Department of Chemistry X-Ray Core Facility
Publication and Co-authorship Policy

(October 2023)

The following are guidelines you should use in determining whether the crystallographer should be included as a co-author for a publication or if an acknowledgment is sufficient. These guidelines are in accord with recommendations from the American Crystallographic Association and consistent with co-authorship guidelines set forth by most academic journals.

Co-authorship

For facility run service structures: If the structural information derived from the X-ray diffraction experiment is a critical part of the intellectual content of the paper, then the crystallographer should be considered for co-authorship on the paper. This includes compounds/structures where other spectroscopy/characterization methods were ambiguous, incomplete or incorrect, structures where absolute stereochemistry was determined and essential to the paper, and structures resulting from crystals that are grown by or in consultation with the facility. The expertise of the facility is available to assist you throughout your publication efforts and our work is not finished with the issuance of the crystal structure report. We will assist with any further analysis requested or required to further enhance the content of the publication. This includes in depth discussions of the metrical data, hydrogen bonding/packing analysis, and similar structure comparisons. We will also work with you to create any additional figures and graphics you may need for publication. The facility would like to review and have the opportunity to give feedback on papers containing structures solved by the facility before the paper is submitted to the journal to check the accuracy of the crystallographic data presented.

For user collected structures: If user collected data requires considerable intervention by the facility in order to obtain a publishable structure, then the crystallographer should be considered for co-authorship on the paper. This includes crystal cutting, selection and mounting, indexing and detwinning of multi-component crystals, space group determination and solution of difficult data sets, and refinement of difficult disorder problems. As with service structures above, we will assist in any way we can to enhance the article and minimize any potential issues that may present themselves during the review process related to difficult crystallographic problems.

Acknowledgment

For facility run service structures: If the structural information derived from the X-ray diffraction experiment is not a critical part of the intellectual content of the paper, then the crystallographer only needs to be acknowledged at the end of the article. This includes compounds/structures where other spectroscopy/characterization methods were unambiguous in identifying the compound and the X-ray structure is only being used to confirm identity, connectivity, regiochemistry, and/or relative stereochemistry determined by other means. If, in these cases, a crystal structure is crystallographically interesting or novel but not central to the paper at hand, the facility may request to publish the crystal structure separately, as a joint publication with the submitting researcher/PI, in a crystallographic journal after the original article is published as to not undermine the original article.

For user collected structures: If user collected data requires minimal to moderate intervention by the facility in order to obtain a publishable structure, then the crystallographer only needs to be acknowledged at the end of the article. This includes consulting on crystal growth/quality/selection, consulting on indexing/unit cell determination, and consulting on data reduction/structure solution/final refinement/checkCIF errors.