Requirements for Depositing X-Ray Crystallographic Data

A procedure described below for submitting Crystallographic Information Files (CIFs) has been implemented for several journals:

• *Crystal Growth & Design* • *Inorganic Chemistry* • *Organic Letters* • *The Journal of Organic Chemistry*

• *Organometallics* • *Journal of the American Chemical Society*

CIF Preparation and Validation

Authors submitting work containing new, unpublished organic, metal-organic, and inorganic crystallographic data intended for publication with their manuscript must prepare this data in the Crystallographic Information File (CIF) format.

It is the responsibility of the author(s) to check all CIFs for the following prior to submission:

- Syntax errors
- Numerical self-consistency of the data
- Possible higher symmetry in the space group assignment

Two programs are recommended for validating CIFs. enCIFer syntax checks are integrated into the CCDC deposition process and a standalone version is distributed freely by the Cambridge Crystallographic Data Centre (CCDC), at http://www.ccdc.cam.ac.uk/free_services/encifer/. CIF-checking software is also available free of charge from the International Union of Crystallography, at http://checkcif.iucr.org/. CheckCIF is now available during deposition to the CCDC.

When possible, CIF errors noted in the checkCIF report should be resolved before depositing the file(s).

Depositing CIFs and Related Files

Note that CIFs, structure factor tables, and checkCIF reports must be submitted to CCDC **prior to manuscript submission.** CCDC will accept organic, metal-organic, and inorganic compounds, including extended molecular solids and also powder data where a constrained refinement has been used. Structural data for inorganic compounds will be transferred by CCDC to the Inorganic Crystal Structure Database after publication and will maintain the original deposition number(s).

Any subsequent revisions to the CIFs or structure factor tables should be deposited directly with CCDC before resubmitting the manuscript in ACS Paragon Plus.

For all other crystallographic data **that are not accommodated by CCDC (for example protein structures, nucleic acids, or metals & alloys),** authors are encouraged to deposit into other available databases (see below) in addition to uploading the data in ACS Paragon Plus during manuscript submission.

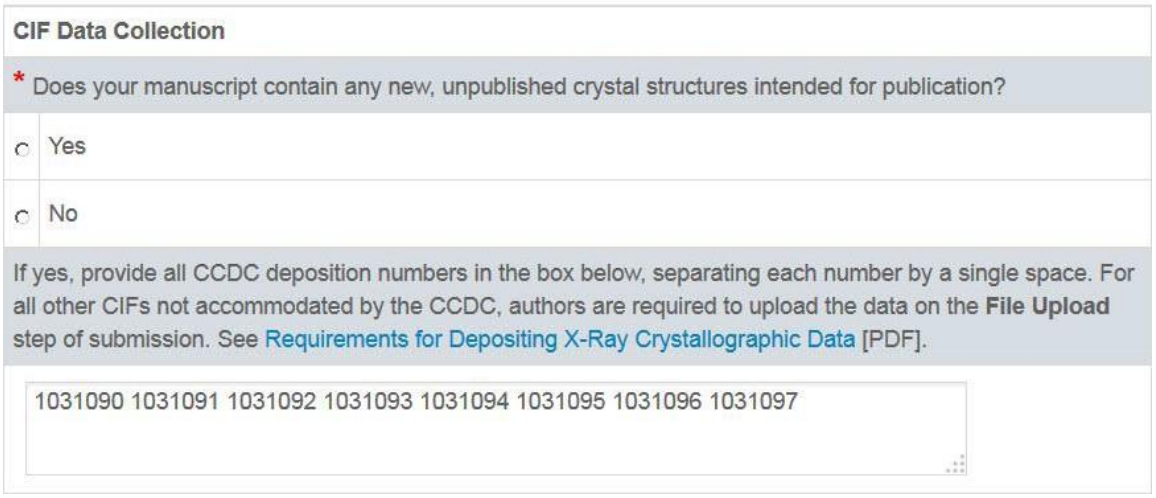
In addition, authors are required to upload the checkCIF output files (combined into one PDF file) as Supporting Information for Review Only. Any A and/or B level alerts must also be addressed prior to submission or otherwise explained in the checkCIF PDF.

Submission of CIFs and Structure Factor Tables to CCDC

To facilitate the reviewing of CIFs, ACS requires that **prior to manuscript submission,** organic, metal-organic, and inorganic CIFs must be deposited with CCDC via http://www.ccdc.cam.ac.uk/services/structure_deposit, even if text tables of crystallographic data are included with the manuscript.

In addition, authors are required to deposit structure factor tables with CCDC alongside their CIFs. Structure factor tables should include h, k, l, Fo, Fc, and σ|Fo| values. The embedded original, unmerged, uncut, unmasked hkl file must be embedded in the CIF.

Upon depositing their CIFs (and structure factor tables) with CCDC, authors will be provided with a CCDC deposition number for each CIF. This number must be entered into ACS Paragon Plus when prompted during the submission process, as shown below.



List of Other Databases

For all other crystallographic data that are not accommodated by CCDC, authors are encouraged to deposit into one of the following databases in addition to uploading the data in ACS Paragon Plus along with the manuscript submission, as Supporting Information. Please indicate whether the other crystallographic data is intended for publication or for review only.

- Protein Data Bank (PDB) for polypeptides and polysaccharides with more than 24 units (http://www.rcsb.org/pdb/)
- Nucleic Acids Data Bank for oligonucleotides (http://ndbserver.rutgers.edu/)
- International Centre for Diffraction Data (ICDD) for powder diffraction data without atomic coordinates (http://www.icdd.com/)
- Incommensurate Structures Database (ICSDB) for incommensurate modulated and composite structures (http://www.cryst.ehu.es)

Peer Review and Acceptance

While the manuscript is undergoing peer review, the CIFs and structure factor tables will be held confidentially in CCDC's archive where they will be accessible only by ACS and reviewers during the peer review process. If the manuscript is accepted and published, ACS will notify CCDC and the data will be released from embargo where it will then be freely accessible through CCDC, via direct link(s) in the article when it is published online.