

Subject: Cif files with incorrect set of group operators

From: Steef Boerrigter <sxmboer@gmail.com>

Date: 2023-02-22 10:07

To: Saulius Gražulis <grazulis@ibt.lt>

Dear Saulius,

My implementation of a cif reader double-checks if the H-M symbol is consistent with the given operators; if they are given. It checks if the International table is consistent etc. What I also want to do is, if a cif only has operators, I want to be able to deduce the spacegroup symbol. Of course, oftentimes the space group is given in non-conventional settings and that leads to bad results. Decomposition of the operators should be an iron-clad test to see if the symmetry is correct.

An iron-clad test to see if the operators are self-consistent is to apply each operator to each other operator which in each case should produce an existing operator. I ran this test on all the database entries and it failed in (only!) 15 cases. In most cases there are missing operators, which means that software that relies on the operators directly will have missing atoms in the unit cell. In other cases, it is clear that the authors attempted to manually edit the spacegroup symmetry operators, but made some mistake in doing so.

I manually went through each case and fixed the issue in a way that requires the least amount of edits to make clear exactly where the mistake was made -- as opposed to just completely replacing the entire operator block.

I have added a diff file of (today's) database entry with the fixed version of the cif. The diff file includes my analysis of what went wrong with the operators. I am also including the fixed cif files.

I used Mercury to view these files. I learned that mercury will typically use the operators, but when the group is incomplete will ignore the symmetry altogether and use the Herman-Mauguin symbol in its favor.

Best Wishes,
Steef Boerrigter

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—Attachments:—

not_closed_fixes.diff	6,6 KB
2003882.cif	7,8 KB
2001551.cif	6,5 KB
2000246.cif	2,9 KB
2003347.cif	9,1 KB
2000404.cif	4,9 KB
2102130.cif	7,3 KB

2006998.cif	11,3 KB
2007181.cif	16,6 KB
2004188.cif	10,1 KB
2004351.cif	6,8 KB
2105675.cif	8,4 KB
2105555.cif	5,7 KB
2105676.cif	9,3 KB
4062540.cif	9,5 KB
8101007.cif	14,9 KB