



2002 IOTA SIGMA PI HONORARY MEMBER AWARD

Professor Janet E. Del Bene, Youngstown State University

Professor Janet E. Del Bene is the **2002 recipient of the Iota Sigma Pi Honorary Member Award**. This is the highest honor that Iota Sigma Pi bestows on outstanding women chemists.

Dr. Del Bene is currently a professor emeritus of chemistry at Youngstown State University. She also holds the position of Adjunct Professor at the Quantum Theory Project, University of Florida, and is currently a BBV Foundation Visiting Fellow at the University of Madrid, Spain. Dr. Del Bene developed CNDO/S, a semi-empirical method for computing electronic excitation energies. Her work with Dr. John Pople led to the prediction of the structures of the hydrogen-based to hydrogen-bonded complexes $(\text{H}_2\text{O})_2$ and $(\text{HF})_2$ and the intermolecular potentials for pairs of HF and H_2O molecules. Her work led to the development of an ab-initio-based model of the hydrogen bond which identified the lone pair and the linear hydrogen bond as primary

structure-determining factors. She performed some of the early studies on hydrogen-bonded complexes containing nucleic acid bases.

Dr. Del Bene has carried out systematic studies of basis set and correlation energy effects on the computed binding energies of neutral, positive-ion, and negative-ion hydrogen-bonded complexes and of the proton affinities and lithium-ion affinities of bases. Recently, she has undertaken detailed studies of the infrared spectroscopic properties of the hydrogen-bonded complexes, with emphasis on the red shift and the increase in the intensity of the X-H band upon formation of the X-H...B hydrogen bond. She has classified hydrogen bonds as traditional, ion-pair, and proton-shared and has demonstrated a relationship between hydrogen-bond type and the computed infrared spectrum. She has studied the NMR properties of hydrogen-bonded complexes. In her collaboration with Dr. Meredith Jordan and Dr. Rodney Bartlett, Dr. Del Bene has demonstrated relationships among the X-Y distance in the X-H-Y hydrogen bond, the proton NMR chemical shift, the anharmonic proton-stretching frequency, and the X-Y spin-spin coupling constant.

Dr. Del Bene has obtained 10 grants totaling 1.53 million dollars, given 43 papers, and published 153 papers. She has given 23 invited talks. Her professional experience includes consulting for Goodyear Tire and Rubber Company and to the National Institutes of Health. She has received NIH and NSF fellowships. In 1972, Dr. Del Bene was awarded the Agnes Fay Morgan research award from Iota Sigma Pi.