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Jerome Karle

Jerome Karle, corecipient of the 1985 Nobel Prize in Chemistry for his contributions to the solution of the crystallographic phase problem, died on 6 June 2013 in Annandale, Virginia. His Nobel feat of physical insight and mathematical power put him into the upper echelon of the greatest scientists of his generation.

Born in Brooklyn, New York, on 18 June 1918, Jerome was raised on Coney Island, for which he retained a lasting affection. He was educated in the New York City public school system and then attended City College of New York. Herbert Hauptman, who graduated with Jerome in 1937, shared the Nobel Prize with him.

Jerome attended Harvard University and received a master's degree in biology in 1938. He spent two years in Albany, New York, working at the state's medical laboratory, where he developed a way of monitoring the concentration of fluorine in the water supply. He then entered the University of Michigan's PhD program in chemistry. In one physical chemistry laboratory class, in which lab partners were assigned alphabetically, he was paired with Polish American student Isabella Lugoski. They would subsequently marry while they were still students. Jerome and Isabella both obtained their PhD degrees with Lawrence Brockway and became experts in the electron diffraction field. That work would later be significant to Jerome's contributions to x-ray structures.

Finishing their PhDs during World War II, the Karles joined the Manhattan Project at the University of Chicago and worked in different research areas of plutonium chemistry. Shortly after the war, they joined the US Naval Research Laboratory (NRL) in Washington, DC. Most of their early work at the NRL was devoted to electron diffraction. Among Jerome's contributions was a new electron diffractometer design that was a considerable advance over machines of the day.

In the early 1950s the phase problem in crystallography was thought to be mathematically impossible to solve, but Jerome and Hauptman realized they could. A typical crystallographic experiment records the direction and intensity of x rays scattered by a crystal. The measured intensity is the square of the structure factor, the Fourier transform of the electron density. One might thus expect that the electron density could be

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obtained by reverse Fourier transform; the peaks in the electron density would correspond to positions of atomic nuclei. But the phase problem arises because the structure factor is a complex quantity. And once the complex structure factor is squared, the phase information is lost. Without the phases, the reverse Fourier transform cannot be constructed to obtain the electron density and the molecular structure.

Jerome and Hauptman realized that the problem is in fact overdetermined: The number of measured data typically far exceeds the number of parameters defining the positions of all the atoms in the crystal's unit cell. But if overdetermined, then a solution must be possible. Ultimately, that solution was found by means of inequalities that hold among the structure factors. Importantly, such inequalities were derivable from a condition that Jerome had employed in his early analysis of electron diffraction data: the mathematical constraint that the electron density must be everywhere positive.

Jerome and Hauptman wrote the mathematical conditions to solve the phase problem, and they announced the same in a 1953 monograph with a title that must have seemed surprising—*The Solution of the Phase Problem I: The Centrosymmetric Crystal*. The mathematics was one thing, but its use to actually show it would lead to solved crystal structures was quite another. Isabella applied the mathematical inequalities to her x-ray measurements and solved structures no one else could. And thus the phase problem of crystallography was solved, theoretically and experimentally. Jerome felt strongly that Isabella's experimental work should have been recognized by her sharing in the Nobel Prize. She was not the first woman or the last to be overlooked by the Nobel committee.

It is difficult now to realize the impact on the world of crystallography by the claim that the phase problem was solved. Jerome summarized it in his official Nobel autobiography: "A large number of fellow-scientists did not believe a word we said." Despite the atmosphere of disbelief, NRL officials never wavered in their steadfast support of the Karles and their work. Jerome insisted that the NRL's support was critically important to the ultimate success of their research.

Jerome learned of his Nobel Prize in a dramatic way on board a Pan American flight from London to Washington, DC, on 16 October 1985. Captain James Green broadcast the announcement: "We are honored to have flying with us today America's newest Nobel Prize winner, and he doesn't even know it." Then the captain invited Jerome to move up to first class.

At the NRL Jerome established the Laboratory for the Structure of Matter in 1968. Dozens of colleagues worked there with him over many years, principally on some aspect of molecular structure, and many deeply appreciated him. He displayed to people an enormous kindness that reflected a natural extension of the love he showed for his own family.

Jerome was always a steady, hard worker. Arriving at the lab, he would often stop at the office of one of us (Huang) to go over work he had taken home the night before. At day's end he would usually stop again to discuss the day's progress. Late into his career he invented with us the field of quantum crystallography, in which x-ray data are used to represent the quantum state of the electrons. Our last paper, published with Jerome after his retirement in 2011, was on using quantum mechanics to predict the explosive properties of high-energy, high-density molecules.

Jerome was more than a great scientist—he was a great man. The Nobel Prize did not change that at all. To us, no characteristic was more manifest than his humility. Despite the importance of his scientific contributions, he led a life of simplicity and modesty. He always made those speaking with him feel comfortable, important, and equal. Jerome's humanity is something to wonder over and emulate.

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