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Enhanced Resolution PDF from Home Lab Based X-ray Scattering. Alex Yokochi[1], Larry Marple[2], [1]Dept. of Chemical, Biological and Environmental Engineering, Oregon State Univ., Corvallis, OR 97331; [2]School of Electrical Engineering and Computer Science, Oregon State Univ., Corvallis, OR 97331.

Synthetic research in coordination chemistry often yields the famous "intractable insoluble material" that resists crystallization. A technique that may yield useful structural insights on the synthesized material is total scattering. In this technique, very high resolution scattering data is collected for the material in question ($Q = 40Å^{-1}$ is typical), from which a radial distribution curve is then reconstructed by Fourier transformation. However, for total scattering to be useful to guide daily activities in the laboratory, the data should be able to be produced in house with a conventional diffractometer. Unfortunately, using current methodology for spectrum reconstruction it is found that resolution limitations resulting from the limited range of data using home laboratory based instruments ($Q_{max} = 24Å^{-1}$ when using AgKα) drastically reduces the usefulness of information obtained with this technique.

A desire to be able to use total scattering techniques from home lab data has led us to investigate the possibility of applying modern signal processing and spectrum reconstruction techniques to enhance the information content of the derived radial distribution curve.

This presentation will report our experiences and insights whilst pursuing this work.