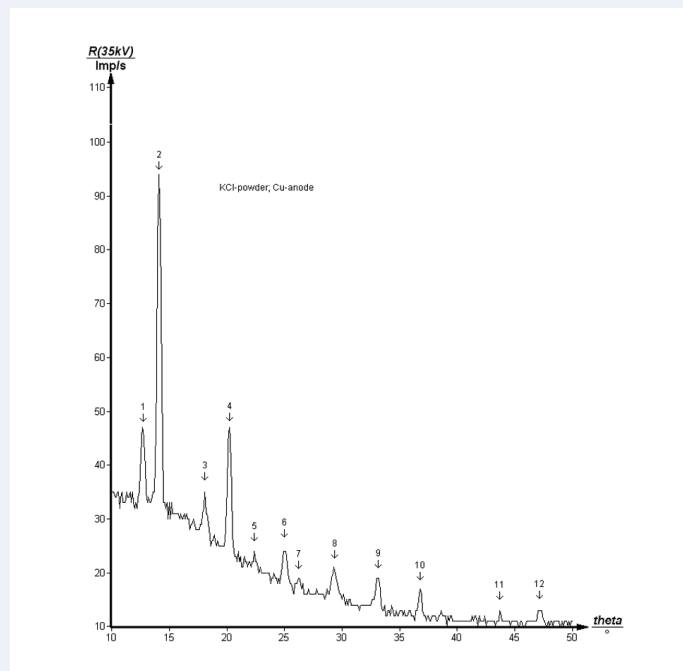
What you need:

X-ray basic unit, 35 kV	09058.99	1
Goniometer for X-ray unit, 35 kV	09058.10	1
Plug-in module with Cu X-ray tube	09058.50	1
Counter tube, type B	09005.00	1
Lithium fluoride monocrystal, mounted	09056.05	1
Universal crystal holder	09058.02	1
Probe holder for powder probes	09058.09	1
Diaphragm tube with nickel foil	09056.03	1
Ammonium chloride, 250 g	30024.25	1
Potassium chloride, 250 g	30098.25	1
Potassium bromide, 100 g	30258.10	1
Molybdenum, 100 g	31767.10	1
Micro spoon, special steel	33393.00	1
Vaseline, 100 g	30238.10	1
Mortar and pestle, $d = 90$ mm	32603.00	1

Recording equipment:

XYt-recorder	11416.97	1
Connecting cable, $l = 100$ cm, red	07363.01	1
Connecting cable, $l = 100$ cm, blue	07363.04	1
<i>or</i>		
Software X-ray unit, 35 kV	14407.61	1
Data cable, 2 x SUB-D, 9 pin	14602.00	1
PC, Windows® 95 or higher		

Complete Equipment Set, Manual on CD-ROM included
Diffractometric Debye-Scherrer patterns of powder samples with the three cubic Bravais lattices
P254 2100



Bragg-Cu- K_{α} and Cu- K_{β} -lines of KCl.

ment of the Bragg lines to the individual lattice planes, their spacings as well as the lattice constants of the samples, and so also the corresponding Bravais lattice type.

Tasks:

1. Record the intensity of the Cu-X-rays back scattered by the four cubic crystal powder samples with various Bravais lattice types as a function of the scattering angle.
2. Calculate the lattice plane spacings appropriate to the angular positions of the individual Bragg lines.
3. Assign the Bragg reflections to the respective lattice planes. Determine the lattice constants of the samples and their Bravais lattice types.
4. Determine the number of atoms in the unit cell.

Related topics

Crystal lattices, crystal systems, Bravais-lattice, reciprocal lattice, Miller indices, structure factor, atomic scattering factor, Bragg scattering, characteristic X-rays, monochromatization of X-rays.

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Equipment

X-ray basic unit, 35 kV	09058.99	1
Goniometer for X-ray unit, 35 kV	09058.10	1
Plug-in module with Cu X-ray tube	09058.50	1
Counter tube, type B	09005.00	1
Lithium fluoride monocrystal, mounted	09056.05	1
Universal crystal holder	09058.02	1
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Molybdenum, 100 g	31767.10	1
Micro spoon, special steel	33393.00	1
Vaseline, 100 g	30238.10	1
Mortar and pestle, $d = 90$ mm	32603.00	1

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XYt-recorder	11416.97	1
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Connecting cable, $l = 100$ cm, blue	07363.04	1
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Tasks

- Record the intensity of the Cu-X-rays back scattered by the four cubic crystal powder samples with various Bravais lattice types as a function of the scattering angle.
- Calculate the lattice plane spacings appropriate to the angular positions of the individual Bragg lines.
- Assign the Bragg reflections to the respective lattice planes. Determine the lattice constants of the samples and their Bravais lattice types.
- Determine the number of atoms in the unit cell.

Fig.1: Experimental set-up



Set-up and Procedure**Sample preparation:**

The sample must be so finely powdered that no grains can be felt when a little of it is rubbed between finger and thumb. A relatively high sample concentration can be obtained by mixing the powder with a little vaseline. To do this, transfer a small amount of the sample onto a sheet of paper and use a spatula to knead it to a firm paste. To achieve the highest concentration of material as possible, use very little vaseline (a spatula tip of it). Fill the relatively solid sample paste into the specimen for powder samples and smooth it flush. Use the universal crystal holder to hold the specimen.

X-ray unit settings:

Acceleration voltage $U_a = 35$ kV, anode current $I_a = 1$ mA. Use the 2 mm diameter double pinhole. Set the goniometer block with line marking at position 4.5. To obtain a good angle resolution, push the counter tube holder to the back stop.

Calibration of the goniometer with the LiF single-crystal:

Exact angular positions of Debye-Scherrer reflections are only to be expected when the goniometer is correctly adjusted. Should the goniometer be out of adjustment for any reason whatever, this can be overcome by stepwise carrying out of the following procedure: In the coupled 2:1 mode, set the LiF single-crystal at an angle of $\vartheta = 22.5^\circ$. Theoretically, the very intense 200 reflection from LiF lies at this angle. Now uncouple the rotation of the crystal and the Geiger-Müller counter tube. Search for the maximum intensity of the reflection by turning the crystal and counter tube alternately and separately through a few 0.1° angular steps. Should the maximum be found at 22.3° , for example, i.e. 0.2° below the theoretical value, then couple the crystal and counter tube together again and turn the crystal through -0.2° past the zero position. Save this corrected zero position by pressing "ENTER". The maximum intensity must now be situated exactly at the angle of 22.5° . Carry out a corresponding positive zero position correction should the maximum be found at an angle greater than 22.5° .

Further settings:

Scanning range: see Figs.: Stepping 0.1° ; Scanning speed: when only the very intense reflection line is to be recorded, then scanning can be relatively rapid at 10 s/ $^\circ$. For the identification of weaker lines, a scanning speed of at least 30 s/ $^\circ$ is required for a better signal-noise ratio. It is also recommended that, for a more exact evaluation, the position of the glancing angle be determined to two decimal places and that the zoom function be used for the region where lines are close together.

Theory and Evaluation

When X-rays of wavelength λ strike a mass of lattice planes of a crystal of spacing d at a glancing angle of ϑ , then the reflected rays will only be subject to constructive interference when Bragg's condition is fulfilled, i.e.:

$$2 d \sin \vartheta = \lambda \quad (1)$$

Bragg's condition implies that all of the waves scattered at the atom are in phase and so amplify each other, whereas partial waves that are scattered in directions not fulfilling Bragg's conditions are of opposite phase and so extinguish each other. A more realistic way of looking at this must, however, take the actual phase relationships of all of the partial waves

scattered by the atom in a certain direction into consideration. When there are N atoms in a unit cell, then the total amplitude of the X-rays scattered by the cell is described by the structure factor F , which is calculated by summing up the atomic scattering factors f of the individual N atoms, taking their phases into account.

In general, the following is valid for F :

$$F_{hkl} = \sum_1^N f_n \cdot e^{2\pi i (hu_n + kv_n + lw_n)} \quad (2)$$

where h, k, l = Miller indices of the reflecting lattice planes and u_n, v_n, w_n are the coordinates of the atoms in fractions of the particular edge lengths of the unit cell.

As F is in general a complex number, the total scattered intensity is described by $|F_{hkl}|^2$.

A cubic simple unit cell contains only one atom with the coordinates 000. According to equation (2), therefore, the structure factor F for this lattice type is given by:

$$F = f \cdot e^{2\pi i (0)} = f \quad ; \quad |F|^2 = f^2 \quad (3)$$

This means that F^2 is independent of h, k and l and all Bragg reflections can therefore occur.

The unit cell of a cubic face-centered lattice has 4 atoms at 000, $1/2 \ 1/2 \ 0$, $1/2 \ 0 \ 1/2$ and $0 \ 1/2 \ 1/2$. The unit cell of a cubic body-centered lattice has in comparison only 2 atoms at 000 and $1/2 \ 1/2 \ 1/2$.

When the lattice only consists of one sort of atom, then the following conditions are valid for the structure factor:

fcc Lattice

$$\begin{aligned} |F|^2 &= 16 f^2 && \text{with } h \ k \ l \text{ only even or only odd} \\ |F|^2 &= 0 && \text{with } h \ k \ l \text{ mixed} \end{aligned}$$

bcc Lattice

$$\begin{aligned} |F|^2 &= 4 f^2 && \text{with } (h + k + l) \text{ even} \\ |F|^2 &= 0 && \text{with } (h + k + l) \text{ odd} \end{aligned} \quad (4)$$

The situation is somewhat different when a lattice is made up of different sorts of atoms.

When, for example, an fcc lattice consists of the atoms A and B , whereby the A atoms lie at 000, $1/2 \ 1/2 \ 0$, $1/2 \ 0 \ 1/2$ and $0 \ 1/2 \ 1/2$, and the B atoms at $1/2 \ 1/2 \ 1/2$, $0 \ 0 \ 1/2$, $0 \ 1/2 \ 0$ and $1/2 \ 0 \ 0$, then the following additional condition is given for the structure factor F :

fcc Lattice with atoms A and B :

$$\begin{aligned} |F|^2 &= 16 (f_A + f_B)^2 && \text{with } (h + k + l) \text{ even and} \\ |F|^2 &= 16 (f_A - f_B)^2 && \text{with } (h + k + l) \text{ odd} \end{aligned} \quad (5)$$

In such fcc lattices, when the atomic scattering factors f of the two atoms are almost equal ($f_A \approx f_B$), then 111 reflections will only be very weak, if they occur at all.

For the cubic crystal system, the spacing d of the individual lattice planes with the indices (hkl) is obtained from the quadratic form:

$$\frac{1}{d_{hkl}^2} = \frac{1}{a^2} (h^2 + k^2 + l^2) \quad (a = \text{lattice constant}) \quad (6)$$

From this and equation (1), with $n = 1$, the quadratic Bragg equation is obtained:

$$\sin^2 \vartheta = \frac{\lambda^2}{4a^2} (h^2 + k^2 + l^2) \quad (7)$$

Examination of fcc lattices

Fig. 2 shows the Debye-Scherrer spectrum of potassium bromide (KBr).

As no filter is used for the monochromatization of the X-rays, when individual lines are evaluated consideration must be given to the fact that the very intense lines that result from K_α -radiation are accompanied by secondary lines that result from the weaker K_β radiation.

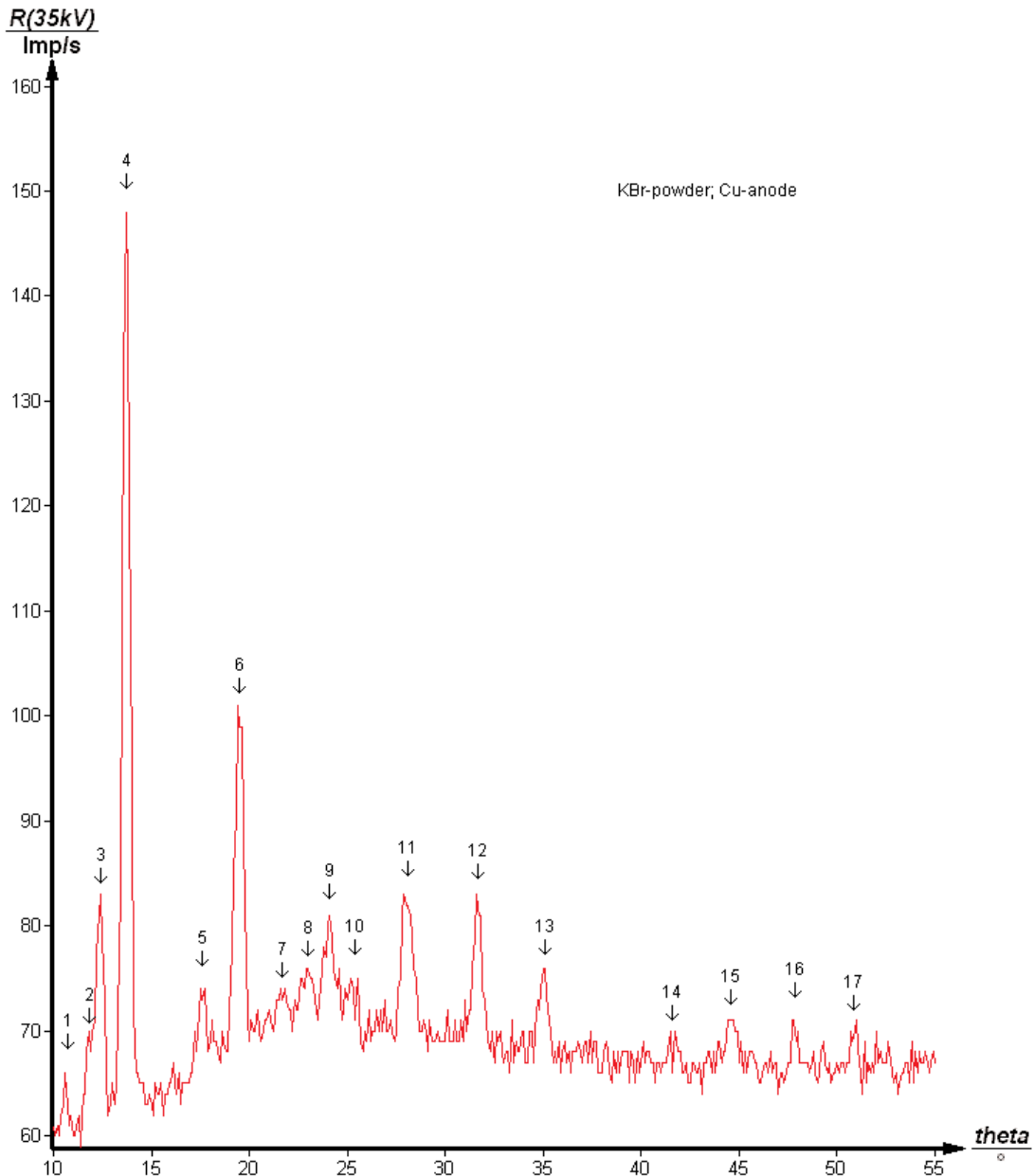
These pairs of lines can be identified by means of equation (1). It is namely approximately true with $\lambda (K_\alpha) = 154.18 \text{ pm}$ and $\lambda (K_\beta) = 139.22 \text{ pm}$:

$$\frac{\lambda (K_\alpha)}{\lambda (K_\beta)} = \frac{\sin \vartheta_\alpha}{\sin \vartheta_\beta} = \frac{154.18 \text{ pm}}{139.22 \text{ pm}} \approx 1.11 \quad (8)$$

These values correspond to the quotients of the $\sin \vartheta$ values (Fig. 2) of the pairs of lines 2-1, 4-3, 6-5 and 9-7, showing that the lines 1, 3, 5 and 7 originate from the K_β radiation.

The correctness of this conclusion can be shown by a control measurement (see Fig. 3) using the diaphragm tube with nickel foil to reduce the intensity of the K_β radiation. The reflexes in Fig. 2 that were previously assigned to the K_β lines are no

Fig. 2: Bragg-Cu- K_α and Cu- K_β -lines of KBr



longer to be seen. As the intensity of the K_{α} - radiation is also somewhat weakened by the Ni foil, the detection of reflexes of weak intensity at larger glancing angles is made difficult when this is used.

The following method for evaluating the spectrum is given as an example, and is representative for that for the spectra of other samples. First determine the $\sin\vartheta$ and $\sin^2\vartheta$ values for each individual reflex from the angle of diffraction ϑ of the particular line. From equation (7), the ratios of the observed $\sin^2\vartheta$ values must be representable by the ratios of the sums of the squares of the three integer numbers (h,k,l) .

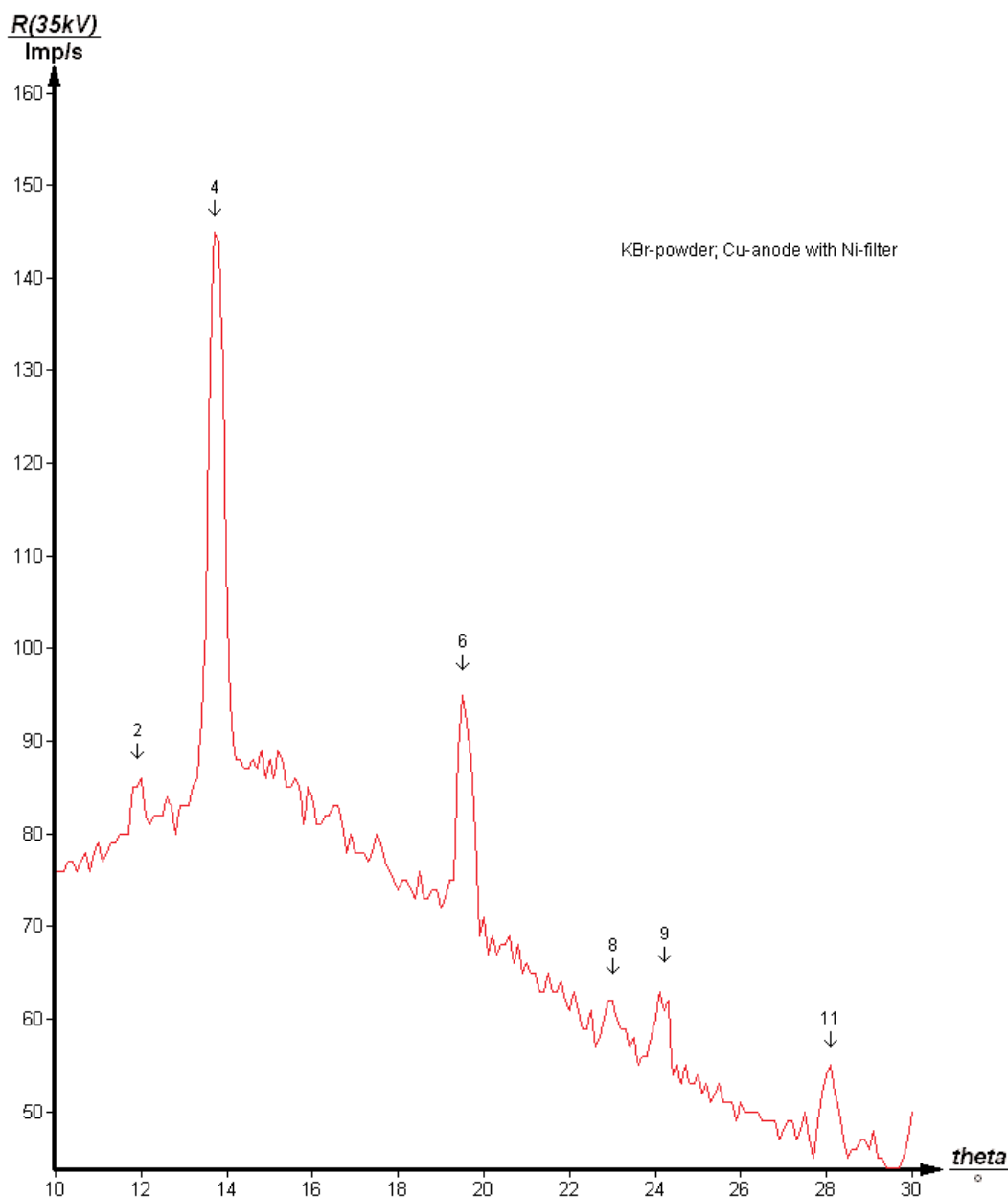
The ratios of the \sin^2 values of the individual lines (n) to the \sin^2 value of the first line (2) are calculated as in column J of Table 1. The numbering in column E relates to the reflex lines indicated in Fig. 2. In column A , all of the possible h,k,l numbers are listed. Columns B , C and D show the individual ratios of the sums of squares of these numbers.

When an attempt is made to allot the indices 100 or 110 to the first reflexes, then no agreement with the ratios of the $\sin^2\vartheta$ values is found. When the index 111 is assigned to the first line, however, then all of the other lines can be assigned hkl index triplets with a certain accuracy.

Only even or odd numbers are now given, no mixed indices hkl triplets. According to this, KBr forms an fcc lattice. The corresponding lattice plane spacings d , calculated using equation (1), are given in column K . Values for the lattice constant a determined from equation (6) are given in column L . Taking both the K_{α} lines and the K_{β} lines into consideration, the mean value of the lattice constant a is found to be:

$a = (655.1 \pm 2.9) \text{ pm}$; $\Delta(a) / a < 0.5\%$;
(literature value: $a = 658.0 \text{ pm}$)

Fig. 3: Bragg-diagram of KBr only with Cu- K_{α} beam (a nickel filter was used here)



On dividing the total mass M of a unit cell by its volume V , the density ρ is given, so that:

$$\rho = \frac{M}{V} = n \cdot m \cdot \frac{1}{a^3} \quad \text{with } m = \frac{m_A}{N} \rightarrow n = \frac{\rho \cdot N \cdot a^3}{m_A} \quad (9)$$

where n = the number of atoms or molecules in the unit cell;
 m = atomic/molecular mass; m_A = atomic/molecular weight;
 $N = 6.022 \cdot 10^{23}$ = Avogadro's number.

On entering the appropriate values for KBr, $\rho = 2.75 \text{ g} \cdot \text{cm}^{-3}$
and $m_A = 119.01 \text{ g}$, in equation (9), it follows that $n = 3.91 \approx 4$,
i.e. the unit cell contains 4 atoms.

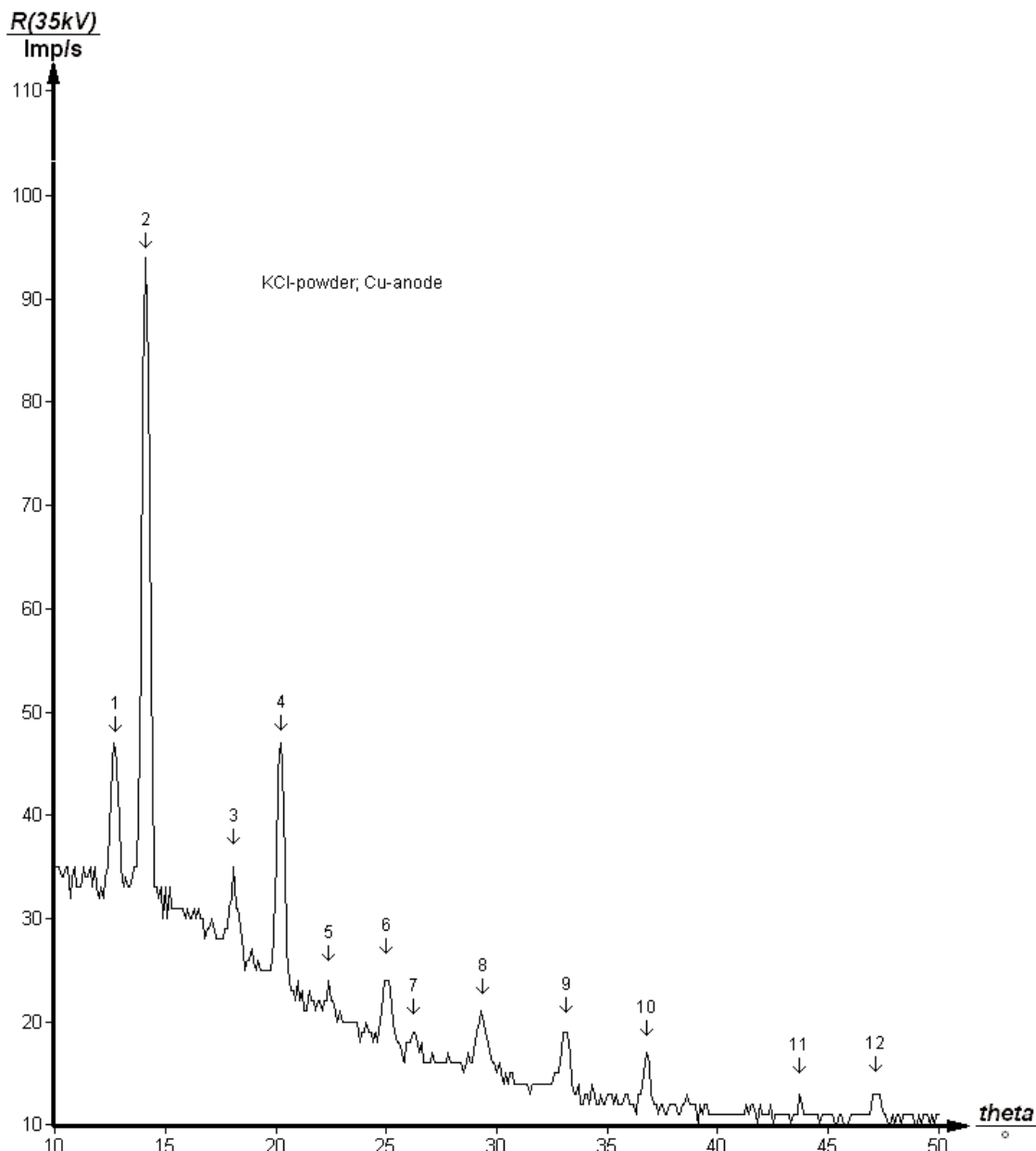
The Debye-Scherrer pattern for potassium chloride (KCl) is shown in Fig. 4, and the evaluation of this with respect to the K_α -radiation is given in Table 3.

The quotients of the sine values of the pairs of lines 2-1, 4-3, 6-5 and 8-7 again give approximately 1.1, so that the lines 1, 3, 5 and 7 can again be assigned to the K_β radiation.

Although KCl forms an fcc lattice, in contrast to KBr it gives exclusively even numbered h,k,l values and no, as expected for an fcc lattice, odd numbered h,k,l index triplets (see Tables 3 and 4). This is understandable when one considers that the atomic scattering factor f is correlated directly with the number of electrons of an atom, among others. As KCl, in contrast to KBr, contains atoms with almost the same scattering power ($Z = 19$ for K and 17 for Cl), it follows from equation (5) that reflexes with odd numbered h,k,l index triplets should not occur.

The mean value found for lattice constant a in the experiment is: $a = (631.3 \pm 1.1) \text{ pm}$; $\Delta(a) / a < 0.2\%$; (literature value: $a = 629.3 \text{ pm}$).

Fig. 4: Bragg-Cu- K_α and Cu- K_β -lines of KCl



From the experimentally determined average value for a and the known values for KCl ($\rho = 1.984 \text{ g} \cdot \text{cm}^{-3}$ and $m_A = 74.56 \text{ g}$), it follows from equation (9) that: $n = 4.04 \approx 4$, i.e. that the unit KCl cell contains 4 atoms.

Examination of bcc lattices

Fig. 5 shows the spectrum of molybdenum (Mo). The evaluation in Table 5 shows that agreement with the ratios of the $\sin^2\vartheta$ - values can only be given when $(h + k + l)$ is even, i.e. that molybdenum forms a bcc lattice.

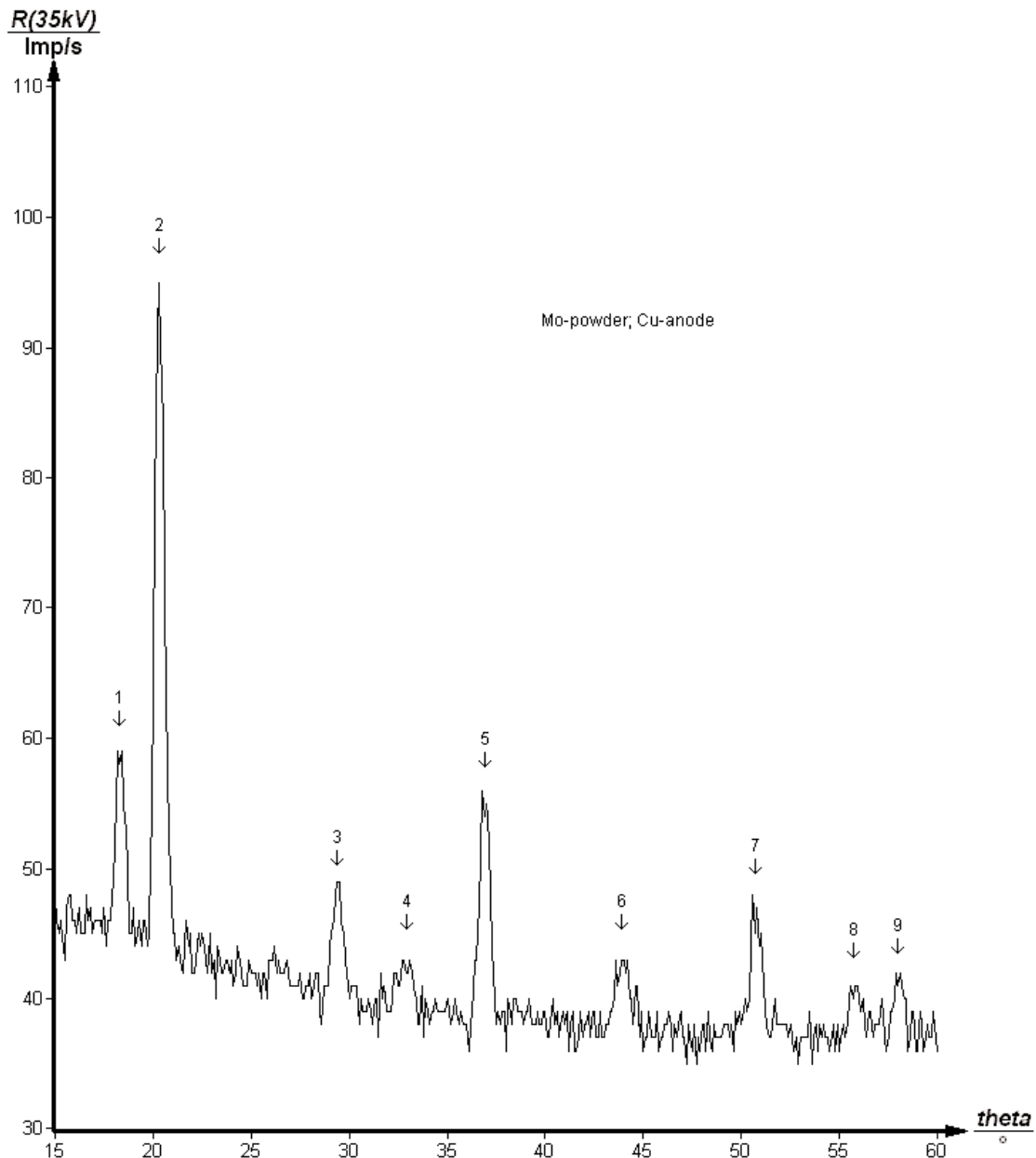
The experiment gives an average value for lattice constant a of $a = (314.22 \pm 0.58) \text{ pm}$; $\Delta(a) / a < 0.2\%$ (literature value: $a = 314.05 \text{ pm}$).

A bcc lattice should contain 2 atoms per unit cell. From the experimentally determined average value for a and the known values for Mo ($\rho = 10.2 \text{ g} \cdot \text{cm}^{-3}$ and $m_A = 95.94 \text{ g}$), it follows from equation (9) that: $n = 1.99 \approx 2$, i.e. that the unit Mo cell does actually contain 2 atoms.

Examination of pc lattices

Fig. 6 shows the Debye-Scherrer spectrum of ammonium chloride (NH_4Cl), the evaluation of which is given in Table 6. Line 2 of the spectrum at $\vartheta = 14.83^\circ$ is not taken into consideration, as the quotient of the $\sin\vartheta$ value of the pairs of lines 3 and 2 is namely $\sin(16.45^\circ) / \sin(14.83^\circ) = 1.11$. Line 2 must therefore be assigned to the K_β radiation (see equation (9)).

Fig. 5: Bragg-Cu- K_α and Cu- K_β -lines of Mo



The quotient of the $\sin^2\vartheta$ values in column *I* is always approximately even-numbered, and could so be assigned both to the bold face numbers in column *B* as well as to column *C*, so that it is not yet possible to make an unambiguous assignment to the reflex planes.

If assignment to column *B* should be correct, then mixed index h,k,l triplets and even-numbered $(h+k+l)$ values would occur. This means that NH_4Cl has neither an fcc lattice nor a bcc lattice, but has rather a cubic simple (pc) cell with a mean lattice constant a (see column *K*) of $a = (384.5 \pm 1.7)$ pm.

If assignment to column *C* should be correct, then only even-numbered $(h+k+l)$ values would occur. This would correspond to a bcc lattice with a mean lattice constant a (see column *L*) of $a^* = (543.7 \pm 2.2)$ pm.

The following consideration helps to solve this dilemma.

The following values are given in Tables for NH_4Cl : $\rho = 1.527 \text{ g} \cdot \text{cm}^{-3}$ and $m_A = 53.49 \text{ g}$.

Using these values and $a = 384.5 \text{ pm}$ in equation (9), $n = 0.977 \approx 1$, i.e. only one molecule is present in the cell. According to this, NH_4Cl crystallizes cubic, simple.

On repeating this same procedure, but with $a^* = (543.7 \pm 2.2) \text{ pm}$, then $n = 2.75$ is obtained.

The number of $2^{3/4}$ molecules in a unit cell can not be brought into accordance with a bcc lattice, as this contains only 2 atoms or molecules. From this it is clear that NH_4Cl forms a cubic simple lattice with the lattice constant $a = (384.5 \pm 1.7) \text{ pm}$; $\Delta(a)/a \leq 0.5\%$.

(Literature value: $a = 386.0 \text{ pm}$).

Fig. 6: Bragg-Cu- K_α and Cu- K_β -lines of NH_4Cl

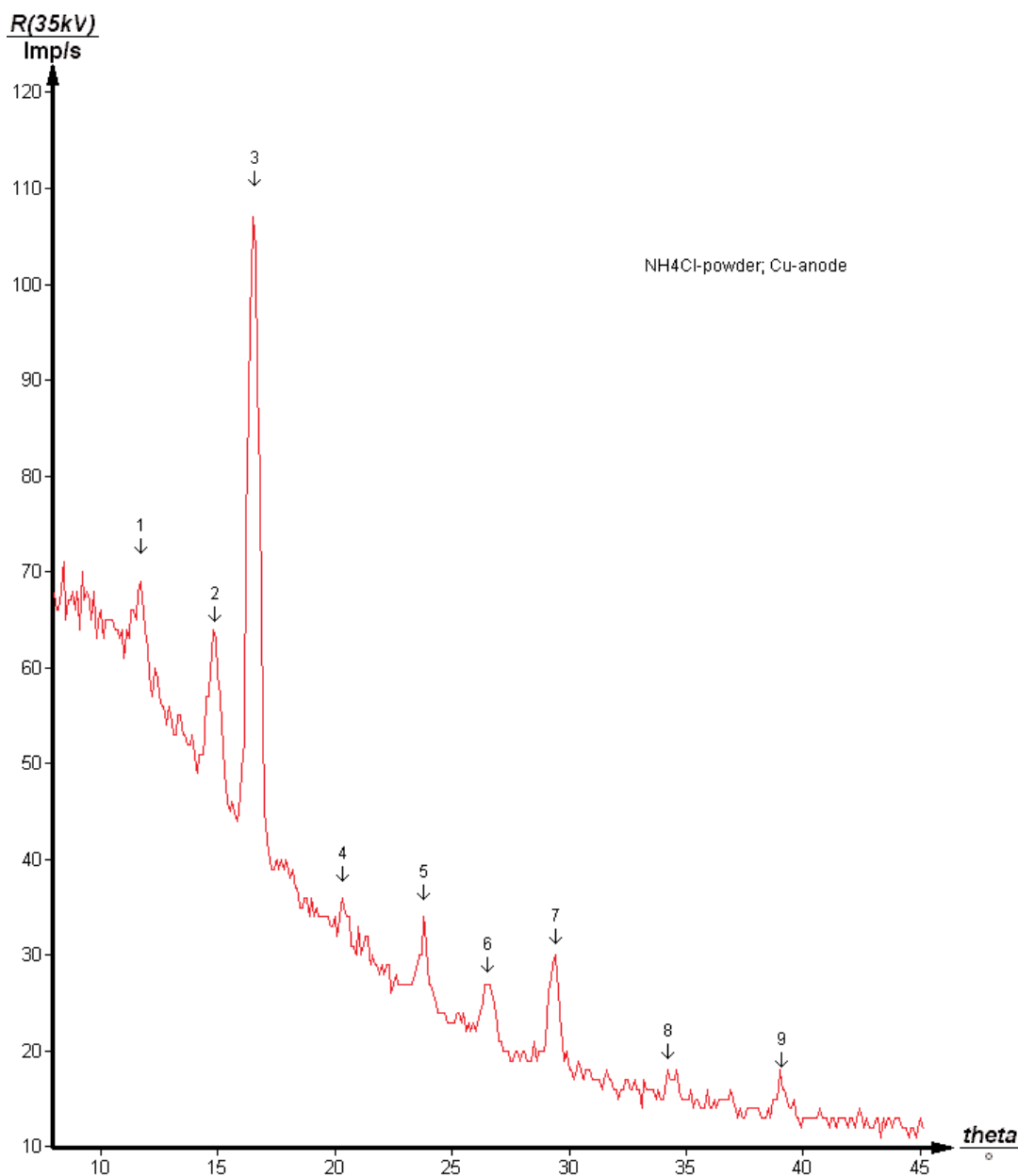


Table 1: Evaluation of the K_{α} -Debye-Scherrer lines of KBr

A	B	C	D	E	F	G	H	I	J	K	L
hkl	$h^2+k^2+l^2$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{011}}$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{111}}$	Reflex no.	Intensity	$\vartheta/^\circ$	$\sin\vartheta$	$\sin^2\vartheta$	$\frac{\sin^2\vartheta(n)}{\sin^2\vartheta(2)}$	d/pm	a/pm
100	1										
110	2	1									
111	3	1.5	1	2	w	11.80	0.20449	0.04182	1.00	377.0	652.9
200	4	2	1.33	4	vs	13.72	0.23718	0.05625	1.34	325.0	650.1
210	5	2.5	1.67								
211	6	3	2								
220	8	4	2.67	6	vs	19.46	0.33315	0.11099	2.65	231.4	654.5
221/300	9	4.5	3								
310	10	5	3.33								
311	11	5.5	3.67	8	w	22.95	0.38993	0.15204	3.64	197.7	655.7
222	12	6	4	9	s	24.08	0.40801	0.16647	3.98	188.9	654.5
320	13	6.5	4.33								
321	14	7	4.67								
400	16	8	5.33	11	s	27.97	0.46901	0.21997	5.26	164.4	657.5
410/322	17	8.5	5.67								
441/330	18	9	6								
331	19	9.5	6.22								
420	20	10	6.67	12	s	31.69	0.52532	0.27596	6.60	146.8	656.3
421	21	10.5	7								
332	22	11	7.33								
422	24	12	8	13	s	35.03	0.57401	0.32948	7.88	134.3	657.9
500/430	25	12.5	8.33								
510/431	26	13	8.67								
511/333	27	13.5	9								
520/432	29	14.5	9.67								
521	30	15	10								
440	32	16	10.67	14	vw	41.61	0.66406	0.44097	10.54	116.1	656.7
522/441	33	16.5	11								
530/433	34	17	11.33								
531	35	17.5	11.67	15	w	44.56	0.70166	0.49232	11.77	109.9	650.0
600/442	36	18	12								
610	37	18.5	12.33								
611/532	38	19	12.67								
620	40	20	13.33	16	w	47.86	0.74151	0.54983	13.15	104.0	657.5
621/540/443	41	20.5	13.67								
541	42	21	14								
533	43	21.5	14.33								
622	44	22	14.67	17	w	50.91	0.77656	0.60242	14.40	99.3	658.5

The K_{β} lines 1, 3, 5 and 7 that occur in Fig. 2 are evaluated in Table 2.

Table 2: Evaluation of the K_{β} -Debye-Scherrer lines of KBr

A	B	C	D	E	F	G	H	I	J	K	L
hkl	$h^2+k^2+l^2$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{011}}$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{111}}$	Reflex no.	Intensity	$\vartheta/^\circ$	$\sin\vartheta$	$\sin^2\vartheta$	$\frac{\sin^2\vartheta(n)}{\sin^2\vartheta(3)}$	d/pm	a/pm
100	1										
110	2	1									
111	3	1.5	1	1	s	10.61	0.18412	0.03390	1.00	378.1	652.9
200	4	2	1.33	3	vs	12.38	0.21439	0.04596	1.36	324.7	650.1
210	5	2.5	1.67								
211	6	3	2								
220	8	4	2.67	5	s	17.61	0.30254	0.09153	2.70	230.1	654.5
221/300	9	4.5	3								
310	10	5	3.33								
311	11	5.5	3.67								
222	12	6	4	7	w	21.73	0.37023	0.13707	4.04	188.0	651.3

Table 3: Evaluation of the K_{α} - Debye-Scherrer lines of KCl

A	B	C	D	E	F	G	H	I	J
$h k l$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{002}}$	Reflex no.	Intensity	$\vartheta/^\circ$	$\sin\vartheta$	$\sin^2\vartheta$	$\frac{\sin^2\vartheta(n)}{\sin^2\vartheta(2)}$	d/pm	a/pm
200	1	2	vs	14.13	0.24412	0.05960	1	315.8	631.6
220	2	4	vs	20.22	0.34562	0.11946	2.00	223.0	630.9
222	3	6	s	25.02	0.42293	0.17887	3.00	182.3	631.4
400	4	8	s	29.30	0.48938	0.23950	4.02	157.5	630.1
420	5	9	s	33.10	0.54610	0.29823	5.00	141.2	631.5
422	6	10	s	36.80	0.59902	0.35883	6.02	128.7	630.5
440	8	11	vw	43.72	0.69113	0.47767	8.01	111.5	630.7
600/442	9	12	w	47.16	0.73326	0.53766	9.02	105.1	630.6

Table 4: Evaluation of the K_{β} - Debye-Scherrer lines of KCl

A	B	C	D	E	F	G	H	I	J
$h k l$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{002}}$	Reflex no.	Intensity	$\vartheta/^\circ$	$\sin\vartheta$	$\sin^2\vartheta$	$\frac{\sin^2\vartheta(n)}{\sin^2\vartheta(2)}$	d/pm	a/pm
200	1	1	vs	12.71	0.22002	0.04841	1	316.4	632.8
220	2	3	s	18.12	0.31101	0.09673	2.00	223.8	633.1
222	3	5	vw	22.40	0.38107	0.14521	3.00	182.7	632.8
400	4	7	vw	26.25	0.44229	0.19562	4.04	157.4	629.6

Table 5: Evaluation of the K_{α} - and K_{β} - Debye-Scherrer lines of Mo

A	B	C	D	E	F	G	H	I	J	K
$h k l$	$h^2+k^2+l^2$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{011}}$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{111}}$	Reflex no.	$\vartheta/^\circ$	$\sin\vartheta$	$\sin^2\vartheta$	$\frac{\sin^2\vartheta(n)}{\sin^2\vartheta(2)}$	d/pm	a/pm
110 (β)	2			1	18.33	0.31449	0.09890		221.34	313.03
110	2	1		2	20.33	0.34743	0.12071	1	221.89	313.78
200	4	2	1	3	29.41	0.49106	0.24114	1.99	156.99	313.98
211 (β)	6			4	32.87	0.54273	0.29456		128.26	314.17
211	6	3	1.67	5	36.89	0.60029	0.36034	2.99	128.42	314.57
220	8	4	2	6	43.95	0.69403	0.48168	3.99	110.08	314.17
310	10	5	2.67	7	50.79	0.77483	0.60037	4.97	99.49	314.62
222	12	6	3.33	9	58.05	0.84851	0.71997	5.96	90.85	314.73
321 (β)	14			8	55.80	0.82708	0.68406		84.16	314.91

Table 6: Evaluation of the K_{α} - Debye-Scherrer lines of NH_4Cl

A	B	C	D	E	F	G	H	I	J	K	L
$h k l$	$h^2+k^2+l^2$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{011}}$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{111}}$	Reflex no.	$\vartheta/^\circ$	$\sin\vartheta$	$\sin^2\vartheta$	$\frac{\sin^2\vartheta(n)}{\sin^2\vartheta(1)}$	d/pm	a/pm	a^*/pm
100	1			1	11.61	0.20125	0.04050	1.00	383.0	383.0	
110	2	1		3	16.45	0.28468	0.08105	2.00	270.8	383.0	541.6
111	3	1.5	1	4	20.34	0.34759	0.12082	2.98	221.8	384.1	543.3
200	4	2	1.33	5	23.79	0.40338	0.16272	4.02	191.1	382.2	541.6
210	5	2.5	1.67	6	26.51	0.44635	0.19923	4.92	172.7	386.2	
211	6	3	2	7	29.36	0.49030	0.24039	5.93	157.2	385.1	543.3
220	8	4	2.67	8	34.40	0.56497	0.31919	7.88	136.4	385.9	540.5
221/300	9	4.5	3								
310	10	5	3.33	9	39.06	0.63013	0.39707	9.80	122.3	386.8	546.1
311	11	5.5	3.67								
222	12	6	4								544.6
320	13	6.5	4.33								
321	14	7	4.67								
400	16	8	5.33								545.6
410/322	17	8.5	5.67								
441/330	18	9	6								
331	19	9.5	6.22								
420	20	10	6.67								546.9