



Re: Crystal calculation

From CARTER FOX <cdfox@wisc.edu>

Date Tue 2/25/2025 9:30 PM

To Liu, Rui <rui.liu@anl.gov>

 1 attachment (57 KB)

NbOI2_CIF_literature.cif;

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Hi Rui,

Thanks, gold is easier for me. Here is the CIF file published by one of the main NbOI2 [papers](#). The lattice parameters are consistent with the other reported values. By looking at the reflections calculated in vesta, I find the following 2*theta angles.

- (200): 10.2272 deg
- (020): 38.7612 deg
- (112): 29.8086 deg
- (002): 20.73 deg
- (110): 19.7852 deg

Best,
Carter

Carter Fox

Dept. of Physics Graduate Student ([Xiao Lab](#))

University of Wisconsin - Madison

cdfox@wisc.edu

From: Liu, Rui <rui.liu@anl.gov>

Date: Tuesday, February 25, 2025 at 8:25 PM

To: CARTER FOX <cdfox@wisc.edu>

Subject: Re: Crystal calculation

Gold is fine, as long as we can see by eyes. Also, could you please send me the cif file?

Rui

From: CARTER FOX <cdfox@wisc.edu>

Sent: Tuesday, February 25, 2025 8:04:14 PM

To: Liu, Rui <rui.liu@anl.gov>

Subject: Re: Crystal calculation

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If we don't need the markers for finding the samples, just for marking the orientation, is nickel still necessary or can I just do Gold?

From: Liu, Rui <rui.liu@anl.gov>
Sent: Tuesday, February 25, 2025 4:28:42 PM
To: CARTER FOX <cdfox@wisc.edu>
Subject: [Attachment Removed] Re: Crystal calculation

From: Liu, Rui
Sent: Tuesday, February 25, 2025 4:21 PM
To: CARTER FOX <cdfox@wisc.edu>
Subject: Crystal calculation

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