

FOR RELEASE: IMMEDIATE

Contact: Bob McGill



Mailed March 9, 1981

YOUNGSTOWN, Ohio - Youngstown State University faculty member Dr. Janet E. DelBene, Girard, was notified recently that she had authored a "classic."

This was a technical, scientific research report. While it's not yet a classic in the sense of music, art, a fashion style or a horse race of champions, it already is a very important milestone in quantum chemistry.

Dr. DelBene, professor of chemistry, was notified by the Institute for Scientific Information (ISI) that her paper on the CNDO/S Method in Spectroscopy "is one of the most frequently cited papers in its field."

Citation of a scientific paper is its use by others as an example, reference or precedent.

According to ISI, "This usually indicates that the cited work has made a significant contribution to the development of scientific knowledge in its field, and has had a lasting effect on the whole of science."

On the average, ISI says, a science paper is cited about four times a year.

Dr. DelBene's paper, which she did as a thesis problem for part of her Ph.D. work in 1968 at the University of Cincinnati, has been cited more than 530 times since it was published in the "Journal of Chemical Physics" that year.

The paper was done in association with Dr. H. H. Jaffe of the University of Cincinnati Chemistry Department.

Because of the wide use and reference to her paper, ISI asked Dr. DelBene to write a brief commentary from a personal standpoint on the background of the research problem, the circumstances surrounding the work, and why her research report is so frequently cited. Her commentary was used as the "Science Citation Classic" feature in the Feb. 16 issue of ISI's "Current Contents."

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In 1966, Dr. DelBene reports, there was a need for a reliable method to calculate the energies of excited electronic states of organic molecules. Dr. Jaffe suggested this as a thesis problem, and although some warned it was a very difficult one, she forged ahead.

The first results after writing and debugging a CNDO computer program were "tangled as badly as a Gordian knot." The successful CNDO/S method came into being only after she subsequently spent six nights a week for three months working it out on computers.

According to Dr. DelBene, her research method is being widely used because it has proven reliable for predicting transition energies in a wide variety of chemical systems; because the computer transition energies have been found to correlate well with various molecular properties; and because the basic methodology in her work has been extended to other important problems.

"It was the right time and we had the right pieces," Dr. DelBene said, adding that unraveling this research problem opened the door for others to solve many related problems.

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NEWS BUREAU
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80 - 237
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YOUNGSTOWN, Ohio - Opera conductor, John DeMain, a native of Youngstown, will speak about his career as part of Youngstown State University's Special Lecture Series at 2 p.m. Thursday, March 12, in Ford Auditorium, Bliss Hall.

The event is free and open to the public.

Mr. DeMain, winner of many honors, is the musical director of the Houston Grand Opera. He is returning here to direct the Youngstown Symphony Society presentation of Gounod's "Faust" March 13 and 14 in Powers Auditorium.

The Special Lecture Committee is made up of administratively appointed administrators, faculty and student representatives.

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NEWS BUREAU
80 - 238