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4.2. X-rays

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4.2.1. Generation of X-rays (By U. W. Arndt)

X-rays are produced by the interaction of charged particles with an electromagnetic field. There are four sources of X-rays that are of interest to the crystallographer.

(1) The bombardment of a target by electrons produces a continuous ('white') X-ray spectrum, called *Bremsstrahlung*, which is accompanied by a number of discrete spectral lines characteristic of the target material. The high-vacuum, or Coolidge, X-ray tube is the most important X-ray source for crystallographic studies.

(2) The decay of natural or artificial radio isotopes is often accompanied by the emission of X-rays. Radioactive X-ray sources are often used for the calibration of X-ray detectors. Mössbauer sources have the narrowest known spectral bandwidth and are used in nuclear resonance scattering studies.

(3) Sources of synchrotron radiation produced by relativistic electrons in orbital motion are of growing importance.

(4) X-rays are also produced in plasmas generated by the bombardment of targets by high-energy laser beams, but to date the yield has been principally in the form of soft X-rays.

The classical text on the generation and properties of X-rays is that by Compton & Allison (1935), which still summarizes much of the information required by crystallographers. There is a more recent comprehensive book by Dyson (1973). X-ray physics has received a new impetus on the one hand through the development of X-ray microprobe analysis dealt with in a number of monographs (Reed, 1975; Scott & Love, 1983) and on the other hand through the increasing utilization of synchrotron-radiation sources (see Subsection 4.2.1.5).

4.2.1.1. *The characteristic line spectrum*

Characteristic X-ray emission originates from the radiative decay of electronically highly excited states of matter. We are concerned mostly with excitation by electron bombardment of a target that results in the emission of spectral lines characteristic of the target elements. The electronic states occurring as initial and final states of a process involving the absorption of emission of X-rays are called *X-ray levels*. Levels involving the removal of one electron from the configuration of the neutral ground state are called *normal X-ray levels* or *diagram levels*.

Table 4.2.1.1 shows the relation between diagram levels and electron configurations. The notation used here is the IUPAC notation (Jenkins, Manne, Robin & Senemaud, 1991), which uses arabic instead of the former roman subscripts for the levels. The IUPAC recommendations are to refer to X-ray lines by writing the initial and final levels separated by a hyphen, *e.g.* Cu $K\text{-}L_3$ and to abandon the Siegbahn (1925) notation, *e.g.* Cu $K\alpha_1$, which is based on the relative intensities of the lines. The correspondence between the two notations is shown in Table 4.2.1.2. Because this substitution has not yet become common practice, however, the Siegbahn notation is retained in Section 4.2.2, in which the wavelengths of the characteristic emission lines and absorption edges are discussed.

Table 4.2.1.1. *Correspondence between X-ray diagram levels and electron configurations; from Jenkins, Manne, Robin & Senemaud (1991), courtesy of IUPAC*

Level	Electron configuration	Level	Electron configuration	Level	Electron configuration
K	$1s^{-1}$	N_1	$4s^{-1}$	O_1	$5s^{-1}$
L_1	$2s^{-1}$	N_2	$4p_{1/2}^{-1}$	O_2	$5p_{1/2}^{-1}$
L_2	$2p_{1/2}^{-1}$	N_3	$4p_{3/2}^{-1}$	O_3	$5p_{3/2}^{-1}$
L_3	$2p_{3/2}^{-1}$	N_4	$4d_{3/2}^{-1}$	O_4	$5d_{3/2}^{-1}$
M_1	$3s^{-1}$	N_5	$4d_{5/2}^{-1}$	O_5	$5d_{5/2}^{-1}$
M_2	$3p_{1/2}^{-1}$	N_6	$4f_{5/2}^{-1}$	O_6	$5f_{5/2}^{-1}$
M_3	$3p_{3/2}^{-1}$	N_7	$4f_{7/2}^{-1}$	O_7	$5f_{7/2}^{-1}$
M_4	$3d_{3/2}^{-1}$				
M_5	$3d_{5/2}^{-1}$				

Table 4.2.1.2. *Correspondence between IUPAC and Siegbahn notations for X-ray diagram lines; from Jenkins, Manne, Robin & Senemaud (1991), courtesy of IUPAC*

Siegbahn	IUPAC	Siegbahn	IUPAC	Siegbahn	IUPAC
$K\alpha_1$	$K\text{-}L_3$	$L\alpha_1$	$L_3\text{-}M_5$	$L\gamma_1$	$L_2\text{-}N_4$
$K\alpha_2$	$K\text{-}L_2$	$L\alpha_2$	$L_3\text{-}M_4$	$L\gamma_2$	$L_1\text{-}N_2$
$K\beta_1$	$K\text{-}M_3$	$L\beta_1$	$L_2\text{-}M_4$	$L\gamma_3$	$L_1\text{-}N_3$
$K\beta_2^{1}$	$K\text{-}N_3$	$L\beta_2$	$L_3\text{-}N_5$	$L\gamma_4$	$L_1\text{-}O_3$
$K\beta_2^{11}$	$K\text{-}N_2$	$L\beta_3$	$L_1\text{-}M_3$	$L\gamma_4'$	$L_1\text{-}O_2$
$K\beta_3$	$K\text{-}M_2$	$L\beta_4$	$L_1\text{-}M_2$	$L\gamma_5$	$L_2\text{-}N_1$
$K\beta_4^{1}$	$K\text{-}N_5$	$L\beta_5$	$L_3\text{-}O_{4,5}$	$L\gamma_6$	$L_2\text{-}O_4$
$K\beta_4^{11}$	$K\text{-}N_4$	$L\beta_6$	$L_3\text{-}N_1$	$L\gamma_8$	$L_2\text{-}O_1$
$K\beta_{4x}$	$K\text{-}N_4$	$L\beta_7$	$L_3\text{-}O_1$	$L\gamma_8'$	$L_2\text{-}N_{6(7)}$
$K\beta_5^{1}$	$K\text{-}M_5$	$L\beta_7'$	$L_3\text{-}N_{6,7}$	L_η	$L_2\text{-}M_1$
$K\beta_5^{11}$	$K\text{-}M_4$	$L\beta_9$	$L_1\text{-}M_5$	Ll	$L_3\text{-}M_1$
		$L\beta_{10}$	$L_1\text{-}M_4$	Ls	$L_3\text{-}M_3$
		$L\beta_{15}$	$L_3\text{-}N_4$	Lt	$L_3\text{-}M_2$
		$L\beta_{17}$	$L_2\text{-}M_3$	Lu	$L_3\text{-}N_{6,7}$
				Lv	$L_2\text{-}N_{6(7)}$

Siegbahn	IUPAC
$M\alpha_1$	$M_5\text{-}N_7$
$M\alpha_2$	$M_5\text{-}N_6$
$M\beta$	$M_4\text{-}N_6$
$M\gamma$	$M_3\text{-}N_5$
$M\zeta$	$M_{4,5}\text{-}N_{2,3}$

In the case of unresolved lines, such as $K\text{-}L_2$ and $K\text{-}L_3$, the recommended IUPAC notation is $K\text{-}L_{2,3}$.

4.2.1.1.1. *The intensity of characteristic lines*

The efficiency of the production of characteristic radiation has been calculated by a number of authors (see, for example, Dyson, 1973, Chap. 3). For a particular line, it depends on the fluorescence yield, that is the probability that the decay of an excited state leads to the emission of a photon, on the statistical weights of the X-ray levels involved, on the effects of the penetration and slowing down of the bombarding electrons in the target, on the fraction of electrons back-scattered out of the target, and on the contribution caused by fluorescent X-rays produced indirectly by the continuous spectrum. The *emerging* X-ray intensity is further affected by the partial absorption of the generated X-rays in the target.

Dyson (1973) has also reviewed calculations and measurements made of the *relative* intensities of different lines in the K spectrum. The ratio of the $K\alpha_2$ to $K\alpha_3$ intensities is very close to