

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 $A_{10}(TO_4)_6X_{2\pm x}$, 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 $Pb_9CuP_6O_{25}$ or $Pb_9Cu(PO_4)_6O$ [2]. The undoped form is $Pb_{10}(PO_4)_6O$. 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: Cu_3P and Pb_2SO_5 [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 $Pb_9CuP_6O_{25}$ 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)

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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 $\text{Pb}_{10-x}\text{Cu}_x(\text{PO}_4)_6\text{O}$ ($x = 0, 1$)

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 apatite. Substituting one Pb here with Cu results in LK99)
2. [LK99-Pb9P6CuO25_Lai](#) (This is the Cu substituted lead apatite. 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 (Cu_3P and Pb_2SO_5)

Source: [MaterialsProject](#)

(a) Cu_3P ([mp-7463: Cu3P \(Hexagonal, P6_3cm, 185\) \(materialsproject.org\)](#))

CIF: [Cu3P_P63cm_mp-7463](#)

(b) Pb_2SO_5 ([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:

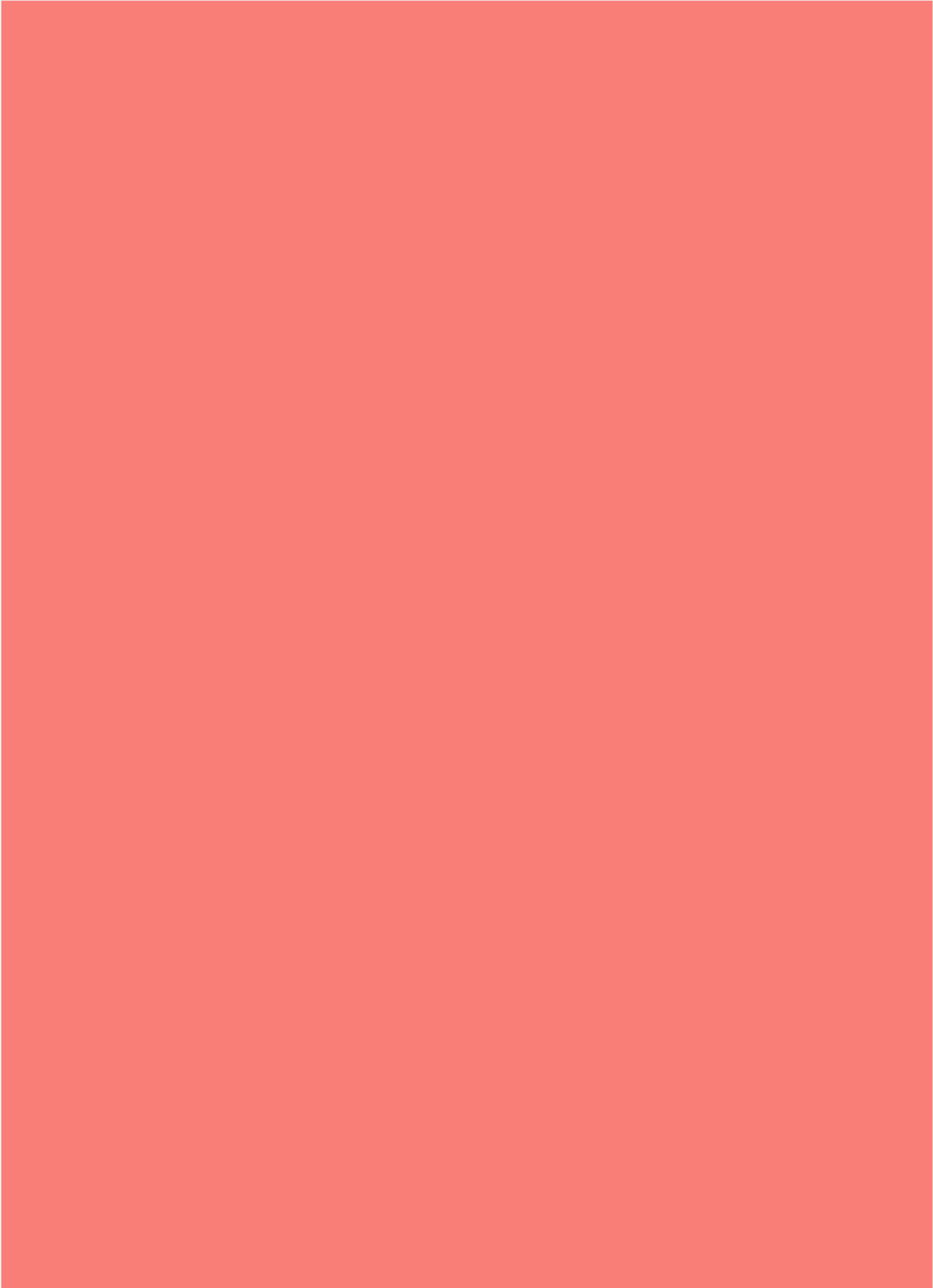
- [1] [\[2307.16892\] Origin of correlated isolated flat bands in copper-substituted lead phosphate apatite \(arxiv.org\)](#)
- [2] [LK-99 - Wikipedia](#)
- [3] [\[2308.03544\] Absence of superconductivity in LK-99 at ambient conditions \(arxiv.org\)](#)

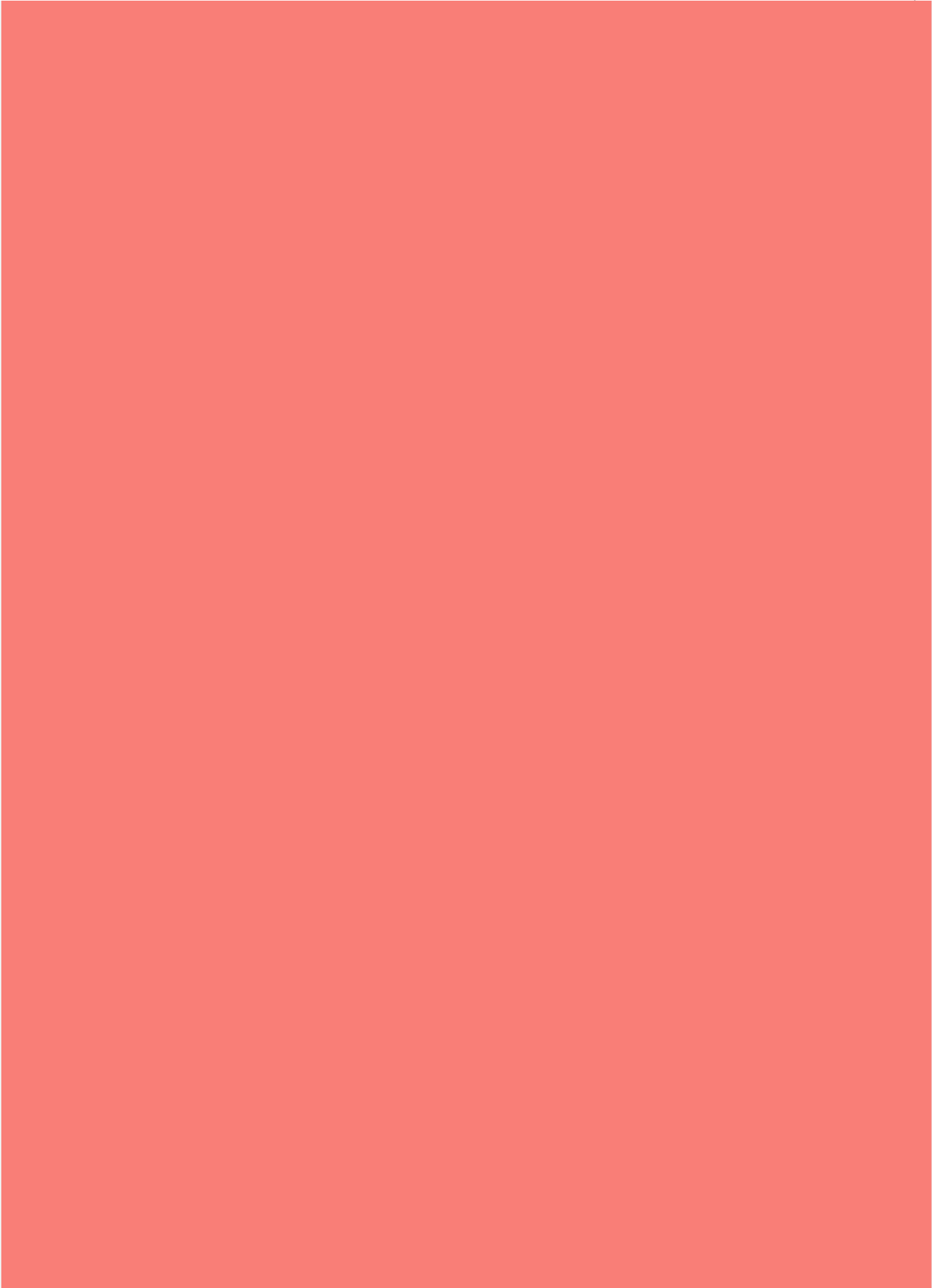


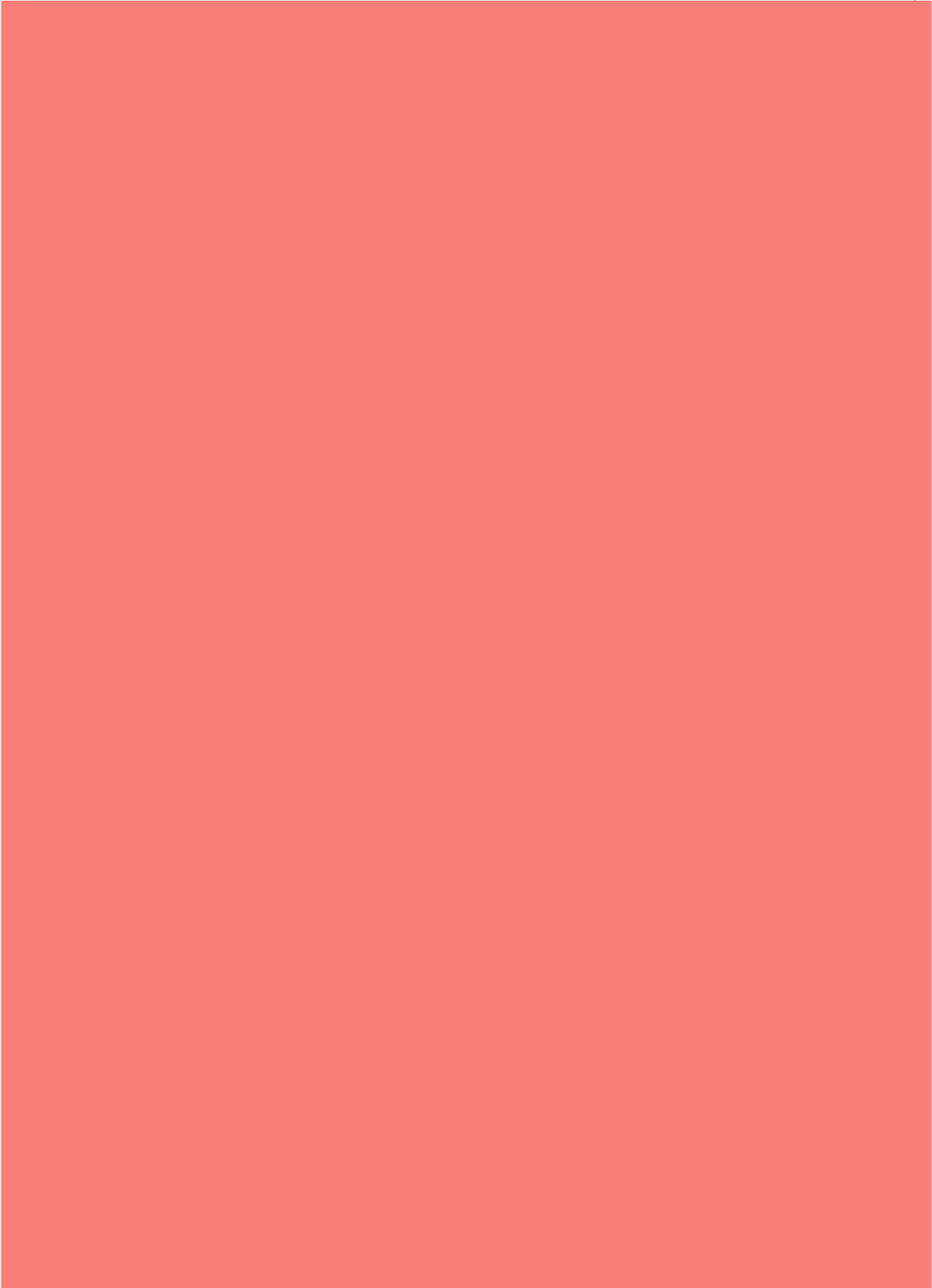
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