K and L edge absorbtion - Moseley's law and Rydberg constant (Item No.: P2541201)

Curricular Relevance

Area of Expertise: ILIAS

Education Level: Physik

Topic: Hochschule

Subtopic: Moderne Physik

Experiment: Röntgenphysik

Difficulty	Preparation Time	Execution Time	Recommended Group Size
Difficult	1 Hour	2 Hours	2 Students

Additional Requirements:

- PC

Experiment Variations:

Keywords:

Bremsstrahlung, characteristic X-radiation, Bragg scattering, Bohr model, energy levels, Moseley’s law, Rydberg frequency, screening constant

Overview

Short description

Principle

Samples of various thicknesses are irradiated with the polychromatic X-rays of a copper X-ray tube. The radiation that passes through the samples is analysed with the aid of a monocrystal. The Rydberg constant is calculated based on the glancing angles of the absorption edges.

This experiment is included in the “XRS 4.0 X-ray structural analysis” upgrade set.
Note: Alternatively, this experiment can also be performed with an iron X-ray tube.

Student's Sheet

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Fig. 1: P2541201

Equipment

Position No.	Material	Order No.	Quantity
1	XR 4.0 expert unit, X-ray unit, 35 kV	09057-99	1
2	XR 4.0 X-ray goniometer	09057-10	1
3	XR 4.0 X-ray Plug-in Cu tube	09057-51	1
4	Geiger-Mueller counter tube, 15 mm (type B)	09005-00	1
5	XR 4.0 X-ray LiF crystal, mounted	09056-05	1
6	XR 4.0 X-ray Chemical set for edge absorption	09056-04	1
7	Silver nitrate, cryst. 15 g	30222-00	1
8	Mortar w. pestle, 70ml, porcelain	32603-00	1
9	Microspoon, steel	33393-00	1
10	XR 4.0 Software measure X-ray	14414-61	1
11	Data cable USB, plug type A/B, 1.8 m	14608-00	1
12	XR 4.0 X-ray Diaphragm tube d = 2 mm	09057-02	1
13	XR 4.0 X-ray Diaphragm tube d = 5 mm	09057-03	1

Tasks

1. Analyse the copper X-radiation with the aid of a LiF monocrystal and as a function of the Bragg angle without and with several K edge absorption samples as absorbers. Determine the K absorption edges of different absorbers based on the spectra.
2. Calculate the Rydberg constant and the screening constant based on the energy values of the K absorption edges.
3. Proceed as described for task 1, but this time with various samples for L edge absorption.
4. Calculate the Rydberg constant based on the energy values of the L absorption edges.

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Safety instructions

When handling chemicals, you should wear suitable protective gloves, safety goggles, and suitable clothing. Please refer to the appendix for detailed safety instructions.

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Setup and Procedure

Setup

Connect the goniometer and the Geiger-Müller counter tube to their respective sockets in the experiment chamber (see the red markings in Fig. 2). The goniometer block with the analyser crystal should be located at the end position on the right-hand side. Fasten the Geiger-Müller counter tube with its holder to the back stop of the guide rails. Do not forget to install the diaphragm in front of the counter tube (see Fig. 3). Insert a diaphragm tube with a diameter of 2 mm (without an absorber) or 5 mm (with an absorber) into the beam outlet of the tube plug-in unit for the collimation of the X-ray beam.

For calibration: Make sure, that the correct crystal is entered in the goniometer parameters. Then, select “Menu”, “Goniometer”, “Autocalibration”. The device now determines the optimal positions of the crystal and the goniometer to each other and then the positions of the peaks.

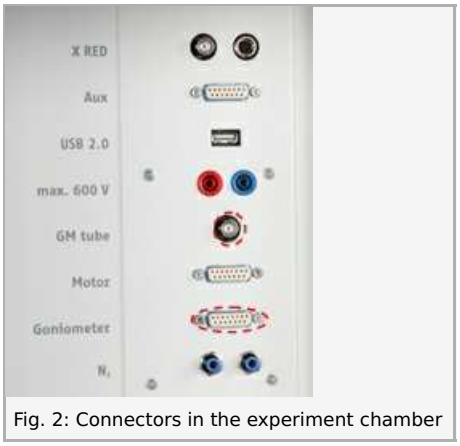

Fig. 2: Connectors in the experiment chamber

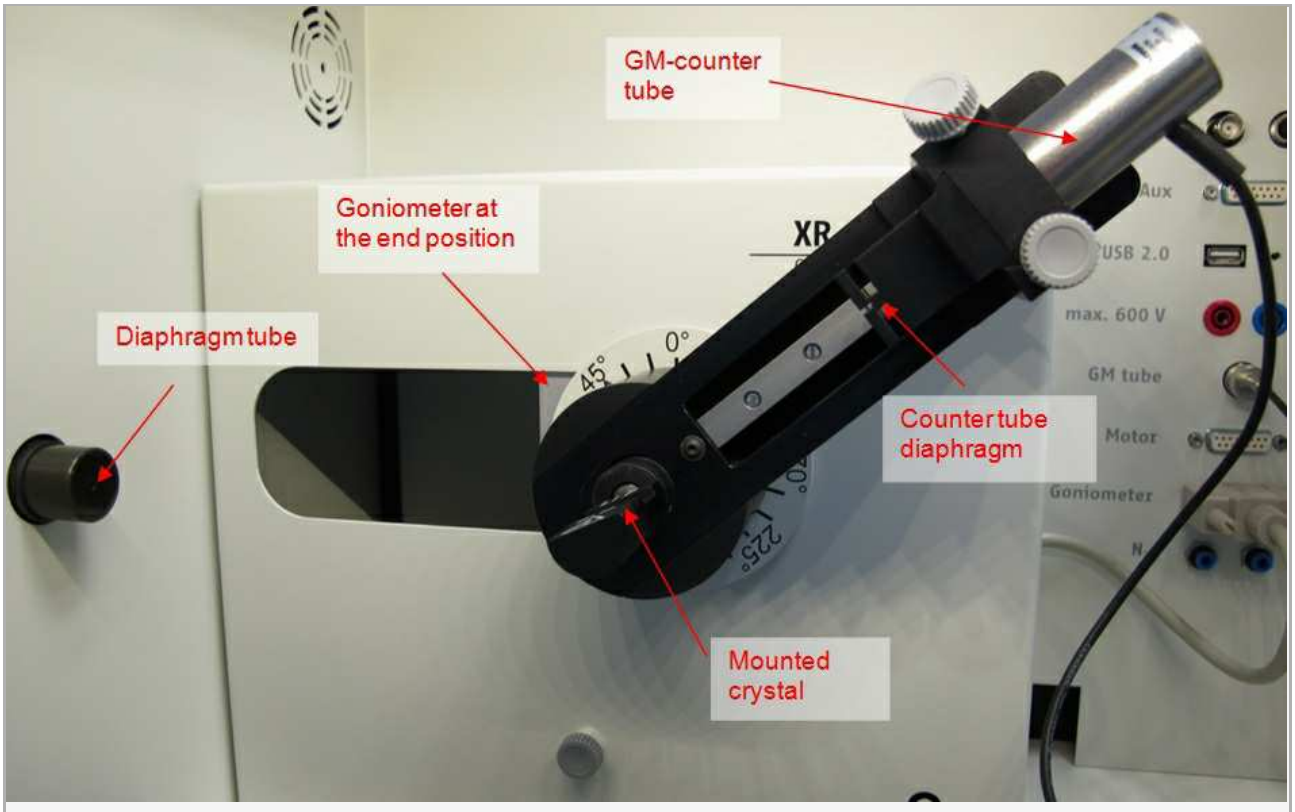

Fig. 3: Set-up of the goniometer

Note

Details concerning the operation of the X-ray unit and goniometer as well as information on how to handle the monocrystals can be found in the respective operating instructions.

Procedure

Theory and Evaluation

Theory

When X-rays interact with matter, they lose energy due to Compton scattering, pair production, and photoelectric effects. The respective strength of these three effects depends on the energy of the radiation. In the range of energy that is available during this experiment, the photoelectric effect plays the most important role. Figure 8 shows the schematic course of the transmission T as a function of the radiation energy E. The cause of the irregularity that is known as “edge absorption” is the photoelectric effect.

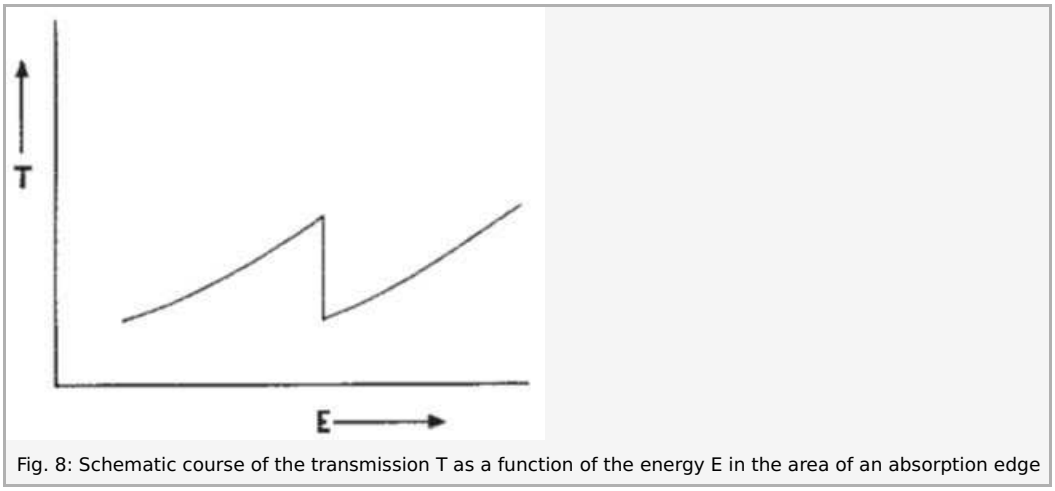

Fig. 8: Schematic course of the transmission T as a function of the energy E in the area of an absorption edge

The binding energy E_n of an electron on the nth shell is approximately:

$E_n = -\frac{m_e e^4}{8\varepsilon_0^2 h^2}(Z-\sigma)^2 \frac{1}{n^2}$ where (n = 1, 2, 3, ...) (1)

Electron mass $m_e = 9.1091 \cdot 10^{-31}$ kg

Elementary charge $e = 1.6021 \cdot 10^{-19}$ As

Planck's constant $h = 6.6256 \cdot 10^{-34}$ Js

Dielectric constant $\varepsilon 0 = 8.8544 \cdot 10^{-12} N^{-1} m^{-2} C^2$

Atomic number Z

Screening constant σ

Principle quantum number n

With the introduction of the Rydberg constant R:

$R = \frac{m_e e^4}{8\varepsilon_0^2 h^2} = 3.28989^1 0 s^{-1}$ (2)

equation (1) becomes:

$E_n = R \cdot h(Z-\sigma)^2 \frac{1}{n^2}$ (3)

For electrons on the K shell (n = 1), the screening constant is σ ~= 1.

Calculation of the energy based on the glancing angles:
Using the Bragg equation

$2dsin\vartheta = n\lambda$ (n = 1, 2, 3,...) (4)

(d = 201.4 pm = interplanar spacing (002) of the LiF crystal)
with n = 1 and together with the energy equation

$E = h \cdot f = \frac{h \cdot c}{\lambda}$ (5)

($c = 2.998 \cdot 10^8 m s^{-1}$ = velocity of light)

we finally obtain the energy (n = 1) based on the glancing angles of the absorption edges:

$E = \frac{h \cdot c}{2dsin\vartheta}$ (6)

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Table 1 shows the ϑ values of the absorption edges of various absorbers that were taken from Figure 9. Equation (6) was used to calculate the energy values E_K of the associated K shells. For comparison, the corresponding literature values are also provided.
Equation (3) is converted in order to calculate the Rydberg constant R.
$Z = \frac{1}{\sqrt{R \cdot h}} \cdot \sqrt{E} + \sigma$ (with n = 1) (7)

Table 1: K edge energies

	Z	$\vartheta Exp/^\circ$	$E_K(exp.)/keV$	$E_K(lit.)/keV$
Zn	30	18.6	9.65	9.66
Ge	32	16.1	11.10	11.10
Se	34	14.0	12.72	12.66
Br	35	13.2	13.48	13.47
Rb	37	11.6	15.31	15.20
Sr	38	11.0	16.13	16.10
Ag	47	6.8	25.99	25.51

Task 1

Analyse the copper X-radiation with the aid of a LiF monocrystal and as a function of the Bragg angle without and with several K edge absorption samples as absorbers. Determine the K absorption edges of different absorbers based on the spectra.

Figure 9 shows the intensity I of the copper X-radiation as a function of the Bragg angle ϑ up to the characteristic $K\beta$ line. The top curve shows the spectrum without any absorber. All of the other curves were recorded with an additional absorber sample. The higher atomic number of the absorber is, the more the absorption edge is shifted towards smaller glancing angles.

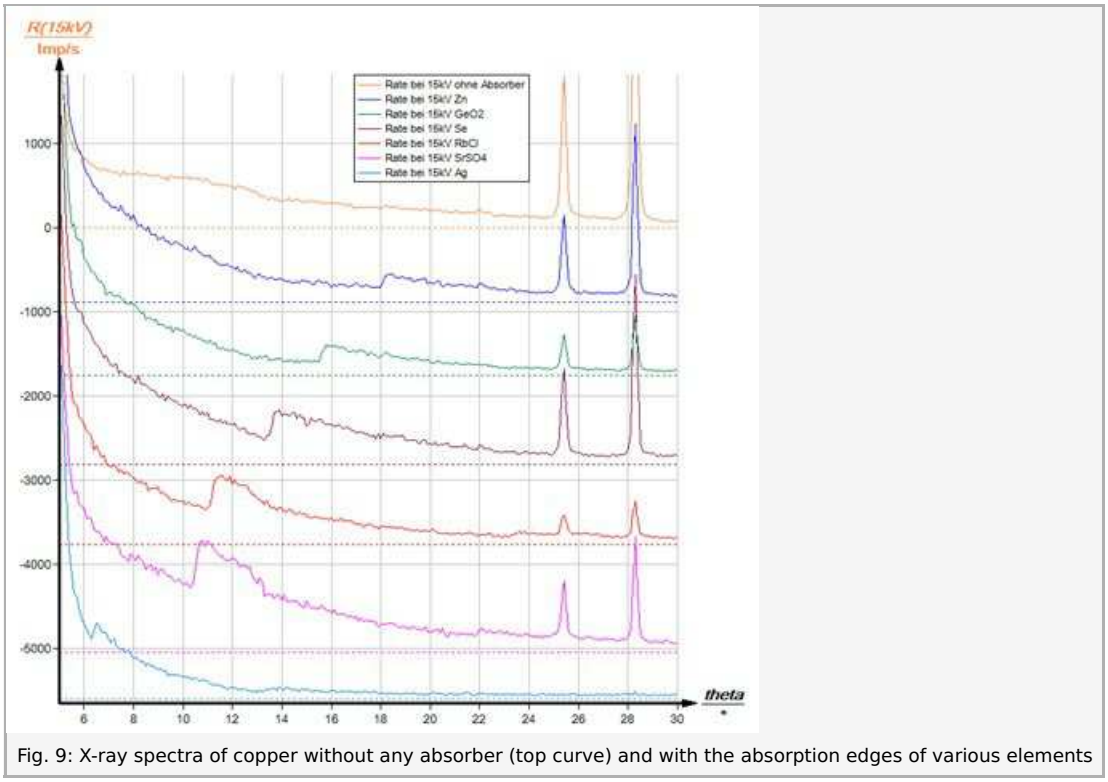

Fig. 9: X-ray spectra of copper without any absorber (top curve) and with the absorption edges of various elements

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Task 2

Calculate the Rydberg constant and the screening constant based on the energy values of the K absorption edges.

With the aid of equation (6), the edge absorption energy values can be obtained.
Figure 10 shows the function $Z = f(\sqrt{E_K})$ based on the energy values E_K (exp.) of table 1.

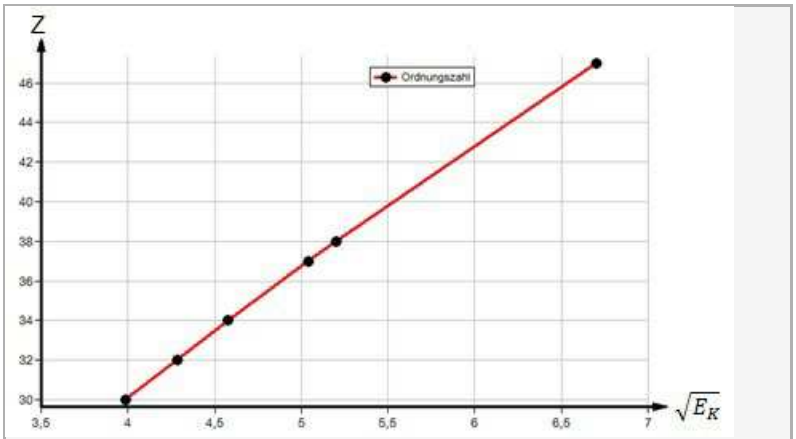

Fig. 10: Moseley line of the K edge absorption to determine the Rydberg constant.

Based on the equation of the straight line

$$a = \frac{1}{\sqrt{R \cdot h}}$$

the following follows for the Rydberg constant:

$$R = \frac{1}{h} \cdot \frac{[\Delta(\sqrt{E})]^2}{(\Delta Z)^2} \qquad (8)$$

With the value for R and the E_K (exp.) values of table 1, equation (3) leads to σ (K) = (3.5 $\pm$ 0.1) as the mean value of the screening constant.

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Task 3

Proceed as described for task 1, but this time with various samples for L edge absorption.

Figure 11 shows bremsspectrum with the absorption edges of elements of a higher atomic number. However, although three edges of the three L shells can be expected in theory, only two can be seen. A separation of the absorption edges of the L_2 and L_3 sub-shells is not possible.

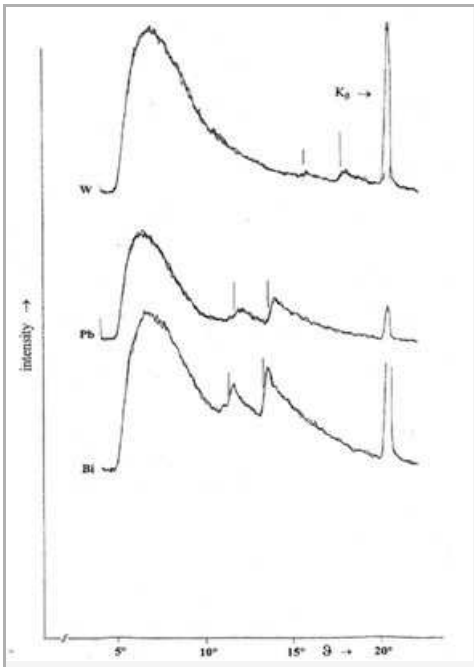

Fig. 11: X-ray spectrum of copper with the L absorption edges of various elements

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Task 4

Calculate the Rydberg constant based on the energy values of the L absorption edges.

Table 2 shows the results concerning the L edge absorption. The literature value $E_{L1,2}$ that is given for comparison has been calculated by taking the mean of the corresponding L_1 and L_2 values.
An evaluation with the aid of equation (1) does not make any sense in this case, since – apart from the Coulomb interaction – other interactive processes must also be taken into account. Nevertheless, equation (1) is helpful in giving a rough idea of the screening of the electrons on L shells. According to (3) and with n = 2 plus the experimental energy values in table 2, the following results:

$$\sigma(K) << \sigma(L_{1,2}\ 15 < \sigma(L_3)\ 20$$

The growth of the screening constant underlines the decreasing influence of the nuclear potential on the electrons on the outer shells.

Table 2: L edge energies

	W (Z = 74)	Hg (Z = 80)	Pb (Z = 82)	Bi (Z = 83)
$\vartheta(L_{1,2})/^\circ$	15.5	12.4	11.6	11.2
$E_{L1,2}exp./keV$	11.52	14.33	15.31	15.85
$E_{L1,2}lit./keV$	11.82	14.52	15.53	16.05
$\vartheta(L_3)/^\circ$	17.6	14.5	13.6	13.2
$E_{L3}exp./keV$	10.20	12.29	13.09	13.48
$E_{L3}lit./keV$	10.21	12.28	13.04	13.42

Figure 12 shows the linear course of the function $Z = f(\sqrt{E_L})$ for $L_{1,2}$ and L_3 (9).

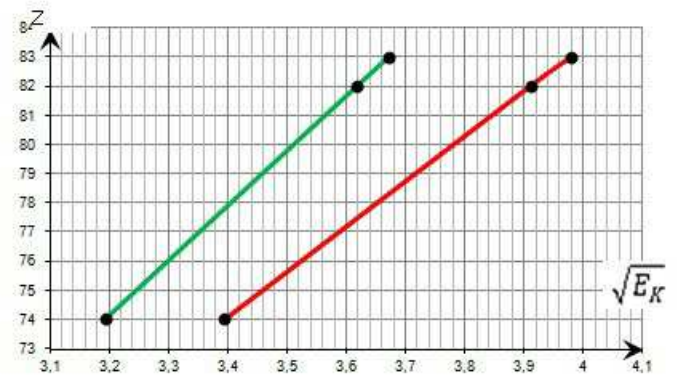

Fig. 12: Moseley lines for the L edge absorption

Note

"measure" software

In order to evaluate the measurements with the aid of the “measure” software, first convert the glancing angles ϑ (crystal angle = x-axis) of the spectra into the corresponding energy values. To do so, proceed as follows:

- “Analysis”, “X-ray spectroscopy”, “Convert x-axis”, and “Energy (n = 1)”.

Moseley lines can be obtained from the converted spectra (Imp/s = f(E/keV) as follows:

- Click “Analysis”, “X-ray spectroscopy”, and “Moseley straight line”.

The window “Moseley straight line” appears. It offers two options: K and L edge absorption. Then, select the middle of the absorption edge as a narrow band with the aid of the marker and click “Accept value”. If necessary, the area of the absorption edge can be zoomed with the aid of the zoom function.
If the absorber and its atomic number were entered into the start window prior to the actual measurement, the corresponding pair values for the edge energy and atomic number are displayed. The latter can also be entered later into the additional window “Moseley straight line”.
Repeat this for the other spectra with different absorbers.
In order to generate the straight line, click “Generate Moseley line”.
The Rydberg constant can be determined by clicking “Analysis”, “X-ray spectroscopy”, and “Determine Rydberg constant”.
With “Display options”, “Channels”, and “Symbol”, the measuring points of the Moseley line can be displayed if desired.

Disposal

Do not dispose of heavy-metal-containing waste via household waste.

Appendix

Hazard symbol, signal word	**Hazard statements**	**Precautionary statements**
Rubidium chloride (RbCl)		
-	--	-
Germanium(IV) oxide (GeO_2)		
	H302: Harmful if swallowed H332: Harmful if inhaled	-
Silver (I) chloride (AgCl)		
 Warning	H400: Very toxic to aquatic life	P273: Avoid release to the environment.
Zinc		
-	-	-
Selenium		
Danger 	H301: Toxic if swalloed H331 Toxic if inhaled H373: Causes damage to organs through prolonged or repeated exposure H413: May cause long lasting harmful effects to aquatic life	-
Potassium bromide (KBr)		
	H315: Causes skin irritation	P261: Avoid breathing dust/fume/gas/mist/vapours/spray.

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	H319: Causes serious eye irritation H335: May cause respiratory irritation	P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
Strontium sulphate $(SrSO_4)$		
-	-	-
Lead(IV) oxide (PbO_2)		
Danger 	H272: May intensify fire; oxidiser H302: Harmful if swallowed H332: Harmful if inhaled H360: May damage fertility or the unborn child H373: Causes damage to organs through prolonged or repeated exposure H410: Very toxic to aquatic life with long lasting effects	P201: Obtain special instructions before use. P220: Keep/Store away from clothing/ .../combustible materials. P273: Avoid release to the environment. P308 + P313: IF exposed or concerned: Get medical advice/attention.
Tungsten(IV) oxide (WO_2)		
 Warning	H335: May cause respiratory irritation	-
Bismuth(III) oxide (Bi_2O_3)		
 Warning	H315: Causes skin irritation H319: Causes serious eye irritation H335: May cause respiratory irritation	P261: Avoid breathing dust/fume/gas/mist/vapours/spray. P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.