Influence of Crystallographic Environment on Scandium *K*-Edge X-Ray Absorption Near-Edge Structure Spectra

—

Electronic Supplementary Information

X-Ray Diffraction Patterns

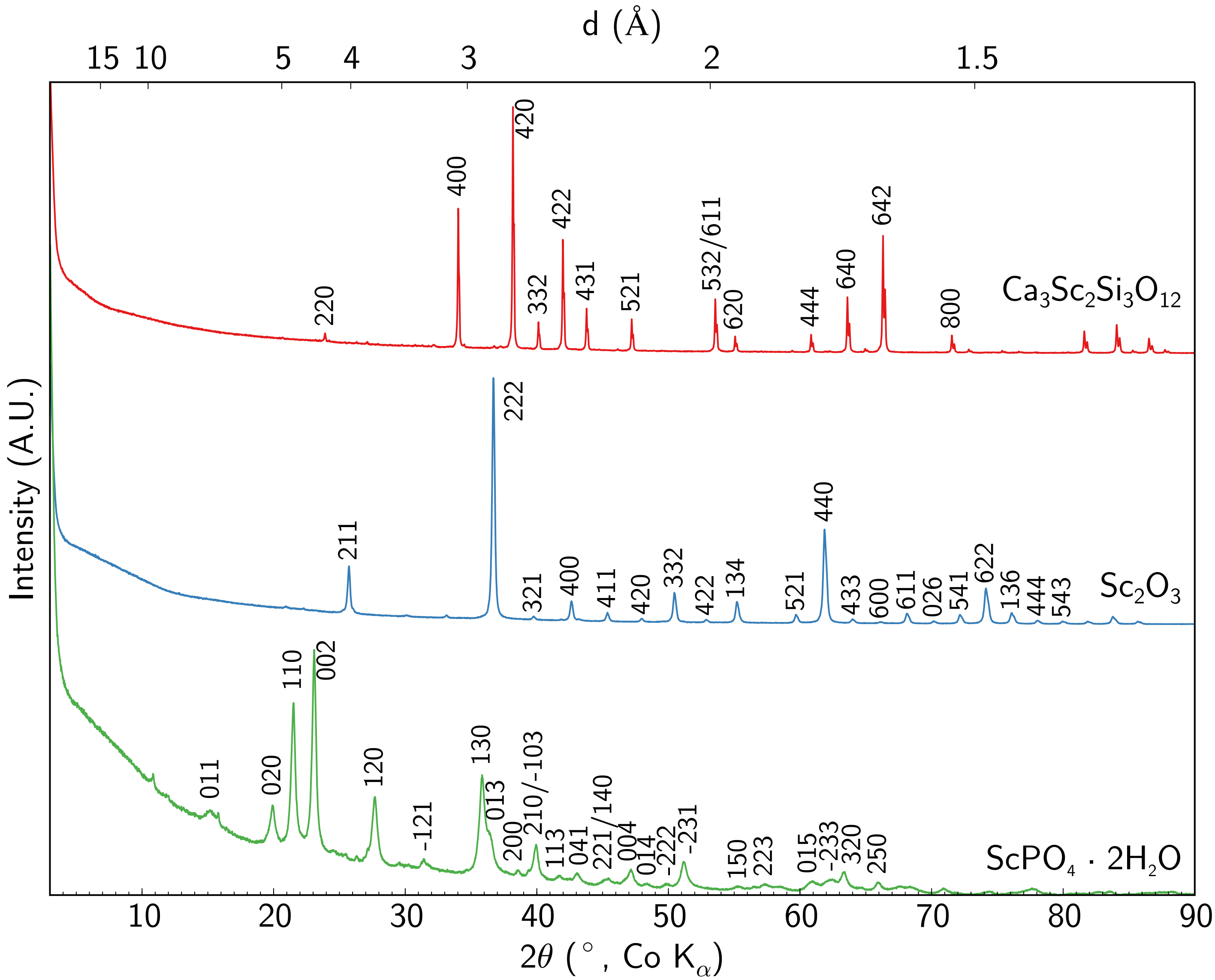

Figure 1 X-ray diffraction patterns of the compounds studied. Miller indices of the lattice plans are indicated above each corresponding diffraction peak. Raw patterns are provided as comma-separated values files.

X-Ray Absorption Near-Edge Structure Spectra

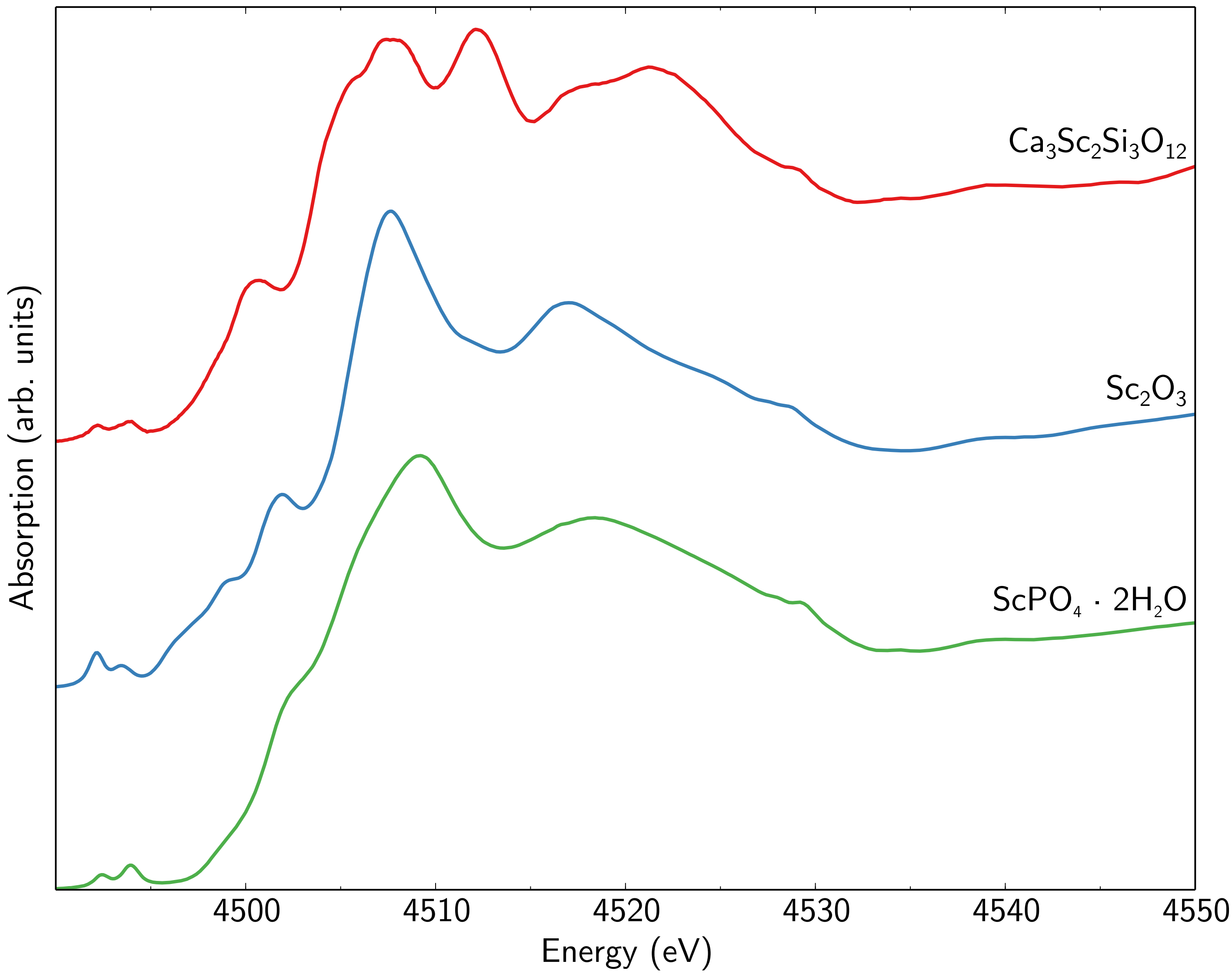

Figure 2 Normalised Sc *K*-edge XANES spectra of $Ca_3Sc_2Si_3O_{12}$, Sc_2O_3 and $ScPO_4 \cdot 2H_2O$. Raw spectra are provided as comma-separated values files.

Expression of the Isotropic Cross Section

Expression of the Electric-Dipole Isotropic Cross Section

X-Ray Polarization Vector.

In an orthonormal reference frame bound to the crystal, the X-ray polarization vector is written:

$$\hat{\varepsilon} = \begin{pmatrix} \sin\theta \cdot \cos\varphi \\ \sin\theta \cdot \sin\varphi \\ \cos\theta \end{pmatrix} \tag{1}$$

The z axis is chosen according to the *International Tables for X-Ray Crystallography*. The x axis is taken parallel to the x axis of the *Tables*. θ is the angle of $\hat{\varepsilon}$ relative to the z axis while φ is the angle of $\hat{\varepsilon}$ relative to the x axis.

Cubic Crystals.

In this case, the angular dependance of the dipolar absorption is isotropic[1]. The electric dipole isotropic cross section, $\sigma^{\mathrm{D}}_{\mathrm{cub}}(0,0)$, does not depend on the direction of the incident polarization vector $\hat{\varepsilon}$ and can be expressed for any $\hat{\varepsilon}$ as:

$$\sigma^{\mathrm{D}}_{\mathrm{cub}}(0,\ 0) = \sigma^{\mathrm{D}}_{\mathrm{cub}}(\hat{\varepsilon}) \tag{2}$$

Monoclinic Crystals.

In monoclinic crystals with a $\mathrm{C_{2h}}$ point group, the angular dependance of the dipolar absorption is trichroic[1]. The electric dipole cross section, $\sigma^{\mathrm{D}}_{\mathrm{C_{2h}}}(\hat{\varepsilon})$, can be expressed as:

$$\begin{aligned} \sigma^{\mathrm{D}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}) = \sigma^{\mathrm{D}}_{\mathrm{C_{2h}}}&(0,\ 0) \\ &- \sqrt{3} \cdot \sin^2\theta \cdot [\cos 2\varphi \cdot \sigma^{\mathrm{Dr}}_{\mathrm{C_{2h}}}(2,\ 2) + \sin 2\varphi \cdot \sigma^{\mathrm{Di}}_{\mathrm{C_{2h}}}(2,\ 2)] \\ &- \frac{1}{\sqrt{2}} \cdot (2 \cdot \cos^2\theta - 1) \cdot \sigma^{\mathrm{D}}_{\mathrm{C_{2h}}}(2,\ 0) \end{aligned} \tag{3}$$

When $\theta = 0$ and $\varphi = 0$:

$$\hat{\varepsilon} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \hat{\varepsilon}_{001} \tag{4}$$

$$\sigma^{\mathrm{D}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_{001}) = \sigma^{\mathrm{D}}_{\mathrm{C_{2h}}}(0,\ 0) - \frac{2}{\sqrt{2}} \cdot \sigma^{\mathrm{D}}_{\mathrm{C_{2h}}}(2,\ 0) \tag{5}$$

When $\theta = \frac{\pi}{2}$ and $\varphi = 0$:

$$\hat{\varepsilon} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \hat{\varepsilon}_{100} \tag{6}$$

$$\sigma^{\mathrm{D}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_{100}) = \sigma^{\mathrm{D}}_{\mathrm{C_{2h}}}(0,\ 0) - \sqrt{3} \cdot \sigma^{\mathrm{Dr}}_{\mathrm{C_{2h}}}(2,\ 2) + \frac{1}{\sqrt{2}} \cdot \sigma^{\mathrm{D}}_{\mathrm{C_{2h}}}(2,\ 0) \tag{7}$$

When $\theta = \frac{\pi}{2}$ and $\varphi = \frac{\pi}{2}$:

$$\hat{\varepsilon} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \hat{\varepsilon}_{010} \tag{8}$$

$$\sigma^{\mathrm{D}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_{010}) = \sigma^{\mathrm{D}}_{\mathrm{C_{2h}}}(0,\ 0) + \sqrt{3} \cdot \sigma^{\mathrm{Dr}}_{\mathrm{C_{2h}}}(2,\ 2) + \frac{1}{\sqrt{2}} \cdot \sigma^{\mathrm{D}}_{\mathrm{C_{2h}}}(2,\ 0) \tag{9}$$

From equation 5, 7 and 9, we show that the electric-dipole isotropic cross section of a monoclinic crystal with a $\mathrm{C_{2h}}$ point group is:

$$\sigma^{\mathrm{D}}_{\mathrm{C_{2h}}}(0,0) = \frac{\sigma^{\mathrm{D}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_{100}) + \sigma^{\mathrm{D}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_{010}) + \sigma^{\mathrm{D}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_{001})}{3} \tag{10}$$

Expression of the Electric-Quadrupole Isotropic Cross section

X-Ray Polarization Vector and Wavevector.

The general coordinates of the vectors are:

$$\hat{\varepsilon} = \begin{pmatrix} \sin\theta\cdot\cos\varphi \\ \sin\theta\cdot\sin\varphi \\ \cos\theta \end{pmatrix} \quad \hat{k} = \begin{pmatrix} \cos\theta\cdot\cos\varphi\cdot\cos\psi - \sin\varphi\cdot\sin\psi \\ \cos\theta\cdot\sin\varphi\cdot\cos\psi - \cos\varphi\cdot\sin\psi \\ -\sin\theta\cdot\cos\psi \end{pmatrix} \tag{11}$$

The angle ψ gives the direction of the wavevector in the plane perpendicular to the polarization vector. The orthonormal axes are chosen as in equation 1.

Cubic Crystals.

For cubic point groups, symmetry considerations lead to the following expression of the electric-quadrupole absorption cross section[1]:

$$\begin{aligned}\sigma^{\mathrm{Q}}_{\mathrm{cub}}(\hat{\varepsilon},\,\hat{k}) = \sigma^{\mathrm{Q}}_{\mathrm{cub}}(0,\,0)& \\ &+\frac{1}{\sqrt{14}}\cdot[35\cdot\sin^2\theta\cdot\cos^2\theta\cdot\cos^2\psi + 5\cdot\sin^2\theta\cdot\sin^2\psi - 4 \\ &+5\cdot\sin^2\theta\cdot(\cos^2\theta\cdot\cos^2\psi\cdot\cos 4\varphi - \sin^2\psi\cdot\cos 4\varphi \\ &-2\cdot\cos\theta\cdot\sin\psi\cdot\cos\psi\cdot\sin 4\varphi)]\cdot\sigma^{\mathrm{Q}}_{\mathrm{cub}}(4,\,0)\end{aligned} \tag{12}$$

For $\theta = 0$, $\varphi = \frac{\pi}{2}$ and $\psi = -\frac{\pi}{2}$:

$$\hat{\varepsilon} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \hat{\varepsilon}_{001}, \quad \hat{k} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \hat{k}_{100} \tag{13}$$

$$\sigma^{\mathrm{Q}}_{\mathrm{cub}}(\hat{\varepsilon}_{001},\,\hat{k}_{100}) = \sigma^{\mathrm{Q}}_{\mathrm{cub}}(0,\,0) - \frac{4}{\sqrt{14}}\cdot\sigma^{\mathrm{Q}}_{\mathrm{cub}}(4,\,0) \tag{14}$$

For $\theta = \frac{\pi}{2}$, $\varphi = \frac{\pi}{4}$ and $\psi = \frac{\pi}{2}$:

$$\hat{\varepsilon} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} = \hat{\varepsilon}_{\frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}0}, \quad \hat{k} = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} = \hat{k}_{-\frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}0} \tag{15}$$

$$\sigma^{\mathrm{Q}}_{\mathrm{cub}}(\hat{\varepsilon}_{\frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}0},\,\hat{k}_{-\frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}0}) = \sigma^{\mathrm{Q}}_{\mathrm{cub}}(0,\,0) + \frac{6}{\sqrt{14}}\cdot\sigma^{\mathrm{Q}}_{\mathrm{cub}}(4,\,0) \tag{16}$$

From equation 14 and 16, we show that the electric-quadrupole isotropic cross section of a cubic crystal is:

$$\sigma^{\mathrm{Q}}_{\mathrm{cub}} = \frac{3\cdot\sigma^{\mathrm{Q}}_{\mathrm{cub}}(\hat{\varepsilon}_{001},\,\hat{k}_{100}) + 2\cdot\sigma^{\mathrm{Q}}_{\mathrm{cub}}(\hat{\varepsilon}_{\frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}0},\,\hat{k}_{-\frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}0})}{5} \tag{17}$$

Monoclinic Crystals.

In monoclinic crystals with a C_{2h} point group, symmetry considerations lead to the following expression of the electric-quadrupole absorption cross section[1]:

$$\begin{aligned}
\sigma^{Q}_{C_{2h}}(\hat{\varepsilon},\,\hat{k}) = {} & \sigma^{Q}_{C_{2h}}(0,\,0) \\
& + \sqrt{\frac{5}{14}} \cdot (3 \cdot \sin^2\theta \cdot \sin^2\psi - 1) \cdot \sigma^{Q}_{C_{2h}}(2,\,0) \\
& + \sqrt{\frac{15}{7}} \cdot [(\cos^2\theta \cdot \sin^2\varphi - \cos^2\psi) \cdot (\sigma^{Qr}_{C_{2h}}(2,\,2) \cdot \cos 2\varphi + \sigma^{Qi}_{C_{2h}}(2,\,2) \cdot \sin 2\varphi) \\
& + 2 \cdot \cos\theta \cdot \sin\psi \cdot \cos\psi \cdot (\sigma^{Qr}_{C_{2h}}(2,\,2) \cdot \sin 2\varphi - \sigma^{Q}_{C_{2h}}(2,\,2) \cdot \cos 2\varphi)] \\
& + \frac{1}{\sqrt{14}} \cdot (35 \cdot \sin^2\theta \cdot \cos^2\theta \cdot \cos^2\psi + 5 \cdot \sin^2\theta \cdot \sin^2\psi - 4) \cdot \sigma^{Q}_{C_{2h}}(4,\,0) \\
& - 2 \cdot \sqrt{\frac{5}{7}} \cdot [(7 \cdot \sin^2\theta \cdot \cos^2\theta \cdot \cos^2\psi + \cos^2\theta \cdot \sin^2\psi - \cos^2\psi) \cdot (\sigma^{Qr}_{C_{2h}}(4,\,2) \cdot \cos 2\varphi + \sigma^{Qi}_{C_{2h}}(4,\,2) \cdot \sin 2\varphi) \\
& - (7 \cdot \sin^2\theta - 2) \cdot \cos\theta \cdot \sin\psi \cdot \cos\psi \cdot (\sigma^{Qr}_{C_{2h}}(4,\,2) \cdot \sin 2\varphi - \sigma^{Qi}_{C_{2h}}(4,\,2) \cdot \cos 2\varphi)] \\
& + \sqrt{5} \cdot \sin^2\theta \cdot [(\cos^2\theta \cdot \cos^2\psi - \sin^2\psi) \cdot (\sigma^{Qr}_{C_{2h}}(4,\,4) \cdot \cos 4\varphi + \sigma^{Qi}_{C_{2h}}(4,\,4) \cdot \sin 4\varphi) \\
& - 2 \cdot \cos\theta \cdot \sin\psi \cdot \cos\psi \cdot (\sigma^{Qr}_{C_{2h}}(4,\,4) \cdot \sin 4\varphi - \sigma^{Qi}_{C_{2h}}(4,\,4) \cdot \cos 4\varphi)]
\end{aligned} \tag{18}$$

For $\theta = 0$, $\varphi = 0$ and $\psi = \frac{\pi}{2}$:

$$\hat{\varepsilon} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \hat{\varepsilon}_1, \quad \hat{k} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \hat{k}_1 \tag{19}$$

$$\begin{aligned}
\sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_1,\,\hat{k}_1) = {} & \sigma^{Q}_{C_{2h}}(0,\,0) \\
& - \sqrt{\frac{5}{14}} \cdot \sigma^{Q}_{C_{2h}}(2,\,0) + \sqrt{\frac{15}{7}} \cdot \sigma^{Qr}_{C_{2h}}(2,\,2) \\
& - \frac{4}{\sqrt{14}} \cdot \sigma^{Q}_{C_{2h}}(4,\,0) - 2 \cdot \sqrt{\frac{5}{7}} \cdot \sigma^{Qr}_{C_{2h}}(4,\,2)
\end{aligned} \tag{20}$$

For $\theta = 0$, $\varphi = \frac{\pi}{2}$ and $\psi = -\frac{\pi}{2}$:

$$\hat{\varepsilon} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \hat{\varepsilon}_2, \quad \hat{k} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \hat{k}_2 \tag{21}$$

$$\begin{aligned}
\sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_2,\,\hat{k}_2) = {} & \sigma^{Q}_{C_{2h}}(0,\,0) \\
& - \sqrt{\frac{5}{14}} \cdot \sigma^{Q}_{C_{2h}}(2,\,0) - \sqrt{\frac{15}{7}} \cdot \sigma^{Qr}_{C_{2h}}(2,\,2) \\
& - \frac{4}{\sqrt{14}} \cdot \sigma^{Q}_{C_{2h}}(4,\,0) + 2 \cdot \sqrt{\frac{5}{7}} \cdot \sigma^{Qr}_{C_{2h}}(4,\,2)
\end{aligned} \tag{22}$$

By combining equations 20 and 22, we obtain:

$$\begin{aligned}
\sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_1,\,\hat{k}_1) + \sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_2,\,\hat{k}_2) = {} & 2 \cdot \sigma^{Q}_{C_{2h}}(0,\,0) \\
& - 2 \cdot \sqrt{\frac{5}{14}} \cdot \sigma^{Q}_{C_{2h}}(2,\,0) - \frac{8}{\sqrt{14}} \cdot \sigma^{Q}_{C_{2h}}(4,\,0)
\end{aligned} \tag{23}$$

For $\theta = \frac{\pi}{2}$, $\varphi = 0$ and $\psi = \frac{\pi}{2}$:

$$\hat{\varepsilon} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \hat{\varepsilon}_3, \quad \hat{k} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \hat{k}_3 \tag{24}$$

$$\begin{aligned}
\sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_3,\,\hat{k}_3) = {} & \sigma^{Q}_{C_{2h}}(0,\,0) \\
& + 2 \cdot \sqrt{\frac{5}{14}} \cdot \sigma^{Q}_{C_{2h}}(2,\,0) + \frac{1}{\sqrt{14}} \cdot \sigma^{Q}_{C_{2h}}(4,\,0) \\
& - \sqrt{5} \cdot \sigma^{Qr}_{C_{2h}}(4,\,4)
\end{aligned} \tag{25}$$

For $\theta = \frac{\pi}{2}$, $\varphi = \frac{\pi}{4}$ and $\psi = \frac{\pi}{2}$:

$$\hat{\varepsilon} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} = \hat{\varepsilon}_4, \quad \hat{k} = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} = \hat{k}_4 \tag{26}$$

$$\begin{aligned} \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_4,\ \hat{k}_4) = \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(0,\ 0) & \\ + 2 \cdot \sqrt{\frac{5}{14}} \cdot \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(2,\ 0) + \frac{1}{\sqrt{14}} \cdot \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(4,\ 0) & \\ + \sqrt{5} \cdot \sigma^{\mathrm{Qr}}_{\mathrm{C_{2h}}}(4,\ 4) & \end{aligned} \tag{27}$$

By combining equations 25 and 27, we obtain:

$$\begin{aligned} \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_3,\ \hat{k}_3) + \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_4,\ \hat{k}_4) = 2 \cdot \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(0,\ 0) & \\ + 4 \cdot \sqrt{\frac{5}{14}} \cdot \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(2,\ 0) + \frac{2}{\sqrt{14}} \cdot \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(4,\ 0) & \end{aligned} \tag{28}$$

By combining equations 23 and 28, we obtain:

$$\begin{aligned} 2 \cdot [\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_1,\ \hat{k}_1) + \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_2,\ \hat{k}_2)] + \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_3,\ \hat{k}_3) + \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_4,\ \hat{k}_4) = & \\ 6 \cdot \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(0,\ 0) - \frac{14}{\sqrt{14}} \cdot \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(4,\ 0) & \end{aligned} \tag{29}$$

For $\theta = \frac{\pi}{2}$, $\varphi = 0$ and $\psi = \frac{\pi}{4}$:

$$\hat{\varepsilon} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \hat{\varepsilon}_5, \quad \hat{k} = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \hat{k}_5 \tag{30}$$

$$\begin{aligned} \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_5,\ \hat{k}_5) = \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(0,\ 0) & \\ + \frac{1}{2} \cdot \sqrt{\frac{5}{14}} \cdot \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(2,\ 0) - \frac{1}{2} \cdot \sqrt{\frac{15}{7}} \cdot \sigma^{\mathrm{Qr}}_{\mathrm{C_{2h}}}(2,\ 2) & \\ - \frac{3}{2 \cdot \sqrt{14}} \cdot \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(4,\ 0) + \sqrt{\frac{5}{7}} \cdot \sigma^{\mathrm{Qr}}_{\mathrm{C_{2h}}}(4,\ 2) - \frac{\sqrt{5}}{2} \cdot \sigma^{\mathrm{Qr}}_{\mathrm{C_{2h}}}(4,\ 4) & \end{aligned} \tag{31}$$

For $\theta = \frac{\pi}{2}$, $\varphi = \frac{\pi}{2}$ and $\psi = \frac{\pi}{4}$:

$$\hat{\varepsilon} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \hat{\varepsilon}_6, \quad \hat{k} = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ 0 \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \hat{k}_6 \tag{32}$$

$$\begin{aligned} \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_6,\ \hat{k}_6) = \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(0,\ 0) & \\ + \frac{1}{2} \cdot \sqrt{\frac{5}{14}} \cdot \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(2,\ 0) + \frac{1}{2} \cdot \sqrt{\frac{15}{7}} \cdot \sigma^{\mathrm{Qr}}_{\mathrm{C_{2h}}}(2,\ 2) & \\ - \frac{3}{2 \cdot \sqrt{14}} \cdot \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(4,\ 0) - \sqrt{\frac{5}{7}} \cdot \sigma^{\mathrm{Qr}}_{\mathrm{C_{2h}}}(4,\ 2) - \frac{\sqrt{5}}{2} \cdot \sigma^{\mathrm{Qr}}_{\mathrm{C_{2h}}}(4,\ 4) & \end{aligned} \tag{33}$$

For $\theta = \frac{\pi}{2}$, $\varphi = \frac{\pi}{4}$ and $\psi = \frac{\pi}{4}$:

$$\hat{\varepsilon} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} = \hat{\varepsilon}_7, \quad \hat{k} = \begin{pmatrix} -\frac{1}{2} \\ \frac{1}{2} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \hat{k}_7 \tag{34}$$

$$\begin{aligned} \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_7,\ \hat{k}_7) = \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(0,\ 0) & \\ + \frac{1}{2} \cdot \sqrt{\frac{5}{14}} \cdot \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(2,\ 0) - \frac{1}{2} \cdot \sqrt{\frac{15}{7}} \cdot \sigma^{\mathrm{Qi}}_{\mathrm{C_{2h}}}(2,\ 2) & \\ - \frac{3}{2 \cdot \sqrt{14}} \cdot \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(4,\ 0) + \sqrt{\frac{5}{7}} \cdot \sigma^{\mathrm{Qi}}_{\mathrm{C_{2h}}}(4,\ 2) + \frac{\sqrt{5}}{2} \cdot \sigma^{\mathrm{Qr}}_{\mathrm{C_{2h}}}(4,\ 4) & \end{aligned} \tag{35}$$

For $\theta = \frac{\pi}{2}$, $\varphi = -\frac{\pi}{4}$ and $\psi = \frac{\pi}{4}$:

$$\hat{\varepsilon} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} = \hat{\varepsilon}_8, \quad \hat{k} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \hat{k}_8 \tag{36}$$

$$\sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_8,\ \hat{k}_8) = \sigma^{Q}_{C_{2h}}(0,\ 0) + \frac{1}{2}\cdot\sqrt{\frac{5}{14}}\cdot\sigma^{Q}_{C_{2h}}(2,\ 0) + \frac{1}{2}\cdot\sqrt{\frac{15}{7}}\cdot\sigma^{Qi}_{C_{2h}}(2,\ 2) - \frac{3}{2\cdot\sqrt{14}}\cdot\sigma^{Q}_{C_{2h}}(4,\ 0) - \sqrt{\frac{5}{7}}\cdot\sigma^{Qi}_{C_{2h}}(4,\ 2) + \frac{\sqrt{5}}{2}\cdot\sigma^{Qr}_{C_{2h}}(4,\ 4) \tag{37}$$

By combining equations 31, 33, 35 and 37, we obtain:

$$\sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_5,\ \hat{k}_5) + \sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_6,\ \hat{k}_6) + \sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_7,\ \hat{k}_7) + \sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_8,\ \hat{k}_8) = 4\cdot\sigma^{Q}_{C_{2h}}(0,\ 0) + 2\cdot\sqrt{\frac{5}{14}}\cdot\sigma^{Q}_{C_{2h}}(2,\ 0) - \frac{6}{\sqrt{14}}\cdot\sigma^{Q}_{C_{2h}}(4,\ 0) \tag{38}$$

For $\theta = \frac{\pi}{4}$, $\varphi = 0$ and $\psi = 0$:

$$\hat{\varepsilon} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \hat{\varepsilon}_9, \quad \hat{k} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \hat{k}_9 \tag{39}$$

$$\sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_9,\ \hat{k}_9) = \sigma^{Q}_{C_{2h}}(0,\ 0) - \sqrt{\frac{5}{14}}\cdot\sigma^{Q}_{C_{2h}}(2,\ 0) - \sqrt{\frac{15}{7}}\cdot\sigma^{Qr}_{C_{2h}}(2,\ 2) + \frac{19}{4\cdot\sqrt{14}}\cdot\sigma^{Q}_{C_{2h}}(4,\ 0) - \frac{3}{2}\cdot\sqrt{\frac{5}{7}}\cdot\sigma^{Qr}_{C_{2h}}(4,\ 2) + \frac{\sqrt{5}}{4}\cdot\sigma^{Qr}_{C_{2h}}(4,\ 4) \tag{40}$$

For $\theta = \frac{\pi}{4}$, $\varphi = \frac{\pi}{2}$ and $\psi = 0$:

$$\hat{\varepsilon} = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \hat{\varepsilon}_{10}, \quad \hat{k} = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \hat{k}_{10} \tag{41}$$

$$\sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_{10},\ \hat{k}_{10}) = \sigma^{Q}_{C_{2h}}(0,\ 0) - \sqrt{\frac{5}{14}}\cdot\sigma^{Q}_{C_{2h}}(2,\ 0) + \sqrt{\frac{15}{7}}\cdot\sigma^{Qr}_{C_{2h}}(2,\ 2) + \frac{19}{4\cdot\sqrt{14}}\cdot\sigma^{Q}_{C_{2h}}(4,\ 0) + \frac{3}{2}\cdot\sqrt{\frac{5}{7}}\cdot\sigma^{Qr}_{C_{2h}}(4,\ 2) + \frac{\sqrt{5}}{4}\cdot\sigma^{Qr}_{C_{2h}}(4,\ 4) \tag{42}$$

For $\theta = \frac{\pi}{4}$, $\varphi = \frac{\pi}{4}$ and $\psi = 0$:

$$\hat{\varepsilon} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \hat{\varepsilon}_{11}, \quad \hat{k} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \hat{k}_{11} \tag{43}$$

$$\sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_{11},\ \hat{k}_{11}) = \sigma^{Q}_{C_{2h}}(0,\ 0) - \sqrt{\frac{5}{14}}\cdot\sigma^{Q}_{C_{2h}}(2,\ 0) - \sqrt{\frac{15}{7}}\cdot\sigma^{Qi}_{C_{2h}}(2,\ 2) + \frac{19}{4\cdot\sqrt{14}}\cdot\sigma^{Q}_{C_{2h}}(4,\ 0) - \frac{3}{2}\cdot\sqrt{\frac{5}{7}}\cdot\sigma^{Qi}_{C_{2h}}(4,\ 2) - \frac{\sqrt{5}}{4}\cdot\sigma^{Qr}_{C_{2h}}(4,\ 4) \tag{44}$$

For $\theta = \frac{\pi}{4}$, $\varphi = -\frac{\pi}{4}$ and $\psi = 0$:

$$\hat{\varepsilon} = \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \hat{\varepsilon}_{12}, \quad \hat{k} = \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \hat{k}_{12} \tag{45}$$

$$\sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_{12},\ \hat{k}_{12}) = \sigma^{Q}_{C_{2h}}(0,\ 0) - \sqrt{\frac{5}{14}}\cdot\sigma^{Q}_{C_{2h}}(2,\ 0) + \sqrt{\frac{15}{7}}\cdot\sigma^{Qi}_{C_{2h}}(2,\ 2) + \frac{19}{4\cdot\sqrt{14}}\cdot\sigma^{Q}_{C_{2h}}(4,\ 0) + \frac{3}{2}\cdot\sqrt{\frac{5}{7}}\cdot\sigma^{Qi}_{C_{2h}}(4,\ 2) - \frac{\sqrt{5}}{4}\cdot\sigma^{Qr}_{C_{2h}}(4,\ 4) \tag{46}$$

By combining equations 40, 42, 44 and 46, we obtain:

$$\sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_9,\ \hat{k}_9) + \sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_{10},\ \hat{k}_{10}) + \sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_{11},\ \hat{k}_{11}) + \sigma^{Q}_{C_{2h}}(\hat{\varepsilon}_{12},\ \hat{k}_{12}) = 4\cdot\sigma^{Q}_{C_{2h}}(0,\ 0) - 4\cdot\sqrt{\frac{5}{14}}\cdot\sigma^{Q}_{C_{2h}}(2,\ 0) + \frac{19}{\sqrt{14}}\cdot\sigma^{Q}_{C_{2h}}(4,\ 0) \tag{47}$$

By combining equations 38 and 47, we obtain:

$$\begin{aligned}
&2\cdot[\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_5,\ \hat{k}_5)+\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_6,\ \hat{k}_6)+\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_7,\ \hat{k}_7)+\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_8,\ \hat{k}_8)]\\
&+\ \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_9,\ \hat{k}_9)+\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_{10},\ \hat{k}_{10})+\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_{11},\ \hat{k}_{11})+\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_{12},\ \hat{k}_{12})=\\
&12\cdot\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(0,\ 0)+\frac{7}{\sqrt{14}}\cdot\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(4,\ 0)
\end{aligned}\tag{48}$$

By combining equations 29 and 48, we show that the electric-quadrupole isotropic cross section of a monoclinic crystal with a $\mathrm{C_{2h}}$ point group is:

$$\begin{aligned}
30\cdot\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(0,\ 0)=&\\
&2\cdot[\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_1,\ \hat{k}_1)+\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_2,\ \hat{k}_2)]+\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_3,\ \hat{k}_3)+\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_4,\ \hat{k}_4)\\
&+\ 2\cdot[2\cdot[\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_5,\ \hat{k}_5)+\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_6,\ \hat{k}_6)+\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_7,\ \hat{k}_7)+\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_8,\ \hat{k}_8)]\\
&+\ \sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_9,\ \hat{k}_9)+\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_{10},\ \hat{k}_{10})+\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_{11},\ \hat{k}_{11})+\sigma^{\mathrm{Q}}_{\mathrm{C_{2h}}}(\hat{\varepsilon}_{12},\ \hat{k}_{12})]
\end{aligned}\tag{49}$$

References

[1] C. Brouder, *Journal of Physics: Condensed Matter*, 1990, **2**, 701–738.