

## Computer Programs Developed for Research Purposes

All these executables have been developed using Fortran77 and Visual Fortran compilers by Dr. R. Saravanan - (IUCr ID: IUCr3611) <http://www.iucr.org/iucr-top/wdc/> You may need a library file 'salflibc.dll' (click to download) to run these executables.

**GUI versions of many of these programs are also available.** Most of these programs are available at the SINCRIS Software database of the IUCr (International Union of Crystallography) in their website (<http://www.iucr.org/>).

**Program 1 (sfac331)** (GUI Available) - For the generation and calculation of the X-ray structure factors and the real and imaginary parts of the structure factors of any crystalline system. **Program 2 (asf88)** (GUI Available) - For the generation and calculation of the X-ray structure factors and the real and imaginary parts of the structure factors of any crystalline system. **Program 3 (sara11)** - Program for the refinement of various parameters of III-V and II-VI semiconductors (ZnS and elemental (diamond) semiconductors. To refine parameters in the harmonic, anharmonic and charge transfer approximations. Refines individual thermal, scale, extinction parameters and the charge transfer from one atom to the other in ZnS type structures. Calculates the real and imaginary phase parts FA and FB of the structure factors. Includes Bijvoet differences in the analysis. Averages the Bijvoet equivalent reflections, etc., etc. **Program 4 (caf2\_ha)** - For CaF<sub>2</sub> structures program to refine parameters in the harmonic approximation. refines individual thermal, scale, extinction parameters in CaF<sub>2</sub> type structures. **Program 5 (caf2\_an)** - For CaF<sub>2</sub> structures program to refine parameters in the anharmonic approximation. refines individual thermal, scale, extinction parameters in CaF<sub>2</sub> type structures. **Program 6 (nacl)** - For NaCl structures program to refine parameters in the harmonic approximation. refines individual thermal, scale, extinction parameters in NaCl type structures. **Program 7 (dremablp)** (GUI Available) - For the data reduction. Single crystal data reduction program. Corrects Lp, and absorption. Applicable to any system. To single crystal spheres. Converts the uncorrected structure factors into Lp and absorption corrected structure factors. **Program 8 (scat771)** (GUI Available) If you have a set of h k l values and powder intensities, you would like to apply Lp and multiplicity corrections for any point group, and convert the intensity data into corresponding structure factors. You may want to calculate the structure factors for the supplied set of h k l values. You may want to correct the structure factors for anomalous dispersion effects for 10 different wavelengths. You may want to calculate the real and imaginary parts of the structure factors. You may want to calculate the sin(theta)/lambda values and the atomic scattering factors of all the atoms that you specify in your structure. You can do all these tasks with this program. Any number atoms (from 212 different kinds of atoms/ions) can be handled in your structures. The program can be wisely used for multiple tasks. There are options to suppress the application of multiplicity correction and absorption correction individually or in combination. Also, simulation of structure factors for a given set of h k l values can be done. No need to supply analytical coefficients, dispersion corrections – all data are pre-connected. Atom names and some preliminary info enough. **Program 9 (cubindex)** Applicable to cubic systems only (!). Many indexing programs for a general crystallographic system are freely available nowadays. Many of them do the indexation

only. This program (at present only for cubic systems), does many useful additional tasks. It does the following; Indexes cubic reflections. Finds the d values if not given. Finds the cell constant. Fits it to a straight line (no graph) using Nelson-Riley function. Gives least-squares results of N-R analysis. Applies multiplicity and polarization corrections to observed powder intensities. Converts them into structure factors. Calculates atomic scattering factors of each element in the system. Calculates the corresponding structure factors. Calculates the real and imaginary parts of the structure factor of each reflection. Does a Wilson-plot analysis using Fobs and Fcal. Gives the least squares results of Wilson plot. Efficient use can result in several information of your system. **Program 10 (datared)** (GUI Available) - Similar to the program dremablp (program 7). If the input is in the form of - left background intensity - peak intensity - right background intensity, you can use this program Program for the data reduction. Single crystal data reduction program. Corrects Lp, absorption and background intensities. Applicable to any system. To single crystal spheres. Converts the uncorrected structure factors into Lp, absorption and background corrected structure factors. **Program 11 (reduce)** (GUI Available) Program reduce - (similar to the program datared (program 10). If the input is in CAD-4 format, u can use this program. Single crystal data reduction program. Corrects Lp, absorption and background intensities. Applicable to any system. To single crystal spheres. Converts the uncorrected structure factors into Lp, absorption and background corrected structure factors.

These programs can be downloaded and used without any charges and warranties. If you use any of these programs, just give me a mail ([saragow@dataone.in](mailto:saragow@dataone.in)) informing me which program you are using.

Other GUI software programs are ;

[Pri1d\\_3\\_win](#) (See GUI Programs)

[sfac331\\_mix](#)

[CMTM4](#)

[sfac332](#) (Similar to sfac331\_mix. But fractional atomic coordinates can be supplied through a file too. Good for normal as well as mixed systems).