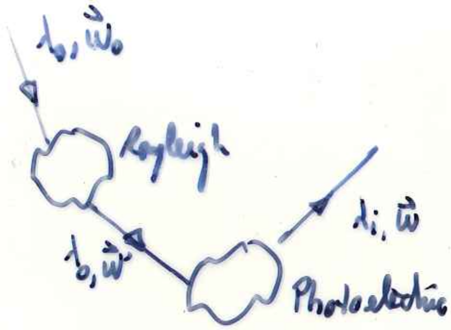
Rayleigh - Photoelectric chain



$$I^{(2)}_{(R,P)}(\vec{\omega},\lambda) = \frac{1-\mathrm{sgn}\,\eta}{2}\;\frac{1+\mathrm{sgn}\,\eta_0}{2}\;\frac{I_0}{|\eta_0|}\;\frac{\delta(\lambda-\lambda_i)}{\frac{\mu_i}{|\eta|}+\frac{\mu_0}{|\eta_0|}}\;\frac{\sigma\, Q_{f_i}(\lambda_0)\left[1-u(\lambda_0-\lambda_{0i})\right]}{4\pi}$$

$$\left\{ \int_0^{2\pi} d\varphi' \int_0^1 \frac{d\eta'}{\eta'}\, \frac{\left[1+(\vec{\omega}'\cdot\vec{\omega}_0^{(+)})^2\right]}{\frac{\mu_i}{|\eta|}+\frac{\mu_0}{\eta'}}\, \frac{F^2(\lambda_0, \vec{\omega}'\cdot\vec{\omega}_0^{(+)}, Z)}{Z} \; + \right.$$

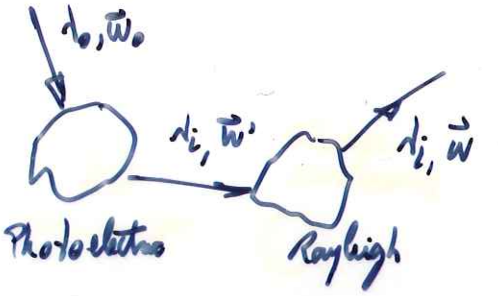
$$\left. + \int_0^{2\pi} d\varphi' \int_0^1 \frac{d\eta'}{\eta'}\, \frac{\left[1+(\vec{\omega}'\cdot\vec{\omega}_0^{(-)})^2\right]}{\frac{\mu_0}{|\eta_0|}+\frac{\mu_0}{\eta'}}\, \frac{F^2(\lambda_0, \vec{\omega}'\cdot\vec{\omega}_0^{(-)}, Z)}{Z} \right\}$$

where

$$\vec{\omega}'\cdot\vec{\omega}_0^{(\pm)} = \pm\,\eta'\eta_0 + \sqrt{1-\eta'^2}\,\sqrt{1-\eta_0^2}\,\cos(\varphi'-\varphi_0)$$

- Discrete $\lambda = \lambda_i \quad (i=1,\dots,N)$
- Azimuthal symmetry
- Modifies only the corresponding photoelectric line

Photoelectric-Rayleigh chain



$$I^{(2)}_{(P,R)}(\vec{\omega}, \lambda) = \frac{1-\operatorname{sgn}\eta}{2} \, \frac{1+\operatorname{sgn}\eta_0}{2} \, \frac{I_0}{|\eta_0|} \, \frac{\delta(\lambda-\lambda_i)}{\frac{\mu_i}{|\eta|} + \frac{\mu_0}{|\eta_0|}} \, \sigma \, \frac{Q_{\lambda_i}(\lambda_0)\left[1 - u(\lambda_0 - \lambda_{E_i})\right]}{4\pi}$$

$$\left\{ \int_0^{2\pi} d\varphi' \int_0^1 \frac{d\eta'}{\eta'} \, \frac{\left[1 + (\vec{\omega}'\cdot\vec{\omega}^{(+)})^2\right]}{\frac{\mu_i}{|\eta|} + \frac{\mu_i}{\eta'}} \, \frac{F^2(\lambda_i, \vec{\omega}'\cdot\vec{\omega}^{(+)}, Z)}{Z} + \right.$$

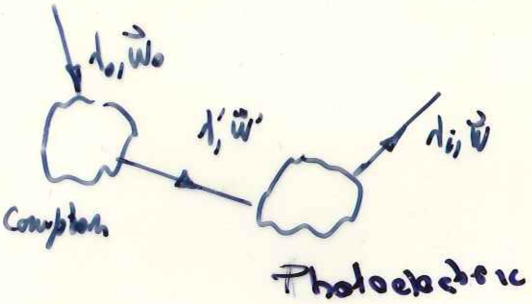
$$\left. + \int_0^{2\pi} d\varphi' \int_0^1 \frac{d\eta'}{\eta'} \, \frac{\left[1 + (\vec{\omega}'\cdot\vec{\omega}^{(-)})^2\right]}{\frac{\mu_0}{|\eta_0|} + \frac{\mu_i}{\eta'}} \, \frac{F^2(\lambda_i, \vec{\omega}'\cdot\vec{\omega}^{(-)}, Z)}{Z} \right\}$$

where

$$\vec{\omega}'\cdot\vec{\omega}^{(\pm)} = \pm \eta'\eta + \sqrt{1-\eta'^2}\,\sqrt{1-\eta^2}\,\cos(\varphi'-\varphi)$$

- Discrete $\lambda = \lambda_i$ $(i = 1, \ldots, N)$
- Azimuthal symmetry
- Modifies only the corresponding photoelectric line

Compton - Photoelectric chain



$$I^{(2)}_{(C,P)}(\vec{w},\lambda) = \frac{1-\operatorname{sgn}\eta}{2}\,\frac{1+\operatorname{sgn}\eta_0}{2}\,\frac{I_0}{|\eta_0|}\,\frac{\delta(\lambda-\lambda_i)}{\frac{\mu_i}{|\eta|}+\frac{\mu_0}{|\eta_0|}}\,\frac{\sigma}{2\pi}\int_{\lambda_0}^{\lambda_0+2\lambda_c}\frac{d\lambda'}{\lambda_c}\,S(\lambda_0,a',z)\,K_{KN}(\lambda',\lambda_0)$$

$$Q_{\lambda_i}(\lambda')\left[1-U(\lambda'-\lambda_{ei})\right]\Bigg\{\underset{(\alpha_2>\alpha_1)}{\int_{\alpha_1}^{\alpha_2}}\frac{d\eta'}{\eta'}\,\frac{1}{\frac{\mu_0}{|\eta|}+\frac{\mu'}{\eta'}}\,\frac{1}{\sqrt{(1-\eta'^2)(1-\eta_0^2)-(a'-\eta_0\eta')^2}}\;+$$

$$+\underset{(\beta_2>\beta_1)}{\int_{\beta_1}^{\beta_2}}\frac{d\eta'}{\eta'}\,\frac{1}{\frac{\mu_0}{|\eta_0|}+\frac{\mu'}{\eta'}}\,\frac{1}{\sqrt{(1-\eta'^2)(1-\eta_0^2)-(a'+\eta_0\eta')^2}}\Bigg\}$$

where
$$a' = 1+\frac{\lambda_0-\lambda'}{\lambda_c}$$

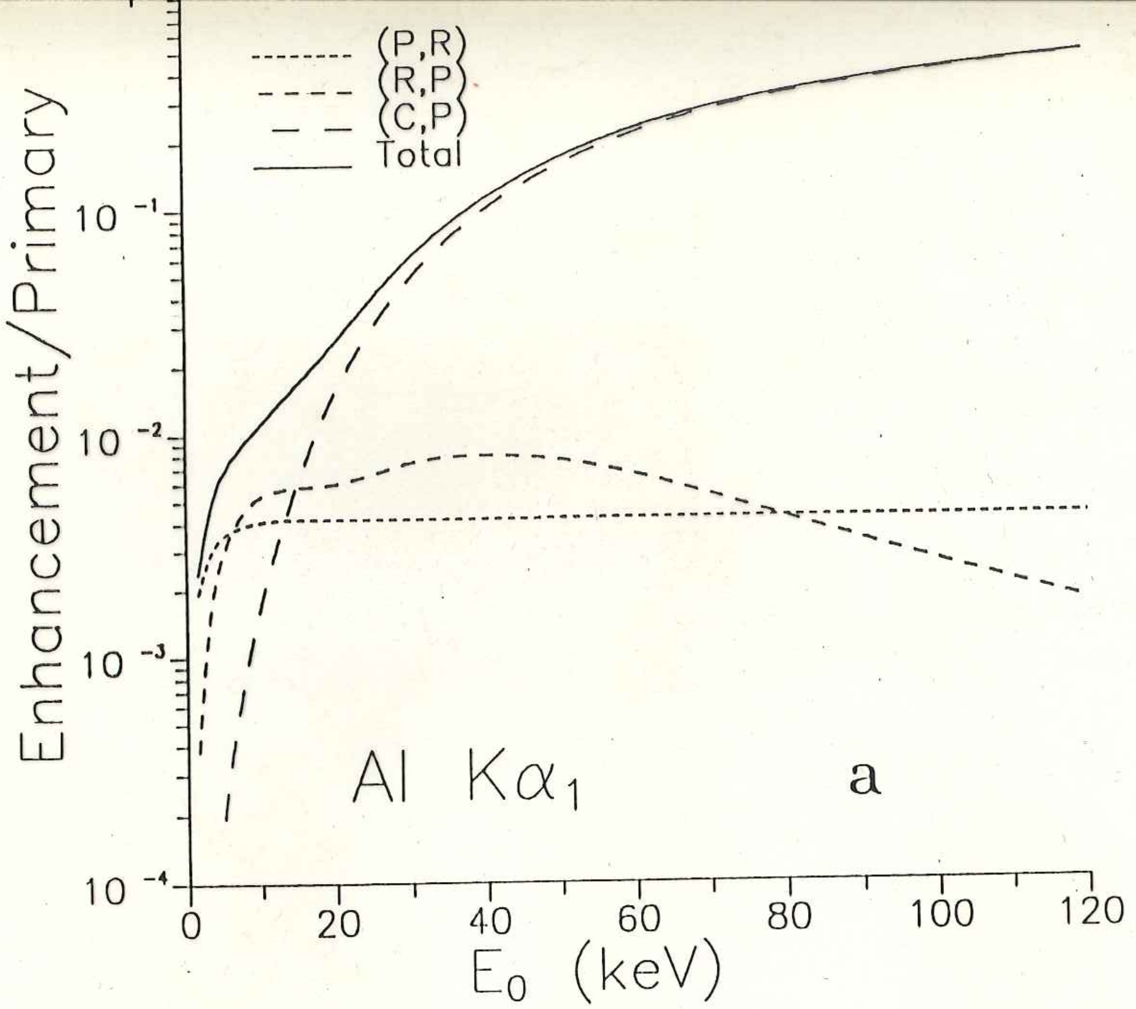
$$\alpha_1 = \max\left(0,\ a'\eta_0-\sqrt{(1-\eta_0^2)(1-a'^2)}\right)$$

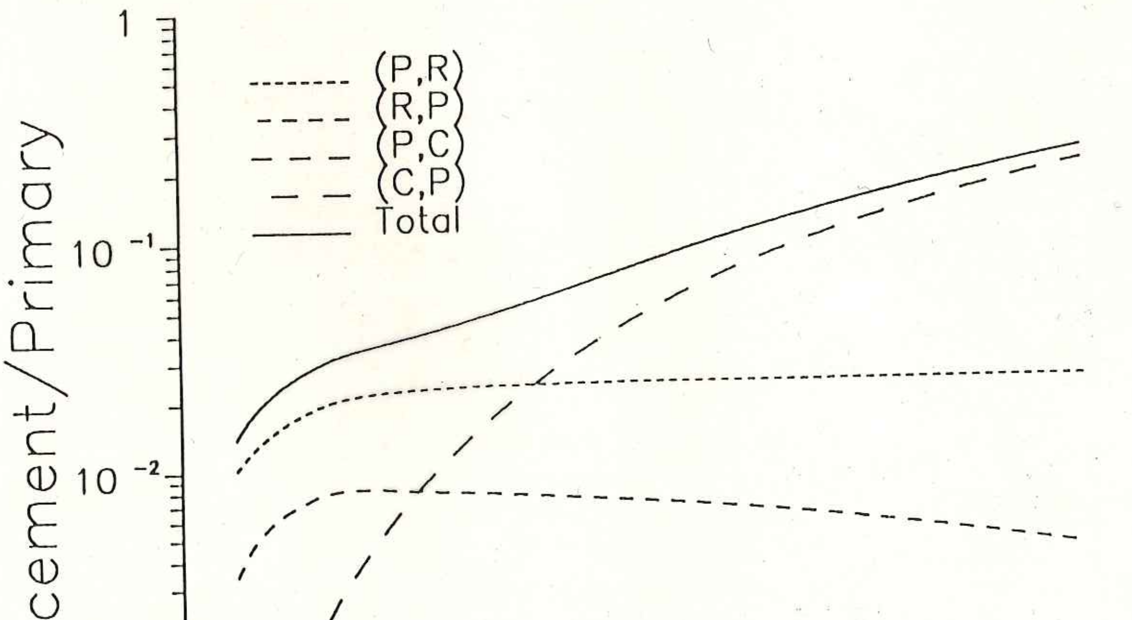
$$\alpha_2 = \min\left(1,\ a'\eta_0+\sqrt{(1-\eta_0^2)(1-a'^2)}\right)$$

$$\beta_1 = -\min\left(0,\ a'\eta_0+\sqrt{(1-\eta_0^2)(1-a')^2}\right)$$

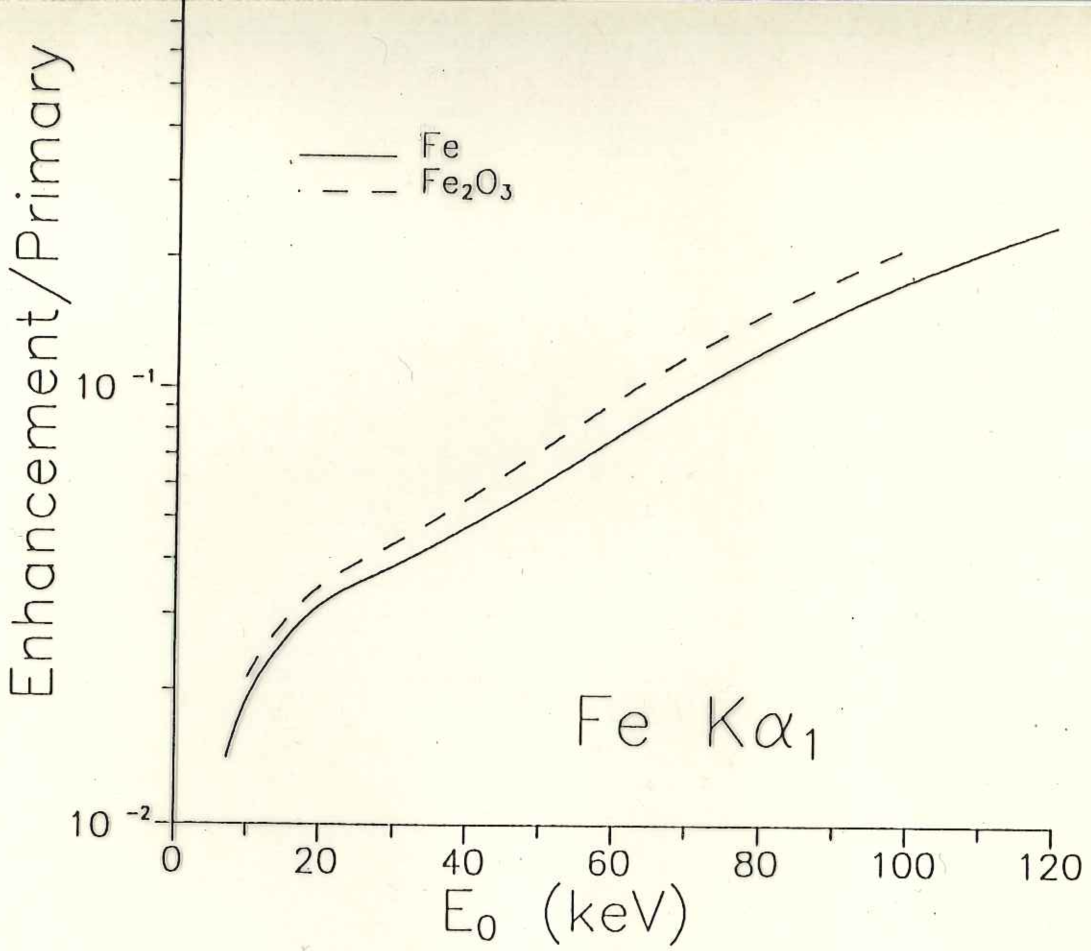
$$\beta_2 = -\max\left(-1,\ a'\eta_0-\sqrt{(1-\eta_0^2)(1-a')^2}\right)$$

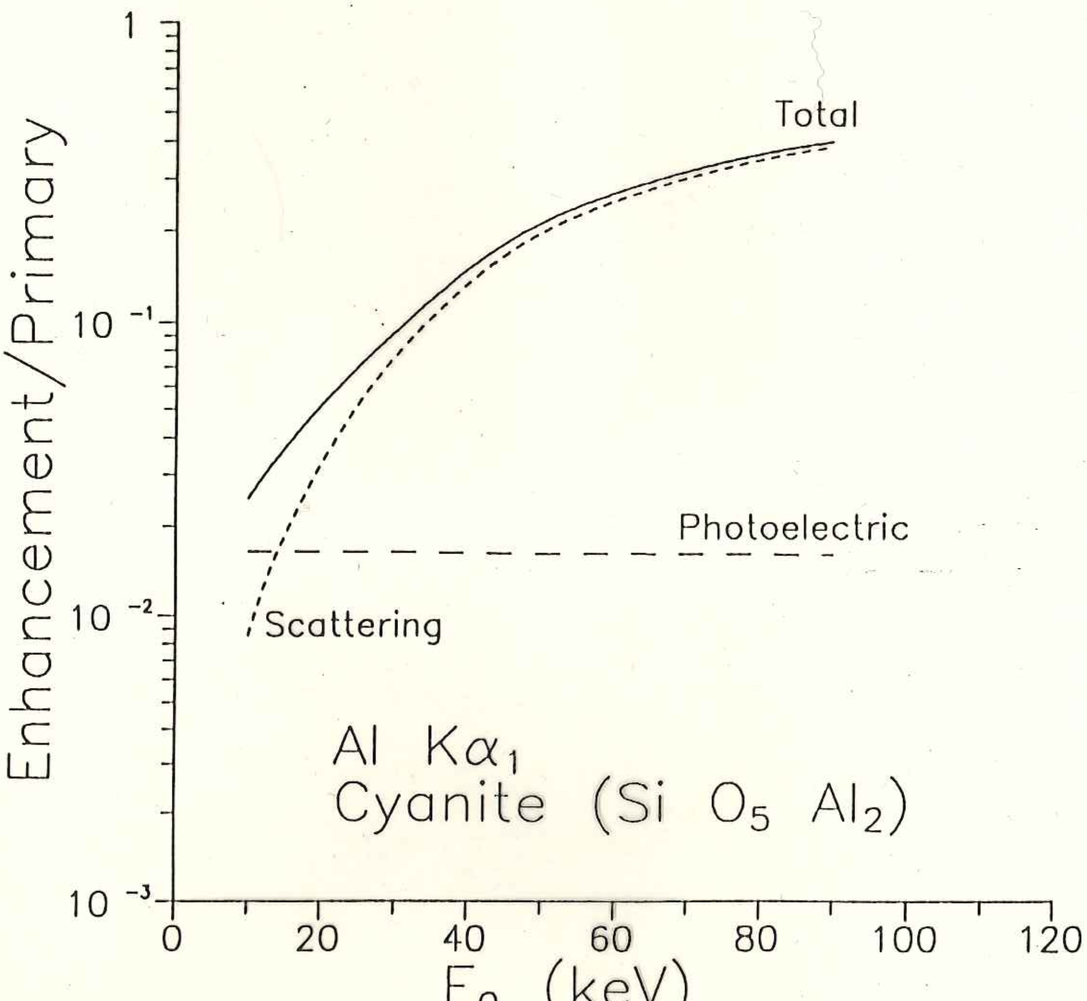
- Discrete $\lambda = \lambda_i$ $(i=1,\dots,N)$
- Azimuthal symmetry
- Mode lin only the corresponding photoelectric line





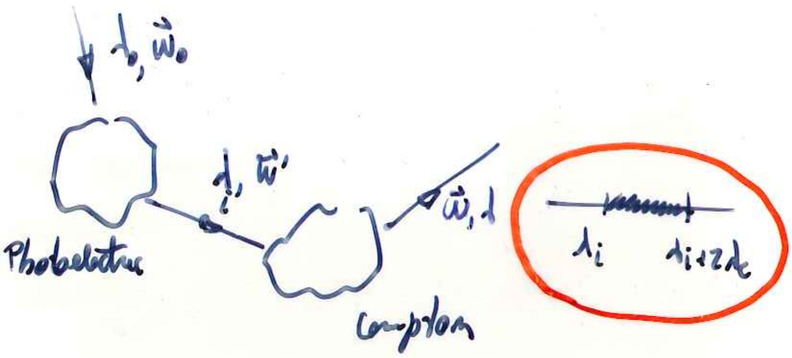
FERNANDEZ, X-RAY SPECTROM. 21, 57 (1992)





FERNANDEZ, X-RAY SPECTROM. 21, 57 (1992)

Photoelectric - Compton chain



$$I^{(2)}_{(P,C)}(\vec{w},\lambda) = \frac{1-\mathrm{sgn}\,\eta}{2}\,\frac{1+\mathrm{sgn}\,\eta_0}{2}\,\frac{I_0}{|\eta_0|\lambda_c}\,\frac{K_{KN}(\lambda,\lambda_i)}{\frac{\mu}{|\eta|}+\frac{\mu_0}{|\eta_0|}}\,\frac{\sigma Q_{\lambda_i}(\lambda_0)\left[1-U(\lambda_0-\lambda_{e_i})\right] S(\lambda_i,a,z)}{2\pi}$$

$$\left\{ \underset{(\alpha_2>\alpha_1)}{\int_{\alpha_1}^{\alpha_2}} \frac{d\eta'}{\eta'}\,\frac{1}{\frac{\mu}{|\eta|}+\frac{\mu_i}{\eta'}}\,\frac{1}{\sqrt{(1-\eta'^2)(1-\eta^2)-(a-\eta\eta')^2}} + \right.$$

$$\left. \underset{(\beta_2>\beta_1)}{\int_{\beta_1}^{\beta_2}} \frac{d\eta'}{\eta'}\,\frac{1}{\frac{\mu_0}{|\eta|}+\frac{\mu_i}{\eta'}}\,\frac{1}{\sqrt{(1-\eta'^2)(1-\eta^2)-(a+\eta\eta')^2}} \right\}$$

where $a = 1+\dfrac{\lambda_i-\lambda}{\lambda_c}$

$$\alpha_1 = \max\left(0,\ a\eta-\sqrt{(1-\eta^2)(1-a^2)}\right)$$

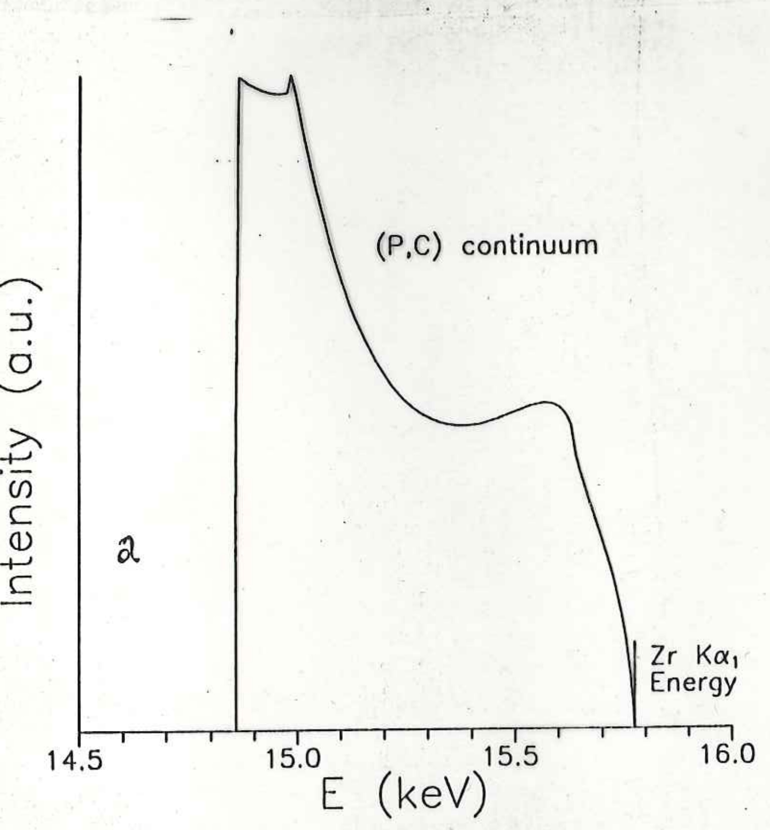
$$\alpha_2 = \min\left(1,\ a\eta+\sqrt{(1-\eta^2)(1-a^2)}\right)$$

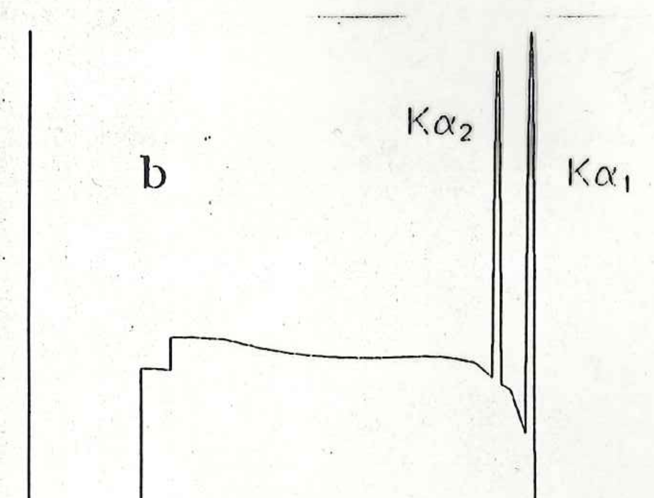
$$\beta_1 = -\min\left(0,\ a\eta+\sqrt{(1-a^2)(1-\eta^2)}\right)$$

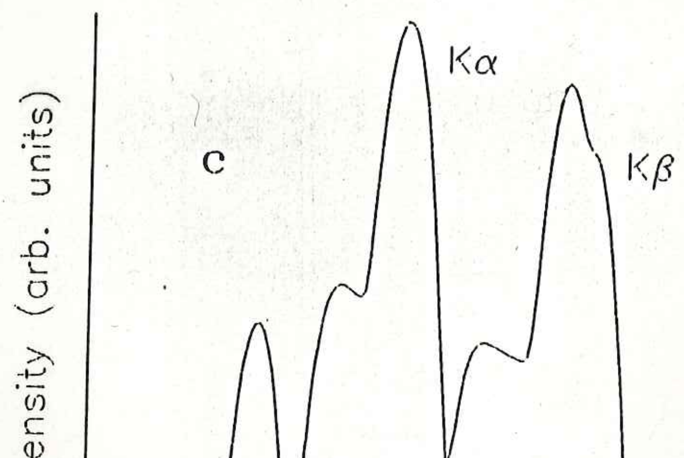
$$\beta_2 = -\max\left(-1,\ a\eta-\sqrt{(1-\eta^2)(1-a^2)}\right)$$

- Continuous $\lambda \in [\lambda_i, \lambda_i+2\lambda_c]$
- Azimuthal symmetry (over the integrated intensity)
- Modifies the line shape (introduces a tail for lower energies than λ_i)
- May overlap to other lines

Fernandez, Hubbell, Hanson and Spencer, Rad. Phys. Chem. 41, 579 (1993)





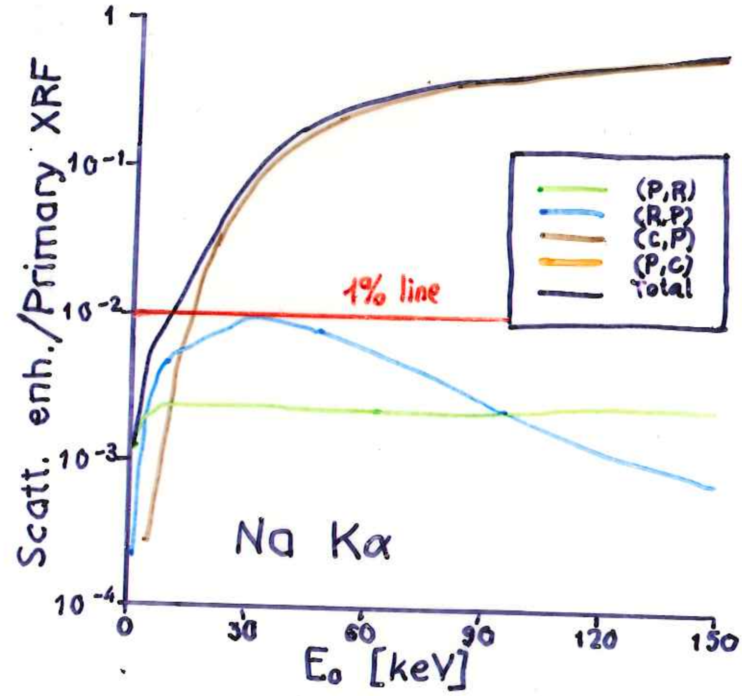


LFS

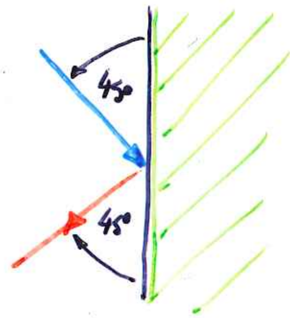
SYSTEMATIC COMPUTATIONS OF SCATTERING CORRECTIONS WITH THE CODE SHAPE

J.E. FERNÁNDEZ AND V.G. MOLINARI
UNIVERSITY OF BOLOGNA

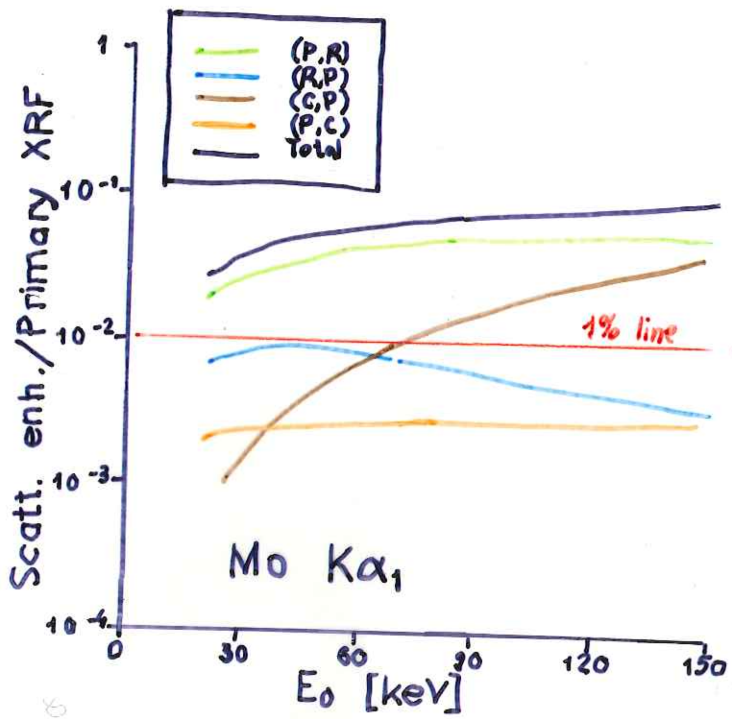
- SCATTERING CORRECTIONS ARE GIVEN FOR $K\alpha_1$ LINES FROM Na ($Z=11$) TO Mo ($Z=42$) PURE ELEMENT SAMPLES. AS A FUNCTION OF EXCITATION ENERGY.



CORRECTION EXCEEDS 1% @ 10 keV AND GROWS RAPIDLY. ~10% @ 30 keV !



EXCITATION-DETECTION GEOMETRY



CORRECTION IS ALWAYS GREATER THAN 3% !

NOTE THAT THIS ARE CORRECTIONS TO $K\alpha$ LINES OF PURE TARGETS (USUALLY ASSUMED AS REFERENCE INTENSITY IN STANDARDLESS ANALYSIS)

DIRECTIONS: COMPLETE THE PERIODICAL TABLE AND INCLUDE A REPRESENTATIVE SET OF MULTICOMPONENT ELEMENTS