

Requirements for X-ray crystal structures

Before submitting a manuscript containing X-ray crystal structure(s), authors are advised to check the consistency and integrity of crystal structure determination by using the CHECKCIF routine on the web site of the International Union of Crystallography (<http://checkcif.iucr.org/>).

Prior to submission of the manuscript to the journal, the author(s) must deposit crystallographic data with the Cambridge Crystallographic Data Centre (CCDC), so that data may be accessed by the referees and checked as part of the refereeing process. The data should be sent in CIF format (excluding structure factors) by e-mail to: deposit@ccdc.cam.ac.uk. In general, author(s) will receive within three working days a summary report containing a CCDC deposition number(s), which should be included with the following standard text in the manuscript:

"CCDC nnnnnn contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif".

Data for inorganic compounds (i.e. those with no C-H bonds) should be deposited with the Fachinformationszentrum Karlsruhe. Data in CIF format should be sent by e-mail to crysdata@fiz-karlsruhe.de. Within a few days, author(s) will receive an answer containing the deposition number(s) which should be included in the manuscript by using the following text:

"Further details of the crystal structure investigation(s) may be obtained from Fachinformationszentrum Karlsruhe, 76344 Eggenstein-Leopoldshafen, Germany (fax: (+49)7247-808-666; e-mail: crysdata@fiz-karlsruhe.de, http://www.fiz-karlsruhe.de/request_for_deposited_data.html) on quoting the CSD-nnnnnn."



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