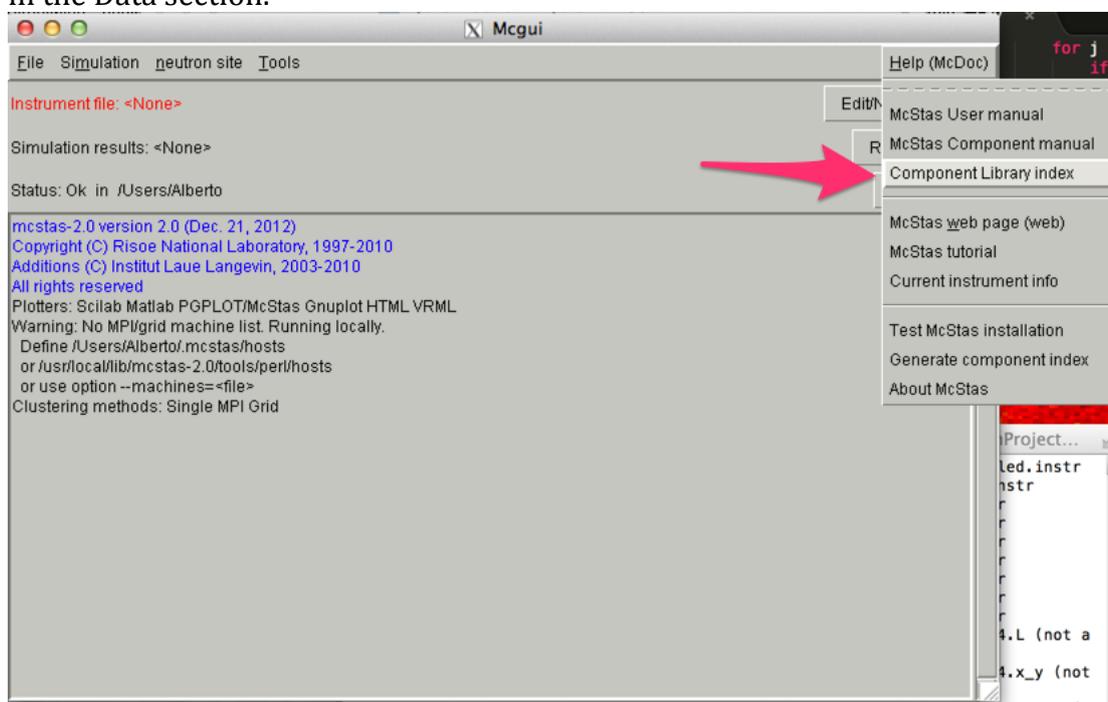


How to make a new .lau file for use with Single_crystal.comp, PowderN or Isotropic_Sqw – by Alberto Cereser & Peter Willendrup, DTU Fysik

- 1) Check that the .lau file is not already available in McStas. To do so, open a mcgui window, and select Help → Component Library index. Then check in the Data section.



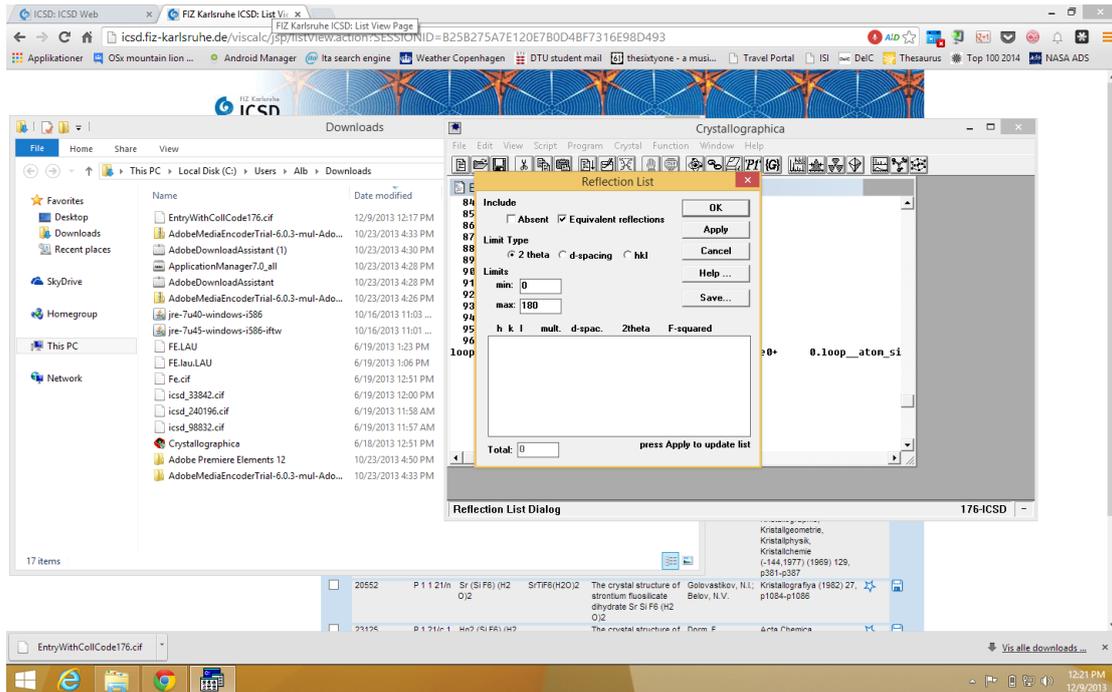
- 2) Install Crystallographica (<http://www.oxcryo.com/cg/crystallographica/>). Crystallographica is for Windows only, so in case you are working with Linux or OSX you should first install a virtual machine running Windows, or use Wine (<http://www.winehq.org/download>);
- 3) In the ICSD database (<http://www.fiz-karlsruhe.com/icsd.html>), look for the crystalline structure you want to study and download the .cif file.



The screenshot shows the ICSD database search results page. The page header includes 'FIZ Karlsruhe ICSD' and 'Welcome to ICSDWeb. IP authenticated (130.225.86.216)'. The search results are displayed in a table with columns: Coll. Code, HMS, Struct. Form., Struct. Type, Title, Authors, and Reference. A red arrow points to the download icon (a small blue square with a white document icon) in the rightmost column of the table.

Coll. Code	HMS	Struct. Form.	Struct. Type	Title	Authors	Reference	
176	C 1 c 1	Si O2	SiO2(mS144)	Kristallstruktur des monoklinen Tief-Tridymits	Kato, K.; Nukui, A.	Acta Crystallographica B (24, 1968-38, 1982) (1976) 32, p2488-p2491	
1109	C 1 c 1	Si O2	SiO2(mS144)	Silicon-oxygen bond lengths, bridging angles Si-O-Si and synthetic low tridymite	Baur, W.H.	Acta Crystallographica B (24, 1968-38, 1982) (1977) 33, p2615-p2619	
4393	C m c m	Ca0.07 (Al0.1629 Si0.8375 O2)	Mordenite-frame	Position of cations and molecules in zeolites with the mordenite-type framework. I. Dehydrated Ca-exchanged ptilolite	Mortier, W.J.; Pluth, J.J.; Smith, J.V.	Materials Research Bulletin (1975) 10, p1037-p1046	
9160	P 42/m n m	Si O2	TiO2(tP6)	Rutile-type compounds. VI. Si O2, Ge O2 and a comparison with other	Baur, W.H.; Khan, A.A.	Acta Crystallographica B (24, 1968-38, 1982) (1971) 27, n2133-n2139	

- 4) Import the file in Crystallographica (File → Import CIF)
- 5) Select Crystal → Radiation → Neutron, and put the lower considered wavelength (this is required to indicate the resolution)
- 6) Select Crystal → Reflections. We suggest to select “Equivalent reflections”. This is however only needed if you intend to use the .lau file with Single_crystal.comp



- 7) Save the obtained file as .dat.
- 8) Open a mcgui window, and select Help → Component Library index. This will return a list of .lau files. Select one, and copy the header on the top of your .dat file. Correct the variables for the material you are using, and save the resulting file as .lau
- 9) Save a copy of your .lau file in the same folder of the .instr file you are working with.