HIGH-STATISTICS MEASUREMENT OF OXIDATION STATE OF FE IN THE ISM USING XMM OBSERVATIONS OF CYG X-1
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Introduction: Comparison of the initial chemistry of the solar nebula with the chemical diversity that we observe today in the solar system in principle can inform our understanding of chemical processing in the early solar system.

Previously, we measured the oxidation state of Fe in the interstellar medium [1], using Chandra x-ray observations of the bright x-ray source Cyg X-1, combined with a library of Fe L-edge spectra of standards acquired by synchrotron-based soft x-ray spectroscopy at the Advanced Light Source (Lawrence Berkeley National Laboratory). Extinction spectra, observed astronomically, cannot be compared directly to absorption spectra measured in the laboratory, so theoretical extinction spectra were derived from absorption spectra via the Kramers-Kronig relation and various assumptions about particle size distribution (e.g., [2]). We concluded that the observations are most consistent with Fe dominated by Fe metal.

Having developed the technique, we are now expanding the effort to survey the oxidation state of Fe in the ISM along lines of sight to numerous x-ray binaries, which serve as quasi-continuum light sources, and to expand our effort to observations by XMM-Newton. XMM has a larger collecting power than Chandra, but poorer energy resolution. Here we present a high-statistics XMM observation of Cyg X-1 to compare to the Chandra observation along the same line of sight, and to explore the adequacy of our standards library to fit high-statistics data.

Methods: We combined multiple spectra of Cyg X-1 taken by the Reflection Grating Spectrometer (RGS) on the XMM-Newton space telescope. We downloaded all fluxed spectra for Cyg X-1 from the XMM-Newton Science Archive but removed observations that have significant contamination from undesirable x-ray phenomena such as overlapping fluorescence lines [4]. We also calculated the orbital phase of the black hole relative to the companion star and chose only those spectra that did not place the black hole in the shadow of the star's atmosphere since we are interested in the composition of the ISM, not the stellar wind.

Analyses: We fit the spectrum using the same technique and code that we used for analysis of Chandra data reported in [1]. We did not include any assumed gas component in the analysis.

We first fit the observations to a combination of metal, sulfide and silicate standards (Fig. 1), as in the Chandra analysis. The best fit was consistent with metal composition (Fig. 2). This conclusion is similar to our previous Chandra analysis, but our improved statistics provide a much smaller confidence interval, allowing for almost no sulfide or silicate content. However, the χ^2 was 210 for 113 degrees of freedom, indicating a significant deficiency in the model. Most of the contribution to χ^2 is at the L-edge structure, and in particular the ratio of the L_3 to L_2 peaks is significantly smaller than that of metal, which has the smallest L_3/L_2 ratio of any of our standards.

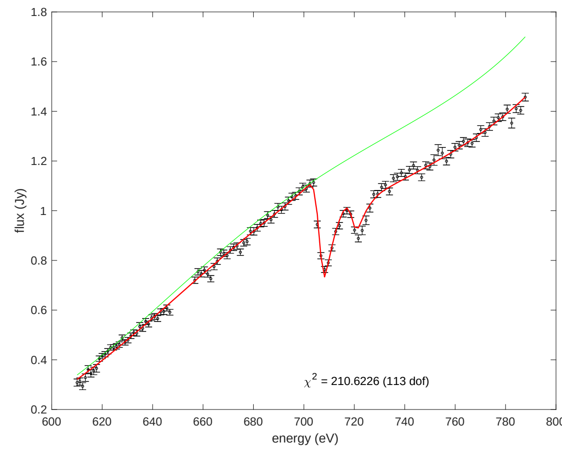

Figure 1: (Red curve) Best fit to (Fe carbide, sulfide, silicate) standard set. Green curve: assumed background, using a third-order polynomial fit to the continuum below the Fe L-edge.

To explore this further, we replaced the metal standard with a carbide spectrum from [3]. The results are shown in Figs. 3 and 4. Here, the fit is somewhat improved, with $\chi^2 = 195$ for 113 degrees of freedom. However, L_3/L_2 is still significantly smaller than the best fit.

We considered the possibility that the deficit in the model may be due to an inadequacy in the dust size model we used which was the Weingartner-Draine distribution with an upper size cutoff as a free parameter. An excess of large grains, which could reduce L3/L2, would also produce significant pre-edge extinction, which is not observed in the observational data. However, we have not yet explored this possibility quantitatively. A deficiency in the quality of the continuum fitting does not appear likely to be significant here since most of the χ^2 contribution comes from the data points within the XANES features and not the pre/post edge.

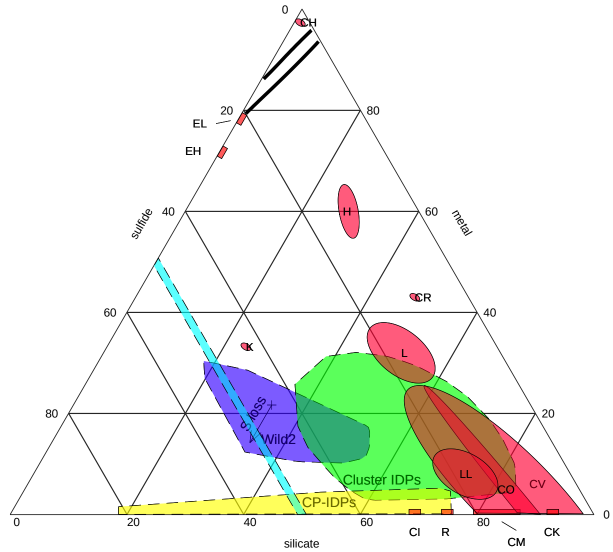

Figure 2: (black lines) Corresponding 1σ and 2σ confidence intervals for Fig. 1. Oxidation states of meteorite families, chondritic porous interplanetary dust particles (CP-IDPs) and comet 81P/Wild 2 are shown for comparison [1 and references therein]

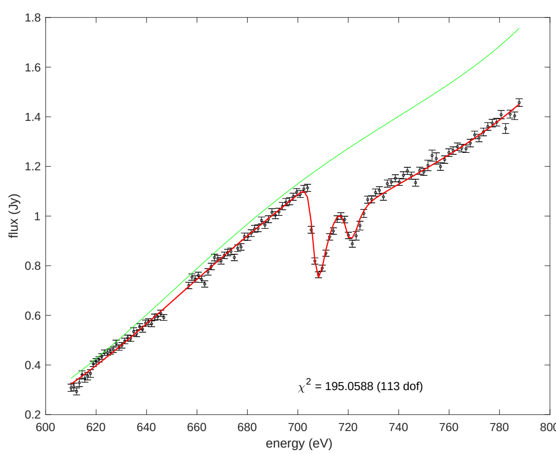

Figure 3: Like Fig. 1, but best fit to (Fe carbide, sulfide, silicate) standard set.

Another possibility is that Fe is present in a phase that is not represented in our standard library. The intensity of the L_3 and L_2 peaks is determined by the chemical bonding environment around the iron. The number of potential phases is vast, and many of the phases are not easily prepared and measured in a synchrotron. Therefore we are computing theoretical XAS spectra using Density Field Theory and Configuration Interaction [9]. A spectrum can be computed in a relatively short time on modern compute clusters, and the "experimental" circumstances are well determined. This is a promising

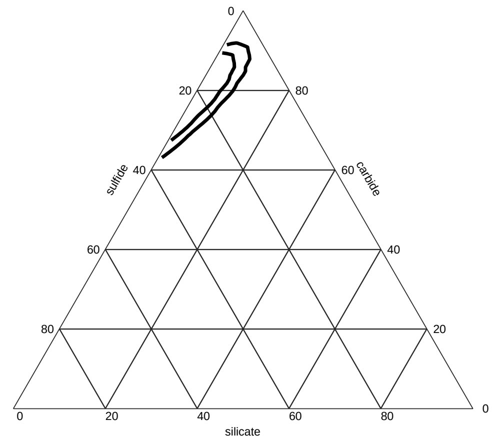

Figure 4: Like Fig. 2, corresponding 1σ and 2σ confidence intervals for Fig. 3.

approach for phases such as FeH molecules, Fe clusters, and nanoparticles dominated by surface area bonding. We explore this avenue in a sister abstract [5].

Finally, measurements of the low energy x-ray polarization of Cyg X-1 are sparse but suggest that X-rays at the Fe-L edge should only be polarized by a few percent [10], and therefore polarization should not dramatically alter the spectra we see. However, it is possible that we must consider polarization of both the photons emitted from the x-ray source as well as transmission through the interstellar medium to obtain the highest quality fits. The upcoming launch of the Imaging X-ray Polarimetry Explorer (IXPE) space telescope should enable measurements that allow us to determine the extent to which polarization influences our ability to measure the phase of interstellar Fe. If polarization is important, then spectra along different sight-lines should have differing L_3/L_2 ratios and shapes since the orientation of the accretion disks in different X-ray sources varies, and the magnetic field orientation of the interstellar medium varies along the different sight-lines as well.

References: [1] Westphal A. J. et al. (2019) *Ap. J.* 872, 66. [2] Weingartner J. C. and Draine B. T. *Ap. J.* 548, 296. [3] Furlan A. et al. (2015) *J. Phys. Condens. Matter* 27, 045002. [4] Gainsforth Z. et al. (2019) *M&M* 25(S2), 258-259. [5] Gainsforth Z. et al. (2021) *LPSC* 2021. [6] Stern, E. A., et al. (1981) *Phys. Rev. B.*, 23, 8, 3781. [7] Hong, S. S., et al. (1980) *A&A* 88,194. [8] Taverna, R. et al. (2020) *arXiv* 2012.06504. [9] Roemelt, M. et al. (2013) *J. Chem. Phys.* 138(20) 204101. [10] Russel, S. & Shahbaz, T. (2014) *MNRAS* 438,2083.