

Hikaru Ishikura,

Attached is a compressed archive containing a Word format data sheet, a couple of png file pictures, and the CIF file for the structure of a crystal from your sample "HI-2-15". I would be grateful if you would take the sample away soon.

diffractometer time: 2 hours (JAB2220) and 3 hours (JAB2220b)

The black-and-white png picture is a simple one intended to provide a basic view of the structure. For presentation purposes I recommend that you use Mercury from the Cambridge Crystallographic Data Centre [either already on your computer or can be obtained from <https://www.ccdc.cam.ac.uk/solutions/csd-core/components/mercury/>] and use this with the CIF file to draw a colour picture in the view and style that you want.

This is not a publishable structure.

I have had a lot of trouble with this sample, and though the results attached here are the best I have been able to get, they are still very poor quality. Every crystal I tried was a twin, and despite collecting data on a second crystal using Cu radiation to spread out the spots (which typically helps with modelling twins) I was unable to get a usable structure.

What I can say is that the compound is probably your expected species, and that it appears to crystallise in a polar space group with two independent molecules (shown in pictures PL1 and PL2).

Andrew

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