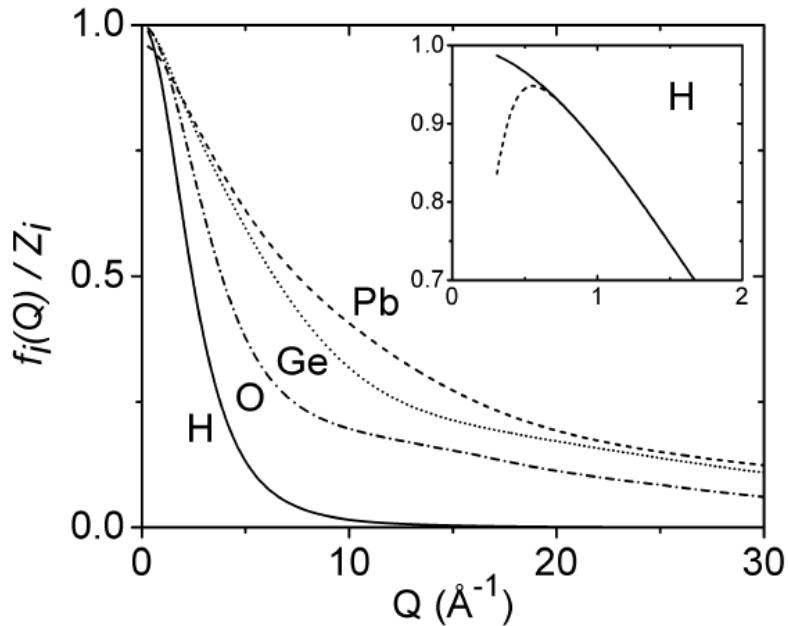
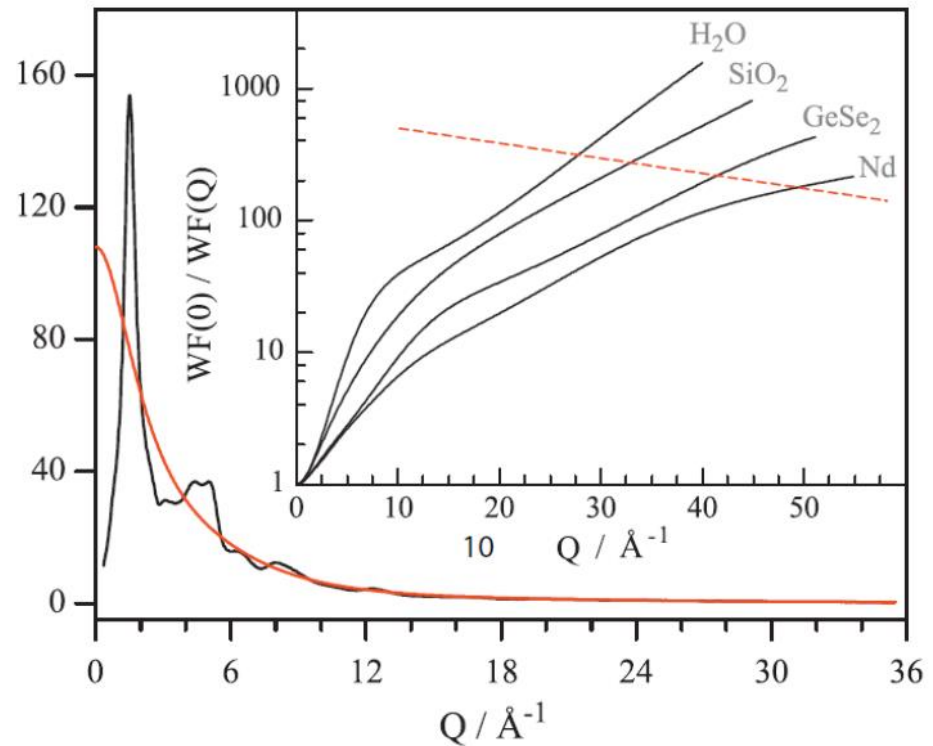


Access to High Momentum Transfers

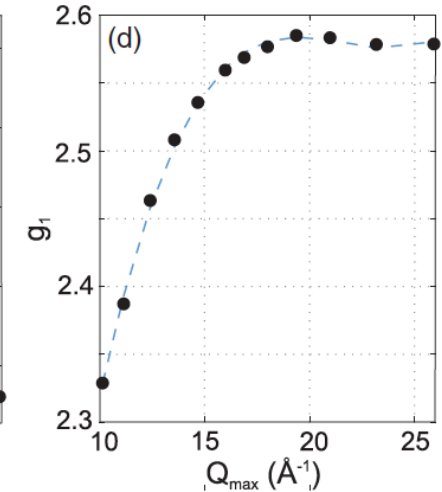
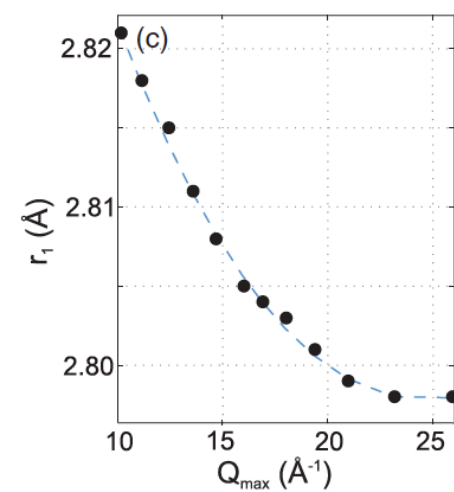
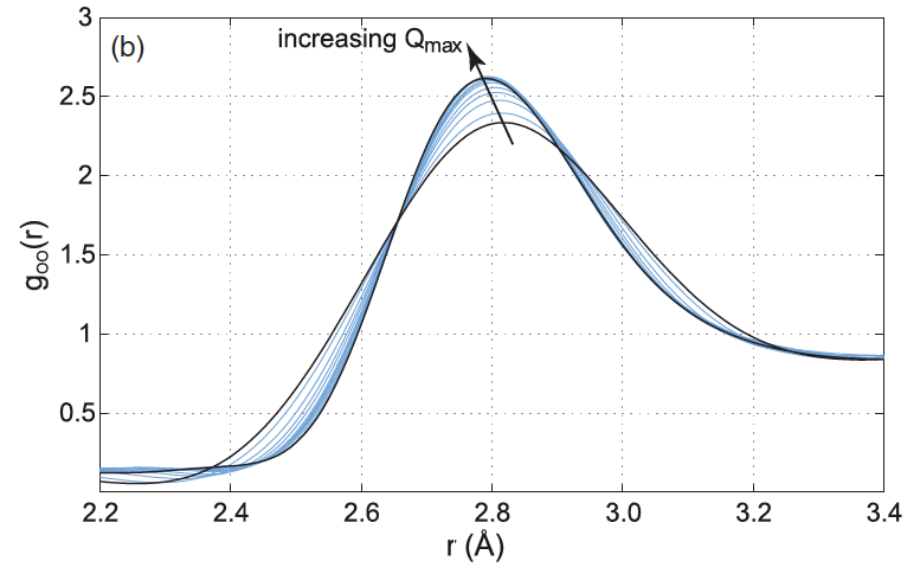
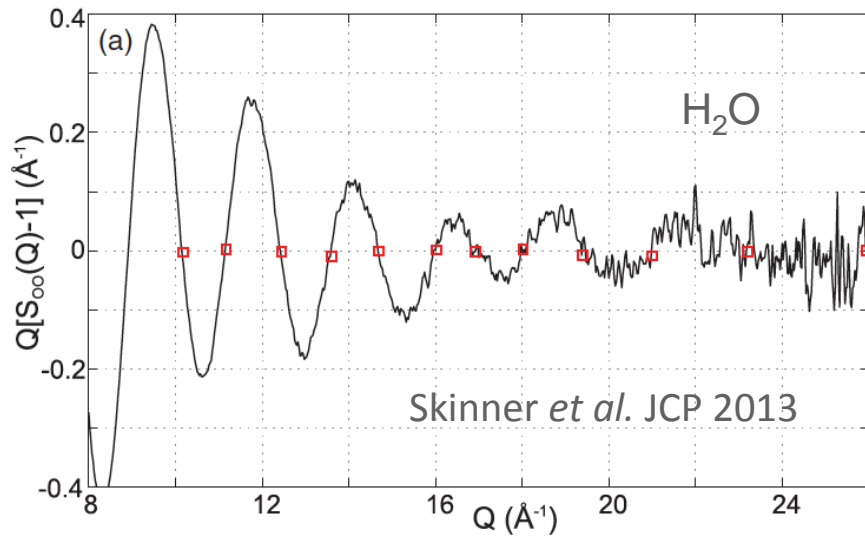


$$S_X(Q) - 1 = \frac{I_X(Q) - FF(Q)}{WF(Q)}$$

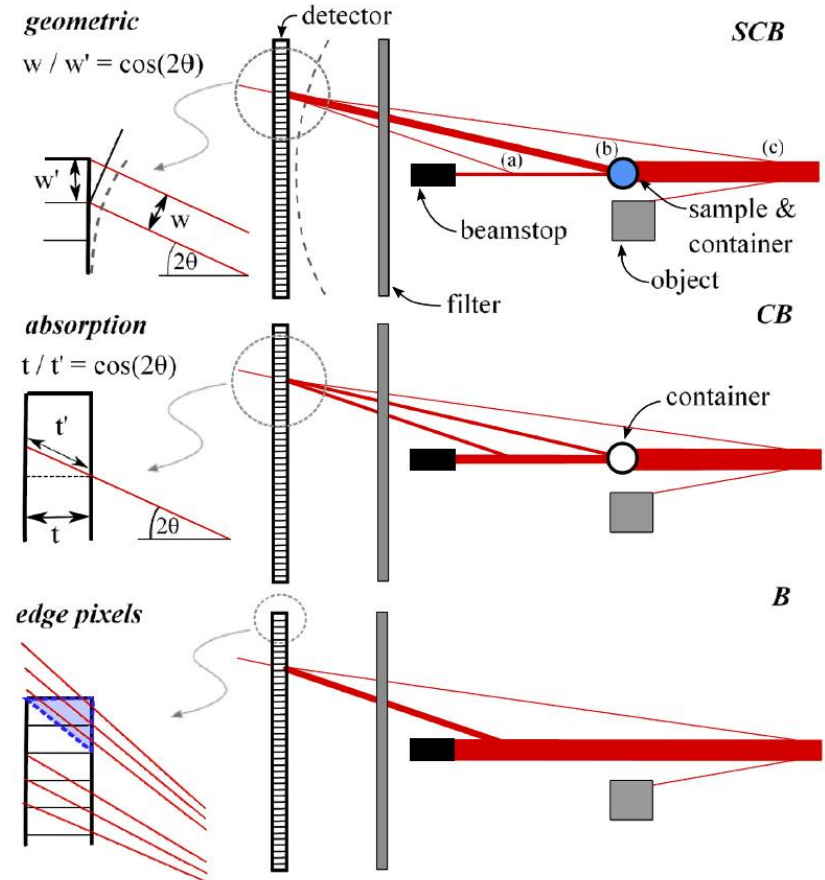
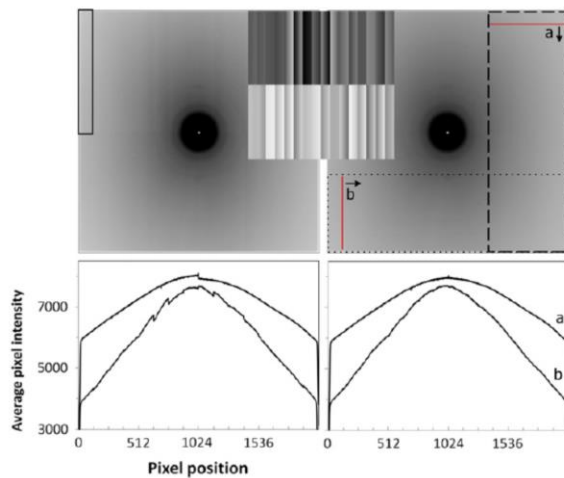
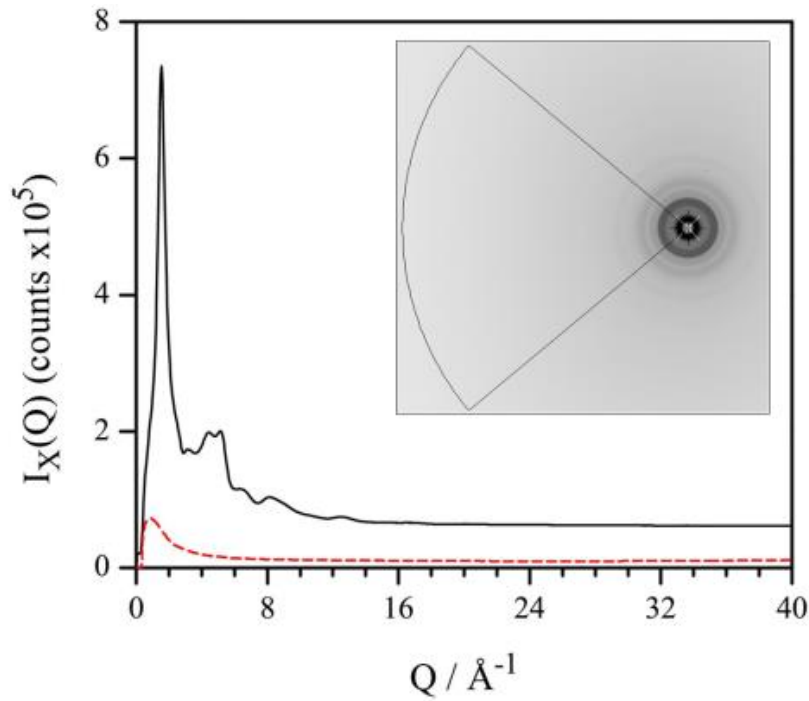
Figure 5. The free atom form factors for the elements H, O, Ge and Pb normalized to their number of electrons at $Q=0$. The insert shows a zoomed in region of the atomic form factor for H using the independent atom approximation (solid line) compared to the modified atomic form factor for H obtained using equation X with $z_{\text{eff}}=0.5$ corresponding to the electron residing halfway along the bond and $\delta=2.0$ obtained from fitting to the quantum mechanical calculations of Wang *et al.* for H_2O .



.. leads to better real space resolution



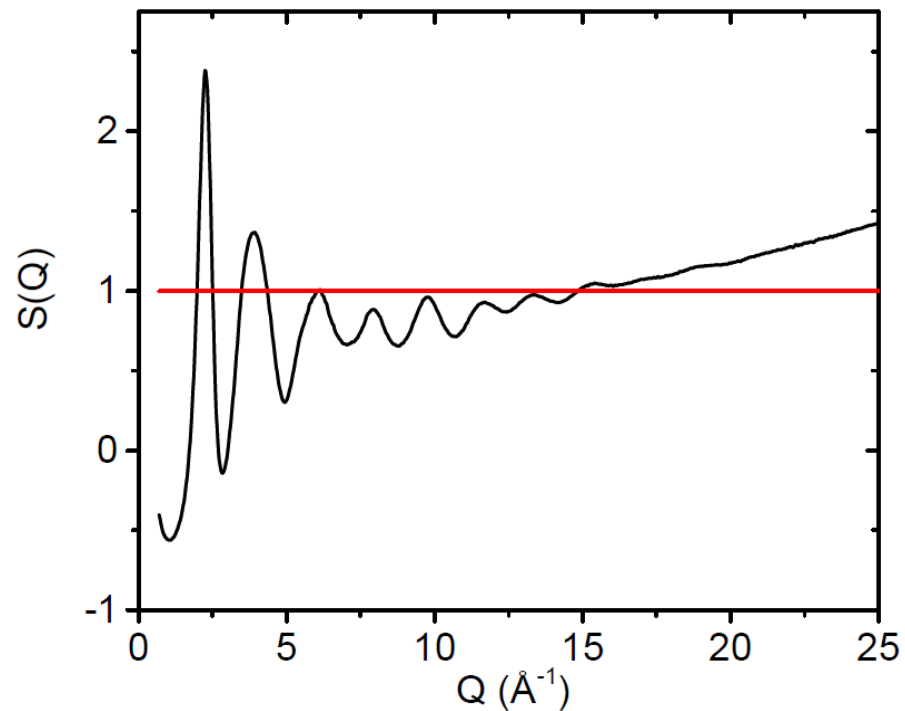
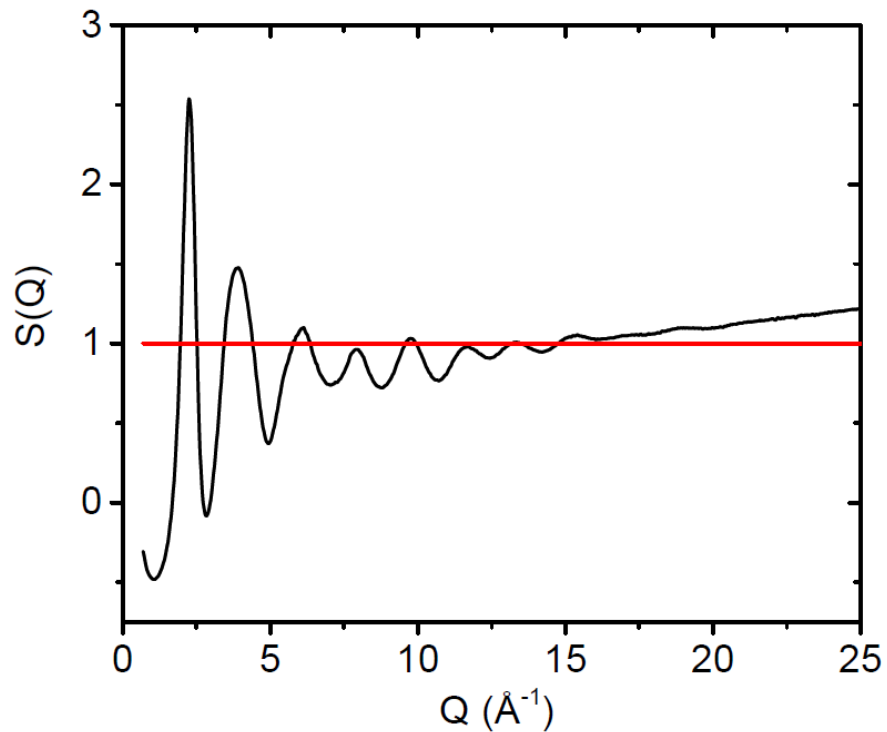
Area detectors for measuring disordered materials



Corrections

Number of input parameters	Sample dependent corrections @100 keV	$I(Q=25)$ correction relative to $I(Q=0)$		% Error in correction	Consequent error in $I(Q)$ (%)	
		SiO ₂	La ₂ O ₃		SiO ₂	La ₂ O ₃
1-4	Sample attenuation	0.99	0.93	2	0.02	0.14
1-4	Fluo. sample attenuation	-	0.79	4	-	0.28 ^a
1	Fluo. detector absorption	-	1.00	1	-	< 0.001
		100 keV	60 keV		100 keV	60 keV
Sample independent corrections						
1	Polarization	1.13	1.38	0.5	0.06	0.14
0	Geometric	1.23	2.04	0.25	0.05	0.13
1	Detector absorption	0.90	0.89	1	0.1	0.1
1	Filter attenuation ^b	1.03	1.11	2	0.06	0.20
Energy dependent Compton corrections^a						
1	Detector energy dep.	1.05	1.07	1	0.05	0.07
1	Filter en. dep.	0.99	0.99	2	0.02	0.02
0	Klein-Nishina	0.95	0.93	< 0.1	< 0.005	< 0.007
				Total	0.34	0.66

How would you correct this data ?



A Practical Guide to Corrections

$$S_{obs}(Q) = \frac{[S(Q) - 1]\gamma + 1 + \beta(Q)}{\alpha}$$

$$= [S(Q) - 1] \frac{\gamma}{\alpha} + \frac{1 + \beta(Q)}{\alpha}$$

Egelstaff's Orange book.

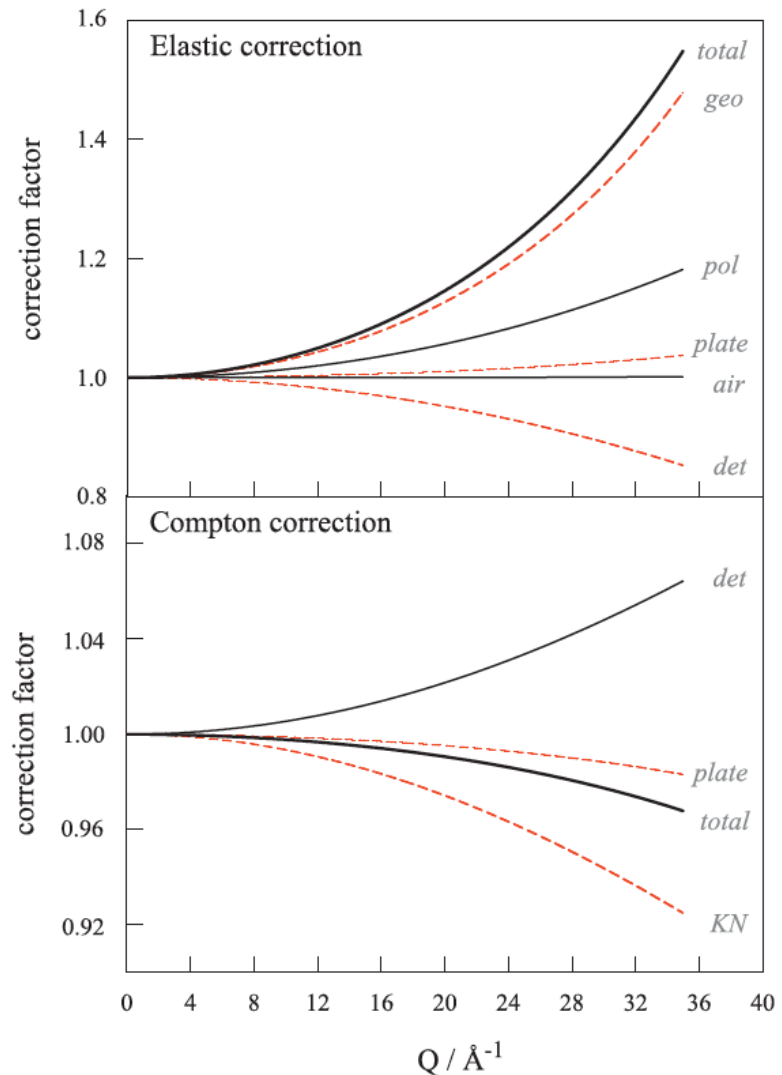
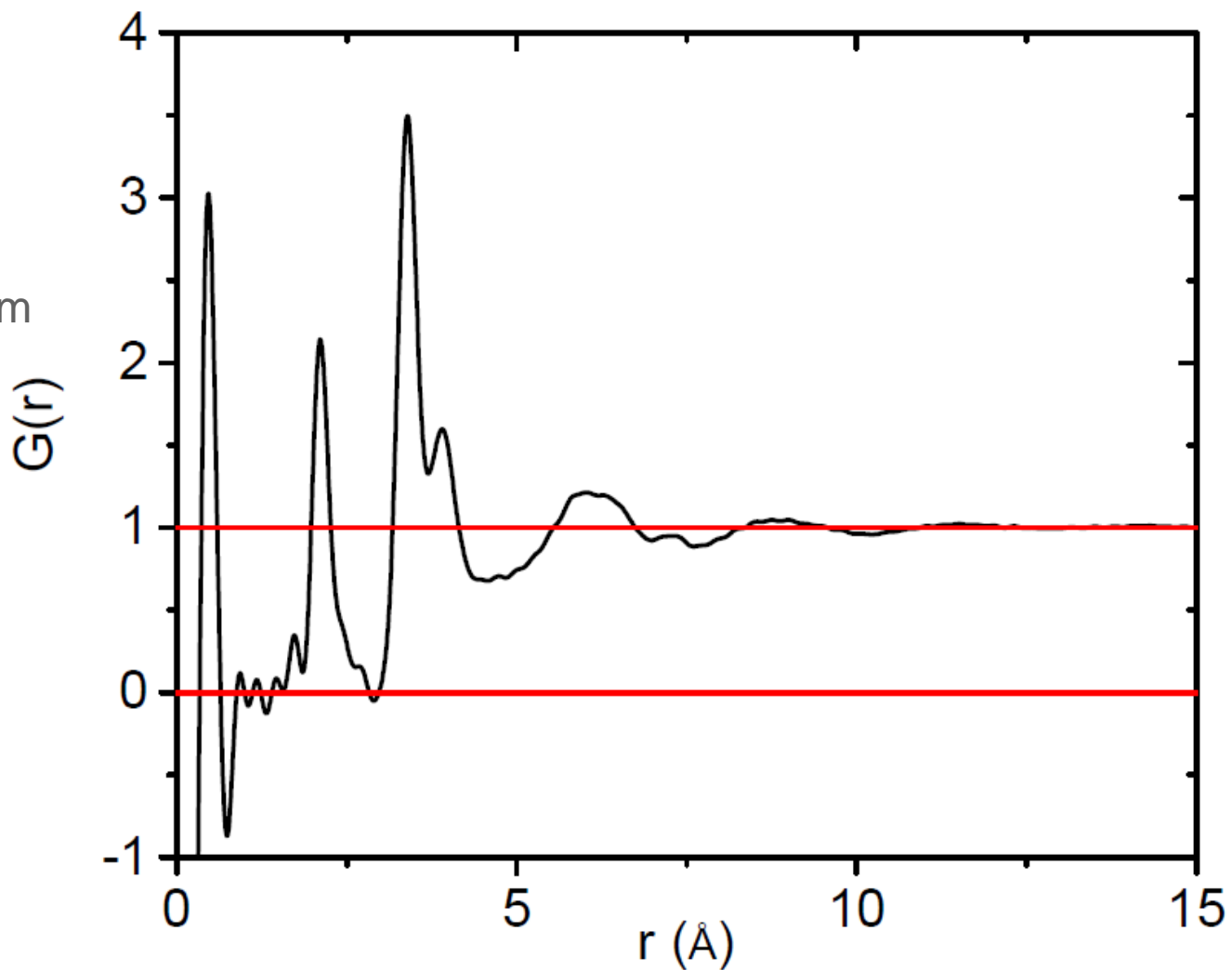


Fig. 6. Top: multiplicative correction factors for a CsI scintillator image plate detector at 115 keV (i.e. the setup at APS beamline 11-ID-C). *Geo*=geometric correction, *pol*=polarization correction, *det*=detector oblique absorption correction, *plate*=plate filter correction, *air*=air absorption correction. Bottom: correction factors to the Compton scattering due to its differing energy (which are additive in $S(Q)$). *KN*=Klein-Nishina quantum mechanical correction to the Compton cross-section.

Sum Rules & Coordination Numbers

HHS
Formalism



When it all goes wrong...

