

W0067

Evaluation of the Different Choice Method of Absorption Correction Used in the Structural Determination in Complex with Heavy Metals. Sauli Santos-Jr^a, Javier Ellena^b, ^aNúcleo de Física, Curso de Engenharia de Alimentos, Univ. Federal do Tocantins – UFT, ^bInst. de Física de São Carlos, Univ. de São Paulo - USP, Brazil.

The determination of three-dimensional structures with heavy metals is a very important tool in the study of complexes that can be able to act as antidotes in the poisoning by ingestion of these kinds of substances. A detailed knowledge of these complexes is important to help in the modeling of new molecular structures and in the determination of more effective procedures in the neutralization of the processes, developed for individuals with chronic heavy metals poisoning. It is known some techniques of X-ray absorption correction for diffraction data from monocrystals. During the data reduction many corrections take place, such as: Lorentz, polarization, absorption and eventually correction for deterioration of the sample. The absorption correction is strongly recommended for crystals with strong absorbers in its structural form. The effect of the absorption of X-ray in crystalline samples had been studied and a comparison of the results using different methods was made. This work that showed different forms of absorption correction, we observed significant differences in the figures of merit, peaks and valleys of residual charge density and parameters of anisotropic displacements. Peaks and valleys of residual charge density that they located close to heavy metals had drastically diminished the height or depth after the appropriate absorption correction, respectively. Bond distances and angles, on the other hand, did not change significantly.