

James Ibers, One of the Pioneers of Modern Crystallography

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Because Jim Ibers so strongly emphasized his contributions to chemistry, his many contributions to crystallographic practice in the early part of his career are often overlooked.

An overview of them will be given.

Jim's Ph.D. work with the legendary Verner Schomaker focused on structure determination by gas-phase electron diffraction; but Jim also calculated electron scattering amplitudes and published a paper about a crystal structure. During his 1954-55 postdoc with John Cowley at the CSIRO in Melbourne Jim used a combination of electron diffraction and powder diffraction to study graphite intercalated with FeCl₃. During 1957-62 he published 15 articles in *Acta Cryst.* based on work he did as an employee of the Shell Development Company in Emeryville, CA.

In 1962 Jim moved to Brookhaven National Lab where he, Walter Hamilton, and Sam La Placa demonstrated that crystal structures could be determined, at least by experts, in a semi-routine way. They developed methods and procedures as they went along; Jim was later recognized as having compiled and integrated an excellent collection of crystallographic software. Data were still mostly collected using film, but later they had a GE quarter-circle diffractometer.

Jim moved to Northwestern University in 1965, where he was a professor (later an emeritus professor) for more than 55 years. There he published nearly 800 papers for a total of *ca.* 870 that have been cited nearly 46,000 times. His name is linked to 640 CSD refcodes and 723 ICSD entries. He mentored dozens of students and postdocs, many of whom went on to establish their own crystallographic labs.

Jim contributions to crystallographic methodology also include co-authoring two tables of structure factors in Vol. III of the "Red Series" of *International Tables*, and editing, with Walter Hamilton, Vol. IV of that series. Jim was involved in planning Vol. I, and claimed to have been responsible for protecting the *b*-unique setting of monoclinic space groups. He wrote software for dispersion corrections and for group refinement. As an editor of *Inorg. Chem.* (1965-79) he set the standards for publication of crystal structures in the chemical literature.

Among crystallographers Jim sometimes referred to himself as the Practicing Crystallographic Idiot, which he most certainly was not. That moniker allowed him to ask simple but penetrating questions about what we do and why we do it. It also revealed his dry sense of humor.