SI: Self-Absorption Correction of NEXAFS Spectra
for Intermediate Sample Thicknesses
applied to Organo-Sulfur Model Compounds

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I. THEORETICAL CALCULATIONS

A. Derivation of the fluorescence count rate

The ansatz for the calculation of the self-absorption correction follows the theory part of Haskel[1]. However, it is rounded up with some additional focus on details as well as a mathematical case analysis for approximations in this work.

Aiming for the correction of the self-absorption effect, one has to model the total process of fluorescence yield NEXAFS spectrometry in order to describe the correlation between the photo-absorption coefficient $\tau(E_0)$ of the examined element and the (normalized) fluorescence count rate. Starting with the differential fluorescence count rate

$$P_f(E_0, z_n)\mathrm{d}z_n = \frac{\Omega}{4\pi}\epsilon_{\mathrm{det}}(E_f)P_0(E_0)e^{-\mu_t(E_0)\frac{z_n}{\sin\vartheta_i}}\epsilon_f\tau(E_0)\frac{\mathrm{d}z_n}{\sin\vartheta_i}e^{-\mu_t(E_f)\frac{z_n}{\sin\vartheta_f}} \tag{1}$$

at the incident energy E_0 originating from an infinitesimally small slice $\mathrm{d}z_n$ in depth z_n of the sample of thickness z_s, with the detected solid angle Ω, detector efficiency ϵ_{det}, incident photon flux $P_0(E_0)$, incident (and fluorescence) beam angle ϑ_i (and ϑ_f), the fluorescence efficiency ϵ_f and the total absorption coefficient $\mu_t(E_0) = \tau(E_0) + \mu_b(E_0)$ with contributions μ_b from all shells and elements in the sample except for the element of interest. The fluorescence energy being denoted by E_f is assumed to be constant.

An integration over the whole sample thickness z_s yields the total fluorescence count rate

$$
\begin{aligned}
P_f(E_0) &= \int_0^{z_s} P_f(E_0, z_n)\mathrm{d}z_n \\
&= \frac{\Omega}{4\pi}\epsilon_{\mathrm{det}}(E_f)P_0(E_0)\epsilon_f\frac{\tau(E_0)}{\sin\vartheta_i}\int_0^{z_s} e^{-\mu_t(E_0)\frac{z_n}{\sin\vartheta_i}}e^{-\mu_t(E_f)\frac{z_n}{\sin\vartheta_f}}\mathrm{d}z_n \\
&= \frac{\Omega}{4\pi}\epsilon_{\mathrm{det}}(E_f)P_0(E_0)\epsilon_f\frac{\tau(E_0)}{\sin\vartheta_i}\left[\frac{e^{-\left(\frac{\mu_t(E_0)}{\sin\vartheta_i}+\frac{\mu_t(E_f)}{\sin\vartheta_f}\right)z_n}}{-\left(\frac{\mu_t(E_0)}{\sin\vartheta_i}+\frac{\mu_t(E_f)}{\sin\vartheta_f}\right)}\right]\Bigg|_0^{z_s} \\
&= \frac{\frac{\Omega}{4\pi}\epsilon_{\mathrm{det}}(E_f)P_0(E_0)\epsilon_f\frac{\tau(E_0)}{\sin\vartheta_i}}{\frac{\mu_t(E_0)}{\sin\vartheta_i}+\frac{\mu_t(E_f)}{\sin\vartheta_f}}\left(1-e^{-\left(\frac{\mu_t(E_0)}{\sin\vartheta_i}+\frac{\mu_t(E_f)}{\sin\vartheta_f}\right)z_s}\right)
\end{aligned}
$$

which, with an eye towards $\tau(E_0)$, simplifies to

$$P_f(E_0) = \frac{\frac{\Omega}{4\pi}\epsilon_{\mathrm{det}}(E_f)P_0(E_0)\epsilon_f\tau(E_0)}{\mu_t(E_0)+\mu_t(E_f)\frac{\sin\vartheta_i}{\sin\vartheta_f}}\left(1-e^{-\left(\mu_t(E_0)+\mu_t(E_f)\frac{\sin\vartheta_i}{\sin\vartheta_f}\right)\frac{z_s}{\sin\vartheta_i}}\right) \tag{2}$$

which occurs in several publications in this or slightly simplified versions[1–9].

B. Calculations of the Taylor expansions for infinitely thin and dilute samples

Relative deviations from the approximation $N(E_0) \approx \bar{\tau}(E_0)$ for the limits $t \ll 1$ and $\zeta \gg 1$ in Equation (2) of the main manuscript can be calculated by Taylor expansion of the fraction

$$\frac{N(E_0)}{\bar{\tau}(E_0)} = \frac{1 + \gamma' + \bar{\beta}}{\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}} \cdot \frac{1 - e^{-\left(\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}\right)t}}{1 - e^{-\left(1 + \gamma' + \bar{\beta}\right)t}}. \tag{3}$$

1. Effective sample thickness $t \ll 1$

For effective sample thickness $t \ll 1$, the coefficient needs to be treated in the limit of $t \to 0$ because the last factor does not exist for $t = 0$. Thus, the Taylor expansion in first order is

$$\frac{N(E_0)}{\bar{\tau}(E_0)}(t \ll 1) = \lim_{t \to 0} \left(\frac{N(E_0)}{\bar{\tau}(E_0)} \right) + \lim_{t \to 0} \left(\frac{\mathrm{d}}{\mathrm{d}t} \frac{N(E_0)}{\bar{\tau}(E_0)} \right) \cdot t + \mathcal{O}(t^2).$$

Following L'Hôpital's Rule and

$$\lim_{t \to 0} \frac{\left(1 - e^{-\left(\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}\right)t} \right)'}{\left(1 - e^{-\left(1 + \gamma' + \bar{\beta}\right)t} \right)'} = \lim_{t \to 0} \frac{\left(\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}\right) e^{-\left(\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}\right)t}}{\left(1 + \gamma' + \bar{\beta}\right) e^{-\left(1 + \gamma' + \bar{\beta}\right)t}} = \frac{\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}}{1 + \gamma' + \bar{\beta}},$$

the limit for the zeroth order yields

$$\begin{aligned}
\lim_{t \to 0} \left(\frac{N(E_0)}{\bar{\tau}(E_0)} \right) &= \lim_{t \to 0} \left(\frac{1 + \gamma' + \bar{\beta}}{\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}} \cdot \frac{1 - e^{-\left(\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}\right)t}}{1 - e^{-\left(1 + \gamma' + \bar{\beta}\right)t}} \right) \\
&= \frac{1 + \gamma' + \bar{\beta}}{\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}} \cdot \lim_{t \to 0} \left(\frac{1 - e^{-\left(\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}\right)t}}{1 - e^{-\left(1 + \gamma' + \bar{\beta}\right)t}} \right) \\
&= \frac{1 + \gamma' + \bar{\beta}}{\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}} \cdot \lim_{t \to 0} \frac{\left(1 - e^{-\left(\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}\right)t} \right)'}{\left(1 - e^{-\left(1 + \gamma' + \bar{\beta}\right)t} \right)'} \\
&= \frac{1 + \gamma' + \bar{\beta}}{\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}} \cdot \frac{\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}}{1 + \gamma' + \bar{\beta}} = 1.
\end{aligned}$$

For the first order coefficient, one needs to evaluate the derivative

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1-\mathrm{e}^{-f_1 t}}{1-\mathrm{e}^{-f_2 t}}\right) &= \frac{\left(1-\mathrm{e}^{-f_1 t}\right)'\left(1-\mathrm{e}^{-f_2 t}\right) - \left(1-\mathrm{e}^{-f_1 t}\right)\left(1-\mathrm{e}^{-f_2 t}\right)'}{\left(1-\mathrm{e}^{-f_2 t}\right)^2} \\
&= \frac{f_1 \mathrm{e}^{-f_1 t}\left(1-\mathrm{e}^{-f_2 t}\right) - \left(1-\mathrm{e}^{-f_1 t}\right) f_2 \mathrm{e}^{-f_2 t}}{\left(1-\mathrm{e}^{-f_2 t}\right)^2} \\
&= \frac{f_1 \mathrm{e}^{-f_1 t} - f_1 \mathrm{e}^{-(f_1+f_2)t} - f_2 \mathrm{e}^{-f_2 t} + f_2 \mathrm{e}^{-(f_1+f_2)t}}{\left(1-\mathrm{e}^{-f_2 t}\right)^2} \\
&= \frac{f_1 \mathrm{e}^{-f_1 t} - f_2 \mathrm{e}^{-f_2 t} - \left(f_1 - f_2\right)\mathrm{e}^{-(f_1+f_2)t}}{\left(1-\mathrm{e}^{-f_2 t}\right)^2}
\end{aligned}
$$

and since this is not defined for $t = 0$, one has to apply L'Hôpital's Rule twice to get

$$
\begin{aligned}
\lim_{t\to 0}\left(\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1-\mathrm{e}^{-f_1 t}}{1-\mathrm{e}^{-f_2 t}}\right)\right) &= \lim_{t\to 0}\left(\frac{f_1 \mathrm{e}^{-f_1 t} - f_2 \mathrm{e}^{-f_2 t} - \left(f_1 - f_2\right)\mathrm{e}^{-(f_1+f_2)t}}{\left(1-\mathrm{e}^{-f_2 t}\right)^2}\right) \\
&= \lim_{t\to 0}\frac{\left(f_1 \mathrm{e}^{-f_1 t} - f_2 \mathrm{e}^{-f_2 t} - \left(f_1 - f_2\right)\mathrm{e}^{-(f_1+f_2)t}\right)'}{\left(\left(1-\mathrm{e}^{-f_2 t}\right)^2\right)'} \\
&= \lim_{t\to 0}\frac{-f_1{}^2 \mathrm{e}^{-f_1 t} + f_2{}^2 \mathrm{e}^{-f_2 t} + \left(f_1 - f_2\right)\left(f_1 + f_2\right)\mathrm{e}^{-(f_1+f_2)t}}{2\left(1-\mathrm{e}^{-f_2 t}\right) f_2 \mathrm{e}^{-f_2 t}} \\
&= \lim_{t\to 0}\frac{-f_1{}^2 \mathrm{e}^{-f_1 t} + f_2{}^2 \mathrm{e}^{-f_2 t} + \left(f_1{}^2 - f_2{}^2\right)\mathrm{e}^{-(f_1+f_2)t}}{2 f_2 \mathrm{e}^{-f_2 t} - 2 f_2 \mathrm{e}^{-2 f_2 t}} \\
&= \lim_{t\to 0}\frac{\left(-f_1{}^2 \mathrm{e}^{-f_1 t} + f_2{}^2 \mathrm{e}^{-f_2 t} + \left(f_1{}^2 - f_2{}^2\right)\mathrm{e}^{-(f_1+f_2)t}\right)'}{\left(2 f_2 \mathrm{e}^{-f_2 t} - 2 f_2 \mathrm{e}^{-2 f_2 t}\right)'} \\
&= \lim_{t\to 0}\frac{f_1{}^3 \mathrm{e}^{-f_1 t} - f_2{}^3 \mathrm{e}^{-f_2 t} - \left(f_1{}^2 - f_2{}^2\right)\left(f_1 + f_2\right)\mathrm{e}^{-(f_1+f_2)t}}{-2 f_2{}^2 \mathrm{e}^{-f_2 t} + 4 f_2{}^2 \mathrm{e}^{-2 f_2 t}} \\
&= \frac{f_1{}^3 - f_2{}^3 - \left(f_1{}^2 - f_2{}^2\right)\left(f_1 + f_2\right)}{-2 f_2{}^2 + 4 f_2{}^2} \\
&= \frac{f_1{}^3 - f_2{}^3 - f_1{}^3 - f_1{}^2 f_2 + f_1 f_2{}^2 + f_2{}^3}{2 f_2{}^2} \\
&= \frac{-f_1 f_2\left(f_1 - f_2\right)}{2 f_2{}^2} \\
&= -\frac{1}{2}\frac{f_1}{f_2}\left(f_1 - f_2\right).
\end{aligned}
$$

Plugging $f_1 = \bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}$ and $f_2 = 1 + \gamma' + \bar{\beta}$, one obtains the first order coefficient

$$
\begin{aligned}
\lim_{t \to 0} \left(\frac{\mathrm{d}}{\mathrm{d}t} \frac{N(E_0)}{\bar{\tau}(E_0)} \right) &= \lim_{t \to 0} \left(\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{1 + \gamma' + \bar{\beta}}{\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}} \cdot \frac{1 - \mathrm{e}^{-\left(\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta} \right) t}}{1 - \mathrm{e}^{-\left(1 + \gamma' + \bar{\beta} \right) t}} \right) \right) \\
&= \frac{1 + \gamma' + \bar{\beta}}{\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}} \cdot \lim_{t \to 0} \left(\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{1 - \mathrm{e}^{-\left(\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta} \right) t}}{1 - \mathrm{e}^{-\left(1 + \gamma' + \bar{\beta} \right) t}} \right) \right) \\
&= \frac{1 + \gamma' + \bar{\beta}}{\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}} \cdot \left(-\frac{1}{2} \frac{\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta}}{1 + \gamma' + \bar{\beta}} \left(\left(\bar{\tau}(E_0) + \gamma(E_0) + \bar{\beta} \right) - \left(1 + \gamma' + \bar{\beta} \right) \right) \right) \\
&= - \frac{\bar{\tau}(E_0) - 1 + \gamma(E_0) - \gamma'}{2}
\end{aligned}
$$

and the first order of the Taylor expansion

$$
\frac{N(E_0)}{\bar{\tau}(E_0)} (t \ll 1) = 1 - \left(\frac{\bar{\tau}(E_0) - 1 + \gamma(E_0) - \gamma'}{2} \right) \cdot t + \mathcal{O}(t^2). \tag{4}
$$

2. *Relative Absorption Coefficient Contributions $\gamma(E_0) + \bar{\beta} \approx \gamma' + \bar{\beta} = \zeta \gg 1$ of the Matrix*

For high matrix contributions to the relative absorption coefficient $\gamma(E_0) + \bar{\beta} \approx \gamma' + \bar{\beta} = \zeta \gg 1$, the coefficient needs to be treated in the limit of $\zeta \to \infty$. In order to perform a Taylor series expansion, the inverse $\eta = \frac{1}{\zeta}$ is introduced with $\eta \to 0$. Thus, the fraction to be expanded is

$$
\frac{N(E_0)}{\bar{\tau}(E_0)} = \frac{1 + \zeta}{\bar{\tau}(E_0) + \zeta} \cdot \frac{1 - \mathrm{e}^{-(\bar{\tau}(E_0) + \zeta)t}}{1 - \mathrm{e}^{-(1 + \zeta)t}} = \frac{1 + \frac{1}{\eta}}{\bar{\tau}(E_0) + \frac{1}{\eta}} \cdot \frac{1 - \mathrm{e}^{-\left(\bar{\tau}(E_0) + \frac{1}{\eta} \right) t}}{1 - \mathrm{e}^{-\left(1 + \frac{1}{\eta} \right) t}} = \frac{\eta + 1}{\eta \bar{\tau}(E_0) + 1} \cdot \frac{1 - \mathrm{e}^{-\left(\bar{\tau}(E_0) + \frac{1}{\eta} \right) t}}{1 - \mathrm{e}^{-\left(1 + \frac{1}{\eta} \right) t}}
$$

and the Taylor expansion in first order is

$$
\frac{N(E_0)}{\bar{\tau}(E_0)} (\zeta \gg 1) = \lim_{\eta \to 0} \left(\frac{N(E_0)}{\bar{\tau}(E_0)} \right) + \lim_{\eta \to 0} \left(\frac{\mathrm{d}}{\mathrm{d}\eta} \frac{N(E_0)}{\bar{\tau}(E_0)} \right) \cdot \eta + \mathcal{O}(\eta^2).
$$

The limit for the zeroth order is trivially

$$
\lim_{\eta \to 0} \left(\frac{N(E_0)}{\bar{\tau}(E_0)} \right) = \lim_{\eta \to 0} \left(\frac{\eta + 1}{\eta \bar{\tau}(E_0) + 1} \cdot \frac{1 - \mathrm{e}^{-\left(\bar{\tau}(E_0) + \frac{1}{\eta} \right) t}}{1 - \mathrm{e}^{-\left(1 + \frac{1}{\eta} \right) t}} \right) = 1.
$$

For the first order coefficient, the following lemma is needed where L'Hôpital's Rule is applied k times

$$\lim_{\eta \to 0} \left(\frac{e^{-\frac{a}{\eta}}}{\eta^k} \right) = \lim_{\eta \to 0} \left(\frac{\eta^{-k}}{e^{\frac{a}{\eta}}} \right)$$

$$= \lim_{\eta \to 0} \frac{\left(\eta^{-k} \right)'}{\left(e^{\frac{a}{\eta}} \right)'}$$

$$= \lim_{\eta \to 0} \left(\frac{-k\eta^{-(k+1)}}{\frac{-a}{\eta^2} e^{\frac{a}{\eta}}} \right)$$

$$= \frac{k}{a} \lim_{\eta \to 0} \left(\frac{\eta^{-(k-1)}}{e^{\frac{a}{\eta}}} \right)$$

$$= \ldots \qquad [\text{(k-1) times L'Hôpital's Rule}]$$

$$= \frac{k!}{a^k} \lim_{\eta \to 0} \left(\frac{1}{e^{\frac{a}{\eta}}} \right) = 0$$

so that for all $a \neq 0$ and k, the limit

$$\lim_{\eta \to 0} \left(\frac{e^{-\frac{a}{\eta}}}{\eta^k} \right) = 0 \tag{5}$$

vanishes. Now, the first order coefficient of the Taylor expansion can be calculated

$$\lim_{\eta \to 0} \left(\frac{\mathrm{d}}{\mathrm{d}\eta} \frac{N(E_0)}{\bar{\tau}(E_0)} \right) = \lim_{\eta \to 0} \left(\frac{\mathrm{d}}{\mathrm{d}\eta} \left(\frac{\eta + 1}{\eta \bar{\tau}(E_0) + 1} \cdot \frac{1 - e^{-\left(\bar{\tau}(E_0) + \frac{1}{\eta} \right)t}}{1 - e^{-\left(1 + \frac{1}{\eta} \right)t}} \right) \right)$$

$$= \lim_{\eta \to 0} \left(\left(\frac{\eta + 1}{\eta \bar{\tau}(E_0) + 1} \right)' \cdot \left(\frac{1 - e^{-\left(\bar{\tau}(E_0) + \frac{1}{\eta} \right)t}}{1 - e^{-\left(1 + \frac{1}{\eta} \right)t}} \right) + \left(\frac{\eta + 1}{\eta \bar{\tau}(E_0) + 1} \right) \cdot \left(\frac{1 - e^{-\left(\bar{\tau}(E_0) + \frac{1}{\eta} \right)t}}{1 - e^{-\left(1 + \frac{1}{\eta} \right)t}} \right)' \right)$$

$$= \lim_{\eta \to 0} \left(\frac{\eta \bar{\tau}(E_0) + 1 - (\eta + 1)\bar{\tau}(E_0)}{\left(\eta \bar{\tau}(E_0) + 1 \right)^2} \cdot \left(\frac{1 - e^{-\left(\bar{\tau}(E_0) + \frac{1}{\eta} \right)t}}{1 - e^{-\left(1 + \frac{1}{\eta} \right)t}} \right) + \left(\frac{\eta + 1}{\eta \bar{\tau}(E_0) + 1} \right) \cdot \right.$$

$$\left. \cdot \frac{\frac{-t}{\eta^2} e^{-\left(\bar{\tau}(E_0) + \frac{1}{\eta} \right)t} \cdot \left(1 - e^{-\left(1 + \frac{1}{\eta} \right)t} \right) - \left(1 - e^{-\left(\bar{\tau}(E_0) + \frac{1}{\eta} \right)t} \right) \cdot \left(\frac{-t}{\eta^2} \right) e^{-\left(1 + \frac{1}{\eta} \right)t}}{\left(1 - e^{-\left(1 + \frac{1}{\eta} \right)t} \right)^2} \right)$$

$$\overset{(5)}{=} 1 - \bar{\tau}(E_0)$$

and the first order of the Taylor expansion yields

$$\frac{N(E_0)}{\bar{\tau}(E_0)}(\zeta \gg 1) = 1 - (\bar{\tau}(E_0) - 1) \cdot \eta + \mathcal{O}(\eta^2),$$

or, in terms of ζ,

$$\frac{N(E_0)}{\bar{\tau}(E_0)}(\zeta \gg 1) = 1 - (\bar{\tau}(E_0) - 1) \cdot \frac{1}{\zeta} + \mathcal{O}\left(\left(\frac{1}{\zeta} \right)^2 \right). \tag{6}$$

II. RESULTS

Table S1 shows the sulfur mass deposition and sample thickness for DPS, DPDS and DMTS from both the transmission and the fluorescence measurements. The sample thickness of DPS is determined to be slightly larger than for DPDS and DMTS. The sulfur mass deposition has the smallest value for DPS though because there is just one sulfur atom per molecule. The second sulfur atom in DPDS and a slightly larger mass density increases the sulfur mass deposition to a value slightly larger than for DPS, despite the lower sample thickness. DMTS does not only have a third sulfur atom, but also shorter carbon chains and the highest mass density of the three molecules, which increases the sulfur mass deposition by more than the factor of 2 compared to DPDS.

Note that only one of the sample films contributed to the fluorescence signal, whereas the transmitted X-ray beam was attenuated by both films. An uneven thickness distribution over the two sample films may lead to a deviation of the measured thickness. The results from transmission and fluorescence agree well with deviations of at most 25% which is consistent with the measurement uncertainties as well as the above mentioned asymmetry.

TABLE S1. Sulfur mass deposition and sample thickness as determined from transmission measurements and reference-free XRF measurements

Molecule		DPS	DPDS	DMTS
Transmission	mass deposition / $\frac{\mu g}{cm^2}$	21.8	27.7	62.6
	sample thickness / μm	0.959	0.678	0.690
Fluorescence	mass deposition / $\frac{\mu g}{cm^2}$	24.2	34.9	78.4
	sample thickness / μm	1.062	0.852	0.865

The Figure S1 below shows the data from Figure 6 for the full energy axis. The residues for the measured transmission and the predicted fluorescence spectra relative to the measured fluorescence spectra of dipropyl sulfide (DPS, blue), dipropyl disulfide (DPDS, orange) and dimethyl trisulfide (DMTS, green) visualize that the forward calculation makes up for the damping of the NEXAFS signal and especially recovers the peak height ratios in the damped fluorescence spectra.
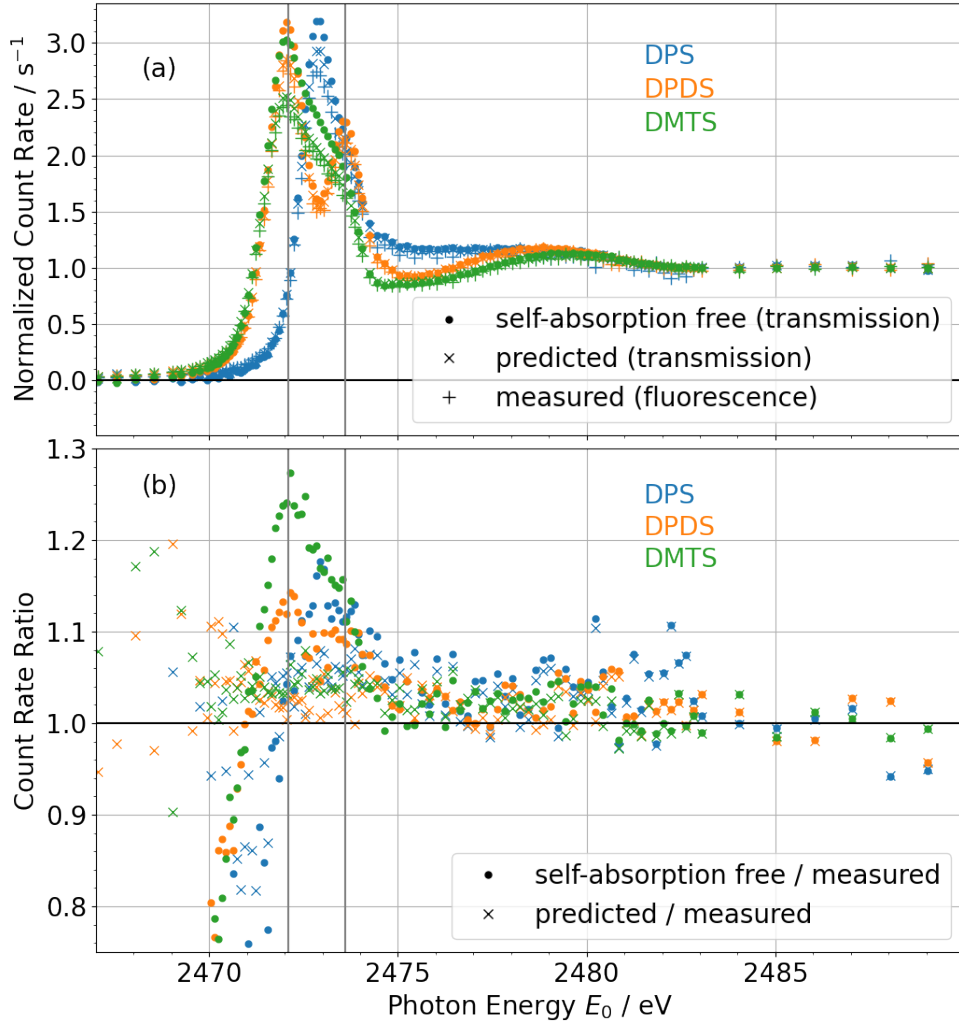
FIG. S1. This figure shows the data from Figure 6 for the full energy axis.

(a) NEXAFS spectra of dipropyl sulfide (DPS, blue), dipropyl disulfide (DPDS, orange) and dimethyl trisulfide (DMTS, green). The self-absorption free (undamped) spectra, directly calculated from transmission measurements, are depicted with dots, the measured fluorescence spectra are marked with pluses, and the crosses in between are the forward calculated fluorescence spectra predicted using transmission and tabulated data. (b) The residues for the measured transmission and the predicted fluorescence spectra relative to the measured fluorescence spectra of dipropyl sulfide (DPS, blue), dipropyl disulfide (DPDS, orange) and dimethyl trisulfide (DMTS, green) visualize that the forward calculation makes up for the damping of the NEXAFS signal and especially recovers the peak height ratios in the damped fluorescence spectra.

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