The discovery of room-temperature superconductivity at ambient pressure in Cu-substituted apatite ('LK99') has sent shockwaves through the scientific community. Social media platforms are abuzz with discussions, and experimentalists and theoreticians alike are diving headfirst into unraveling the secrets of this remarkable phenomenon.

As a computational materials scientist, I understand the excitement and the challenges that come with starting your own exploration. One common hurdle is obtaining accurate starting structures for simulations or modeling real materials for your own Density Functional Theory (DFT) simulations. But worry not! I've done some legwork to make your journey smoother.

In this blog post, I share a collection of CIF and POSCAR files containing the reported structures (atomic coordinates and lattice parameters) of the LK99 material to date.
I hope to save you from the hassle of searching the literature, downloading supplementary PDFs, and manually extracting data.
Therefore, I provide you with a one-stop solution.

Let's save time and effort together!

LK99

Apatites are materials with the general formula $\mathrm{A_{10}(TO_4)_6X_{2\pm x}}$, where A = alkaline or rare earth metal; T = Ge, Si, or P; and X = halide, O, or OH [1]. Lk99 is supposed to be a copper (Cu) doped Lead Apatite with the formula Pb9CuP6O25 or Pb9Cu(PO4)6O [2]. The undoped form is Pb10(PO4)6O. So essentially, a Pb atom is replaced/doped with the Cu atom in LK99.

A study from India was able to synthesize the Cu-doped Lead Apatite from the precursors: Cu3P and Pb2SO5 [3]. Their experimental x-ray diffraction pattern indeed matched well with the theoretical structure obtained by DFT optimization. [3]

Here are some visualizations of the Pb9CuP6O25 structure from ref [1] created with CrysX – 3D Viewer.

This slideshow requires JavaScript.

and a Jsmol interactive visualization here

LK99-Pb9P6CuO25_Cu_on_Pb(1)

About/Help

PS: I have also created a GitHub repo (https://github.com/manassharma07/LK99) providing the files below. Please '*star*' it if you find it useful!

Well, enough of chit-chat. Below you will find the structures of LK99 and related materials reported in the literature.

Reported Structures

1. Origin of correlated isolated flat bands in copper-substituted lead phosphate apatite

Author: Sinéad M. Griffin
Link: https://arxiv.org/abs/2307.16892

Structures provided in the Supporting Information:

CIFs:

1. LK99-Pb9P6CuO25_Cu_on_Pb(1) (page 12) (This is the actual LK99 material as the simulated XRD pattern compares well with [3])
2. LK99-Pb9P6CuO25_Cu_on_Pb(2) (page 13) (Cu substitution on Pb(2) does not result in flat bands so it is not probably LK99)
3. LK99-Pb9P6CuO26H2_Cu_on_Pb(1) (page 11) (This is also a candidate for LK99 but with a slightly different formula)
4. LK99-Pb9P6CuO26H2_Cu_on_Pb(2) (page 12) (Again, Cu substitution on Pb(2) is not useful)

POSCARs:

2. First-principles study on the electronic structure of Pb10−xCux(PO4)6O (x = 0, 1)

Authors: Junwen Lai, Jiangxu Li, Peitao Liu a, Yan Sun, Xing-Qiu Chen
Link: https://doi.org/10.1016/j.jmst.2023.08.001

Structures provided in the Supporting Information:

CIFs:

1. Lead_apatite_undoped-Pb10P6O25 (This is the undoped or pure lead apatitie. Substituting one Pb here with Cu results in LK99)
2. LK99-Pb9P6CuO25_Lai (This is the Cu substituted lead apatitie. This has the same formula as LK99 but with slightly different lattice parameters than reported by [1])
3. Pb9P6AuO25_Lai (Au doped Lead Apatite)
4. Pb9P6NiO25_Lai (Ni doped Lead Apatite)
5. Pb9P6ZnO25_Lai (Zn doped Lead Apatite)
6. Pb9P6AgO25_Lai (Ag doped Lead Apatite)

POSCARs:

1. Lead_apatite_undoped-Pb10P6O25
2. LK99-Pb9P6CuO25_Lai
3. Pb9P6AgO25_Lai
4. Pb9P6AuO25_Lai
5. Pb9P6NiO25_Lai
6. Pb9P6ZnO25_Lai

3. Structures of Precursors (Cu3P and Pb2SO5)

Source: MaterialsProject

(a) Cu3P (mp-7463: Cu3P (Hexagonal, P6_3cm, 185) (materialsproject.org))

CIF: Cu3P_P63cm_mp-7463

(b) Pb2SO5 (mp-21497: Pb2SO5 (Monoclinic, C2/m, 12) (materialsproject.org))

CIF: Pb2SO5_mp-21497

So, that's it for now. Hope you guys find this useful! I will keep this post updated with new structure files as soon as I find some in literature.

If you also have a structure file and would like to contribute it then please leave a comment down below.

References:

[1] [2307.16892] Origin of correlated isolated flat bands in copper-substituted lead phosphate apatite (arxiv.org)

[2] LK-99 – Wikipedia

[3] [2308.03544] Absence of superconductivity in LK-99 at ambient conditions (arxiv.org)

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I'm a physicist specializing in computational material science with a PhD in Physics from Friedrich-Schiller University Jena, Germany. I write efficient codes for simulating light-matter interactions at atomic scales. I like to develop Physics, DFT, and Machine Learning related apps and software from time to time. Can code in most of the popular languages. I like to share my knowledge in Physics and applications using this Blog and a YouTube channel.

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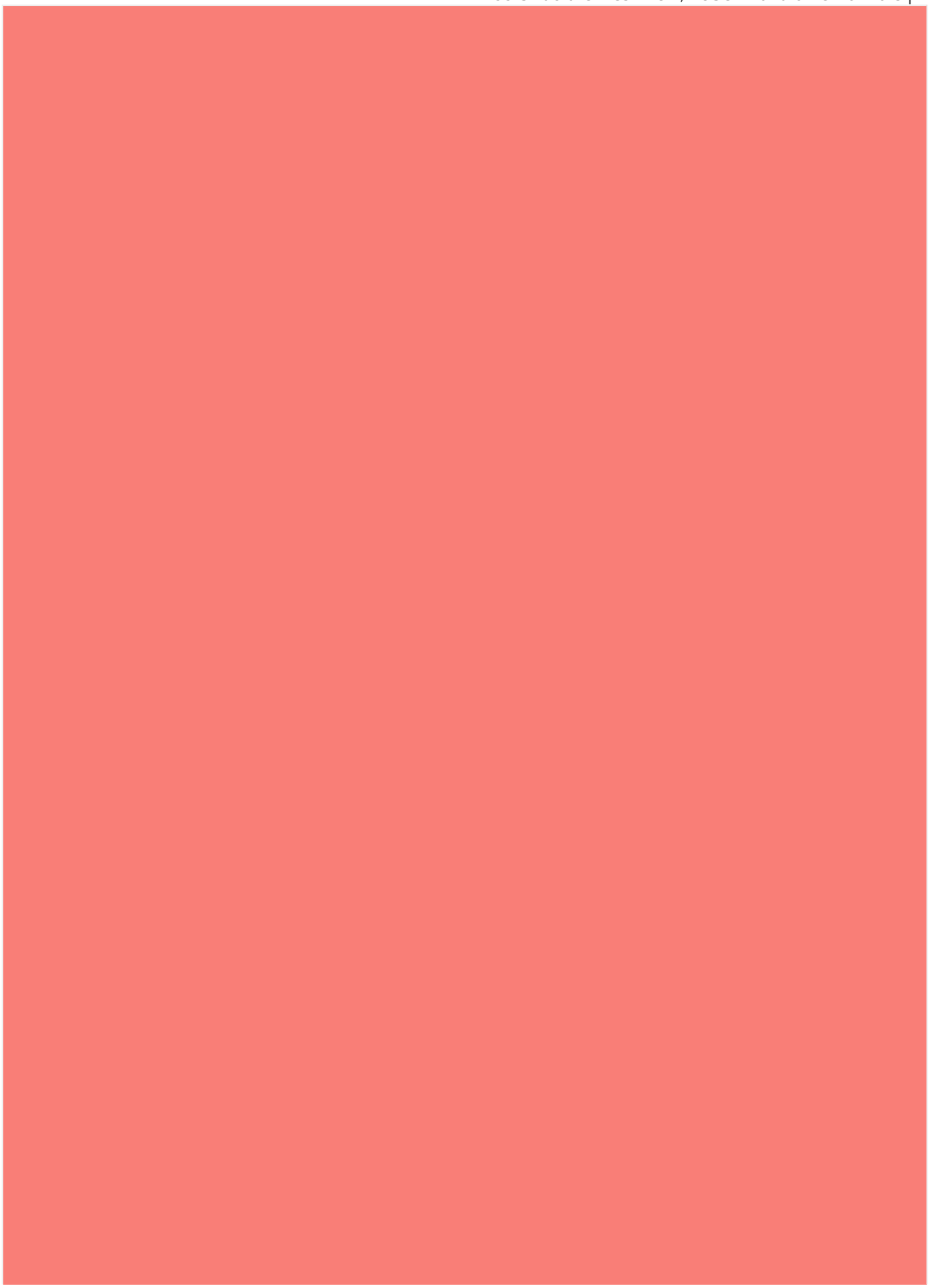

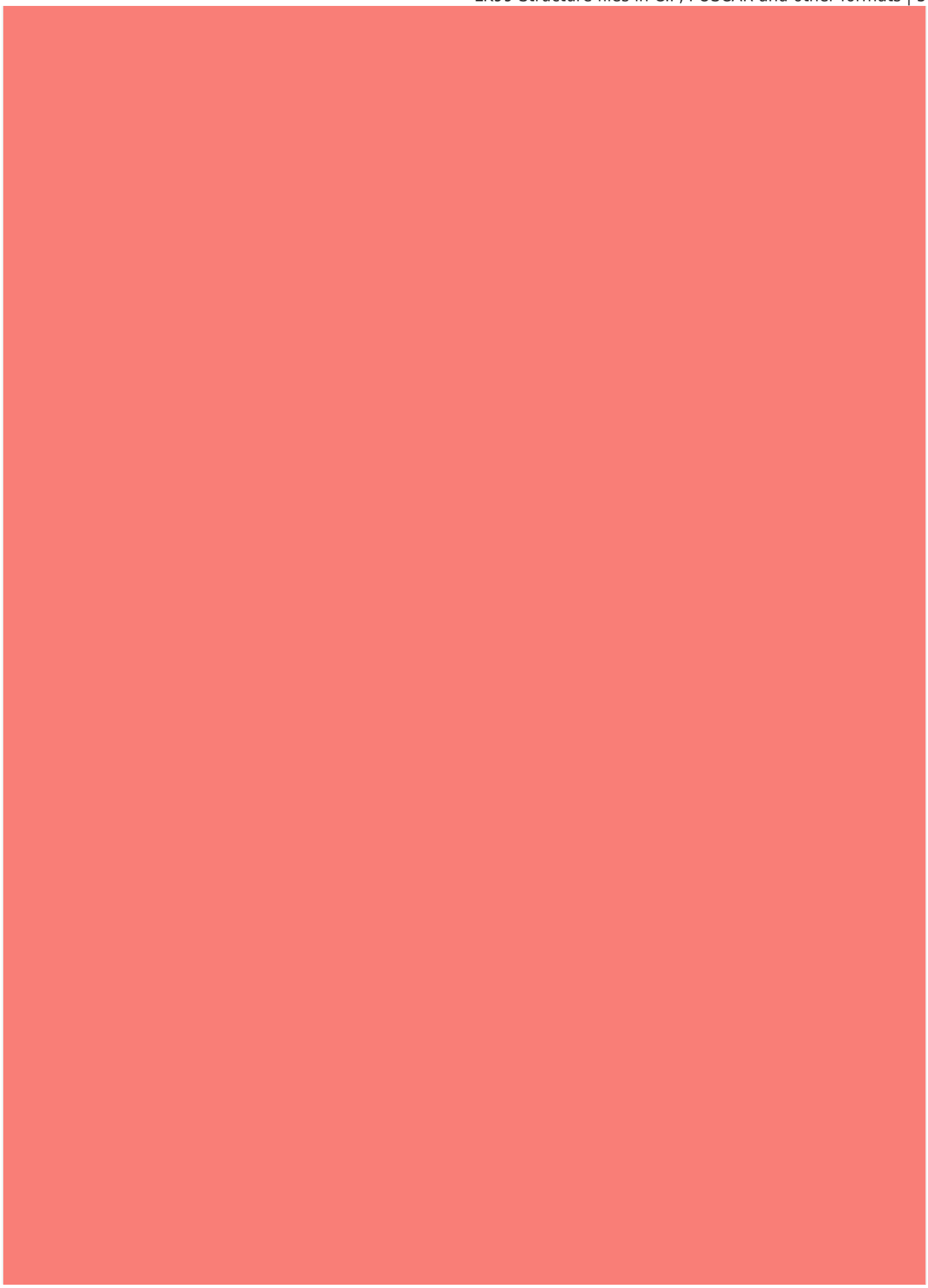

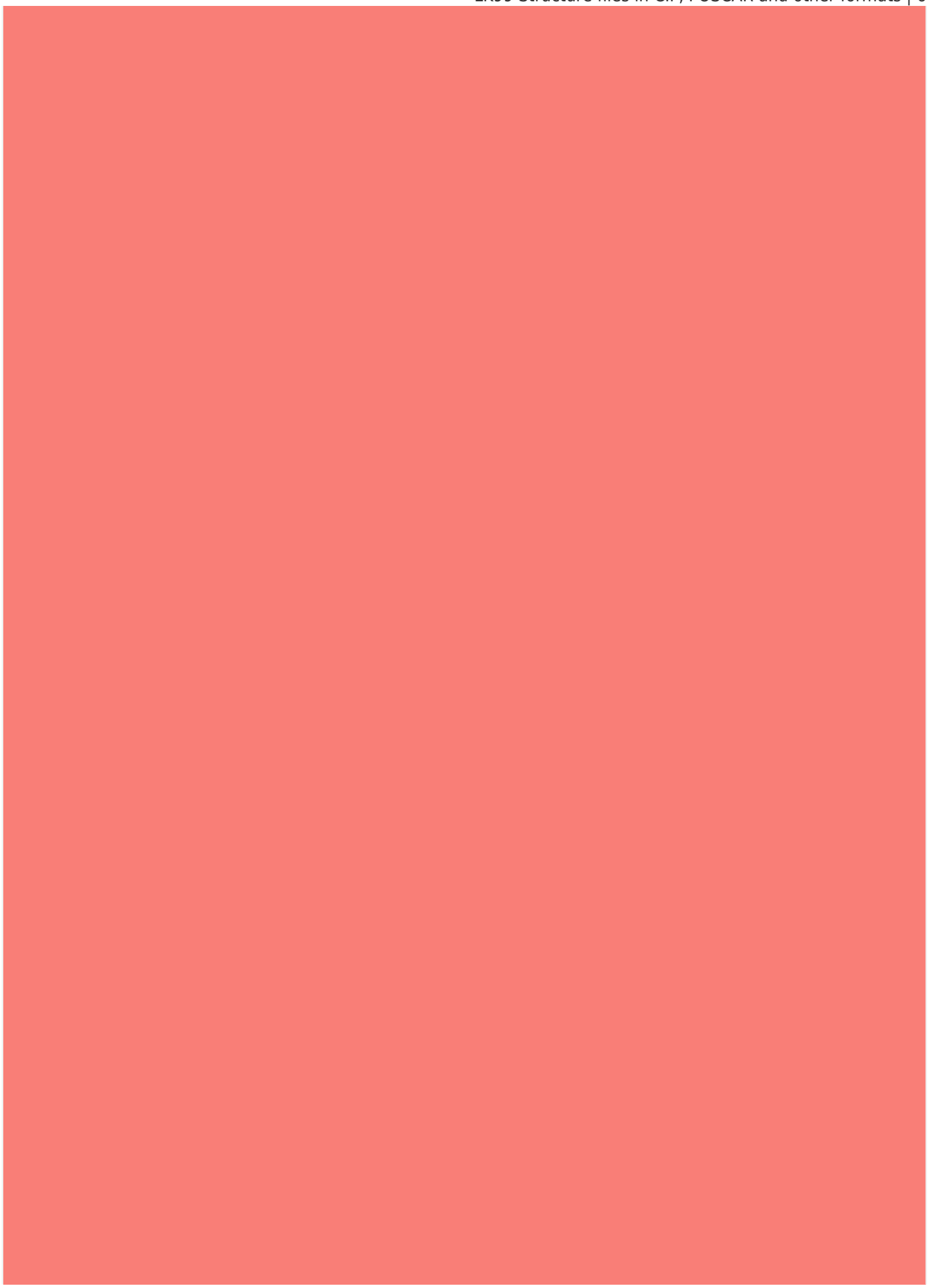

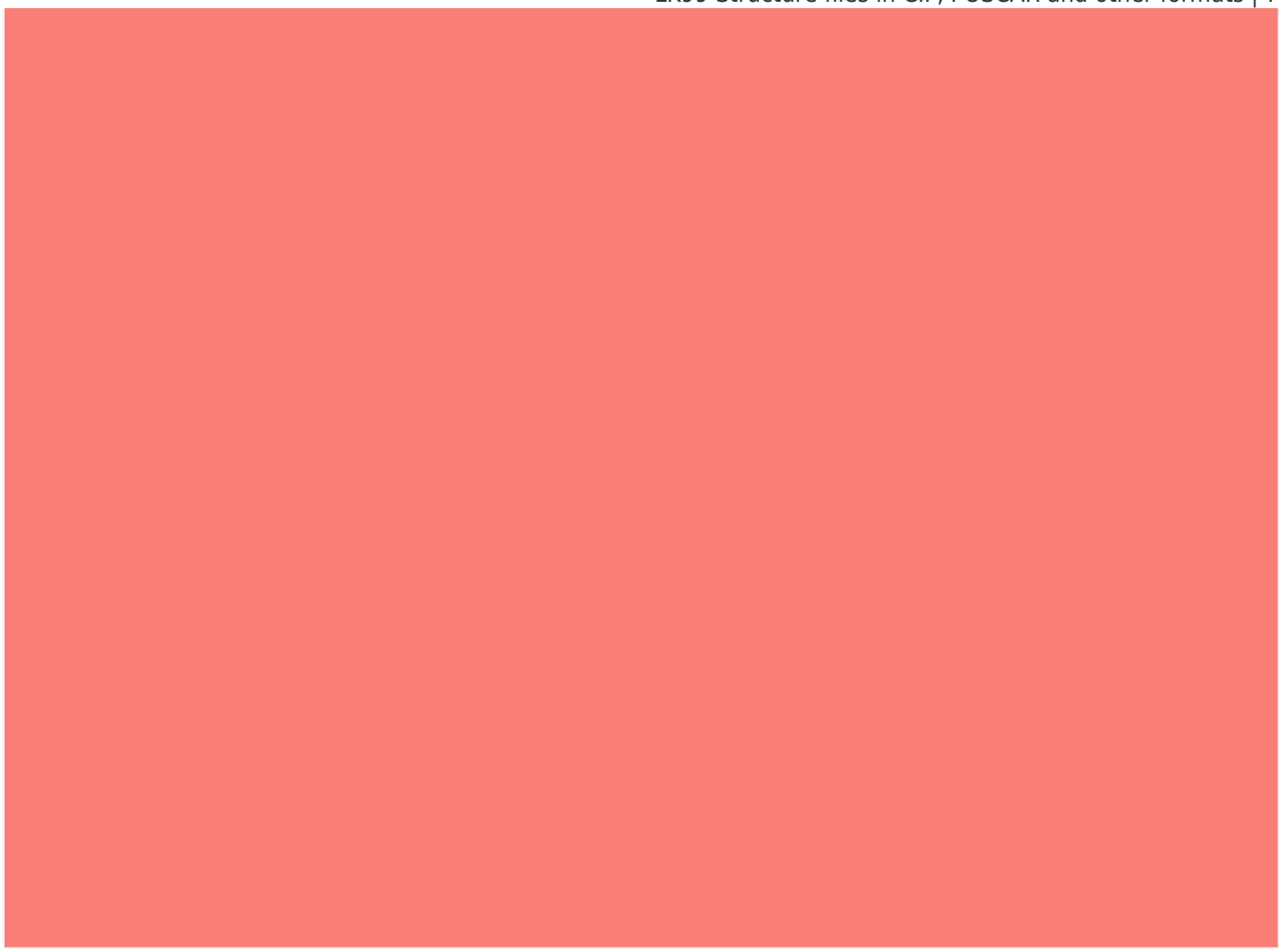

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