**The Difficult Chore of Measuring Coordination Number with EXAFS**

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**Abstract**

Neither the theory nor the interpretation of Extended X-Ray Absorption Fine Structure (EXAFS) spectroscopy requires assumptions of crystallographic symmetry or periodicity. As a result, EXAFS is a tool applied to a wide range of scientific disciplines and applied to a wide variety of experimental systems. One common use of the EXAFS measurement is the determination of coordination chemistry. A simple enumeration of the atoms in the coordination environment of the absorber is often the primary goal of an EXAFS experiment. There are, however, a number of pitfalls in the way of an accurate determination of coordination number. These include statistical limitations of the EXAFS fitting problem, empirical effects due to sample preparation or detector response, and the assumptions made about the physical structure surrounding the absorber in the course of data analysis. In this poster we examine several of these pitfalls and their effects upon the determination of coordination number. Where possible, we offer suggestions for avoiding or mitigating the pitfalls. We hope this poster will help guide the general EXAFS practitioner through the difficult chore of accurately determining coordination number. 

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**Modeling Complicated Distributions in IFEFFIT**

These data are best fit by a skewed Gaussian distribution. The skewed Gaussian distribution is shown below in a situation where the skewed Gaussian (i.e., with a third cumulant) using the same centroid, width, and skewness parameters. The skewed Gaussian distribution drops sharply at low R and more gradually at high R. It’s peak is also shifted inward for the same centroid. Using the skewed Gaussian in a situation where the Gamma should be used will introduce systematic error into your determination of coordination number. 

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**Local Disorder in Barium Tantalum Oxynitride**

Data were measured on the Ta K-edge of BaTaO$_2$N at 10, 100, 200, and 300 K. Fitting the nominally cubic perovskite BaTaO$_2$N using a cumulant distribution was unsuccessful. The fit quality was quite poor and the refined values of the fitting parameters were impossible to interpret as physically meaningful parameters. Subsequently, a structural model based on an energy minimization of a box of 4x4x4 unit cells. The different ionic sizes and electrostatics of O and N resulted in a multi-modal distortion to the local structure. The two- and three-body atomic arrangements from the energy-minimized box were collected in bins, as shown in the figures below. A FEFF calculation was made for each bin and the position and height of each bin was used as A and B in the FEFF equation. Our fitting results suggest that this is a true three-atom representation of the structure. Although not perfect, the fit is vastly improved and the fitting parameters (including some σ parameters and a lattice expansion coefficient) were all physically reasonable.

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**Conclusions**

Accurate determination of coordination number is not trivial in EXAFS data analysis. At best, coordination number must be interpreted from the amplitude term refined in a fit, given that coordination is highly or completely correlated to $S$. And to various aspects of sample preparation and data processing.

For complicated systems, accurate determination of coordination number requires sophisticated structural modeling. Any information that can be drawn from other measurements, or from representation of some sort can be leveraged to solving the EXAFS problem. The references box cites several examples of using a path expansion for complicated, non-Gaussian distributions. A variety of useful tutorials and presentations discussing the many issues covered in this short paper can be found on the web at http://xafs.org.