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This Week's Citation Classic

Busing W R, Martin K O & Levy H A. *OR FLS, a FORTRAN crystallographic least-squares program.* Oak Ridge, TN: Oak Ridge National Laboratory, August 1962, ORNL-TM-305. 75 p.
[Chemistry and Mathematics Divisions, Oak Ridge National Laboratory, Oak Ridge, TN]

This report describes a computer program to perform the least-squares refinement of crystal structure parameters based on x-ray or neutron diffraction measurements. The program is written mostly in the FORTRAN language to facilitate modification and to permit its use on various machines. Detailed instructions for its use are included, and the required card decks may be obtained from the authors. [The *SCI*® indicates that this paper has been cited over 3,035 times since 1962.]

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"Crystallographers measure the intensities of many x-ray or neutron reflections from a crystal (sometimes several thousand) and use various techniques to deduce the approximate atomic arrangement. Finally, the structure is refined by adjusting the coordinates of the atoms and parameters which describe their thermal motion so as to produce the best agreement between observed and calculated intensities. Our 1962 report describes a least-squares computer program for performing this refinement.

"I arrived at Oak Ridge National Laboratory in 1954 and began learning crystallography, neutron diffraction, and computing from Henri Levy. We had access to the ORACLE, a vacuum tube computer with 1,024 40-bit words of cathode-ray tube memory and paper tape input and output. Programming was done in hexadecimal machine language. We wrote a least-squares program to refine the two coordinates and six temperature factors of calcium hydroxide[1] based on 53 neutron diffraction intensities. We then generalized this program to handle other problems under study at Oak Ridge. It was capable of adjusting a maximum of 30 parameters, and when they doubled the memory to 2,048 words, we were able to increase this number to 54.

"Following the acquisition of an IBM 704 with 8 k words of memory in 1957, we rewrote the program for that machine using assembly language. A computing conference at the National Bureau of Standards in November of that year made it clear that many crystallographers had access to this machine, so we made binary card decks available to them and wrote a report[2] with instructions for its use.

"In 1961, with the arrival of the IBM 7090, and with other computers on the horizon, it became apparent that it would be worth rewriting the program in FORTRAN. Kay Martin of the mathematics division worked closely with us and did the actual programming and testing. Again, a report was written to provide instructions, and this is the work which has been highly cited. The program has been greatly improved by various users so that the present version lists nine coauthors. It is often used to adjust from 200 to 400 parameters. Instructions are now included as part of the source program, so the users generally identify it by citing the 1962 report. Apparently it has been successful because it is a versatile program with test examples and clear instructions, and because it performs a job which is routinely needed.

"We have sent out 395 copies of the program on request, and there has been much indirect propagation. There have been several newer least-squares programs developed by other authors,[3] often incorporated into comprehensive crystallographic computing systems. Nevertheless, we still get requests for this program, 59 since 1975."

1. **Busing W R & Levy H A.** Neutron diffraction study of calcium hydroxide. *J. Chem. Phys.* **26**:563-8, 1957.
2. ——————————. *A crystallographic least squares refinement program for the IBM 704.* Oak Ridge, TN: Oak Ridge National Laboratory, April 1959, ORNL-CF-59-4-37. 138 p.
3. **Stewart J M,** ed. *The X-ray system of crystallographic programs.* College Park, MD: Computer Science Center, University of Maryland, March 1976, TR-445. 232 p.

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