

## Biography of Roald Hoffmann

Roald Hoffmann was born in a Polish Jewish family in Złoczów, Poland (now in the Ukraine), on July 18, 1937, the son of Clara (Rosen) and Hillel Safran. He later became the stepson of Paul Hoffmann. Having survived the Nazi occupation, in 1946 he left Poland with his family for Czechoslovakia, Austria, Germany and arrived in the U.S.A. on February 22, 1949, at the age of 11. He continued his primary education in New York City (P.S. 93 Queens, P.S. 16 Brooklyn) and graduated from Stuyvesant High School there in 1955. In the same year he became a naturalized citizen of the U.S.A. He entered Columbia College in New York as a Pulitzer Free Scholar and received his B.A., summa cum laude, majoring in chemistry, in 1958. During the summers of his college career he worked at the National Bureau of Standards with E. S. Newman on the thermochemistry of cement compounds and with R. E. Ferguson on the pyrolysis of hydrocarbons. He also spent a summer with J. B. Cumming at Brookhaven National Laboratory working on the  $C^{12}(p,pn)C^{11}$  reaction.

Roald Hoffmann began graduate study at Harvard University in 1958, obtaining a M.A. in physics in 1960 and a Ph.D. in chemical physics in 1962. His thesis work was done under the joint supervision of Martin Gouterman and William N. Lipscomb and dealt with the molecular orbital theory of polyhedral molecules, particularly boron hydrides, and with the application of second quantization methods to the study of excited states of helical polymers. The latter work was the product of a nine-month stay at Moscow University in the USSR during the academic year 1960-61. This stay was under the auspices of the graduate student exchange between the U.S.A. and the USSR. At Moscow University Dr. Hoffmann worked with A. S. Davydov on exciton theory.

In 1962 R. Hoffmann was elected a Junior Fellow in the Society of Fellows of Harvard University. He remained in this position until 1965. During this period he developed further a semiempirical method of calculation of the electronic structure of molecules, the extended Hückel method, as a direct outgrowth of thesis work on the boron hydrides with W. N. Lipscomb. Through the encouragement of E. J. Corey, he became interested in structural and mechanistic problems in organic molecules. At the end of this stay at Harvard he began his collaboration with R. B. Woodward on the theory of concerted reactions.

In 1965 Dr. Hoffmann joined the Department of Chemistry at Cornell University as Associate Professor of Chemistry. In 1968 he was appointed Professor of Chemistry in the same department, and in 1974 he became the John A. Newman Professor of Physical Science. Since 1996 he is the Frank H.T. Rhodes Professor of Humane Letters, and a Professor of Chemistry.

Dr. Hoffmann received the 1969 American Chemical Society Award in Pure Chemistry sponsored by Alpha Chi Sigma; the 1969 Fresenius Award of Phi Lambda Upsilon; the 1969 Harrison Howe Award of the Rochester Section of the American Chemical Society, and the 1970 Award of the International Academy of Quantum Molecular Sciences. In 1973 Dr. Hoffmann,

jointly with R. B. Woodward, received the first Arthur C. Cope Award in Organic Chemistry from the American Chemical Society. Dr. Hoffmann received the 1974 Pauling Award of the Puget Sound and Oregon Sections and the 1981 Nichols medal of the New York Section of the American Chemical Society. In 1981 he shared the Nobel Prize in Chemistry with Kenichi Fukui. In 1982 he received the ACS Award in Inorganic Chemistry sponsored by the Monsanto Company. In 1983 he was awarded the National Medal of Science, and in 1986 the Dickinson College Award in memory of Joseph Priestley and the National Academy of Sciences Award in the Chemical Sciences. In 1990 he received the Priestley Medal of the American Chemical Society, its highest honor. In 1991 Dr. Hoffmann received the first (and last) Gold Medal in honor of N.N. Semenov, awarded by the Academy of Sciences of the USSR. In 1994 he received the Centennial Medal of the Graduate School of Arts and Sciences of Harvard University. In 1996 he received the Pimentel Award in Chemical Education of the American Chemical Society. In 1997 Dr. Hoffmann received the first Elizabeth A. Wood Science Writing Award of the American Crystallographic Association. In 1998 Prof. Hoffmann received the Jawaharlal Nehru Birth Centenary Award of India. In 1999 he was made an Honorary Member of the German Chemical Society, and in 2002 he was made Honorary Member of the Chemical Society of Japan. In 2006 he received the Gold Medal of the American Institute of Chemists.

In 1977 Dr. Hoffmann received an honorary Doctor of Technology degree from the Royal Institute of Technology, Stockholm, Sweden, on the occasion of their 150th anniversary. He has been awarded honorary Doctor of Science degrees from Yale University (1980); University of Hartford (1982); Columbia University (1982); City University of New York (1983); University of Puerto Rico (1983); Universidad de la República-Uruguay (1984); University of La Plata, Argentina (1984); SUNY at Binghamton (1985); Colgate University (1985); Univ. of Rennes, France (1986); Ben Gurion University of the Negev, Beer Sheva, Israel (1989); Lehigh University (1989); Carleton College (1989); University of Maryland (1990); University of Arizona (1991); Bar-Ilan University (1991); University of Central Florida (1991); University of Athens (1991); University of Thessaloniki (1991); University of St. Petersburg (1991); University of Barcelona (1992), Ohio State University (1993), Northwestern University (1996), The Technion (1996), Brandeis University (1997), Georgetown Univ. (2000), Durham University (2000), Luther College (2001), Gustavus Adolphus College (2001), Nagoya University (2003), Duke University (2005).

Professor Hoffmann has been a Centenary Lecturer of the Chemical Society, the John William Draper Lecturer at Hampden-Sydney College, the Corn Products Lecturer at Pennsylvania State University, the Lucy Pickett Lecturer at Mt. Holyoke College, the 3M Lecturer at the University of Minnesota, the Steward Lecturer of Notre Dame, the Venable Lecturer at the University of North Carolina, the Arthur D. Little Lecturer at Northeastern University, the Centennial Lecturer at Loyola University, the Seydel-Wooley Lecturer at Georgia Tech, the Friend E. Clark Lecturer at the University of West Virginia, The Werner Lecturer at the University of Kansas, the Lind Lecturer of the East Tennessee Section of the American Chemical Society, the Killpatrick Lecturer at Illinois Institute of Technology, the American Cyanamid Lecturer at the University of Connecticut, the Walker-Ames Lecturer at the University of Washington, the first Jeremy Musher Lecturer at Hebrew University, Jerusalem, the Barton Lecturer at the University of Oklahoma, the FMC Lecturer at Princeton, the Renaud Lecturer at

Michigan State University, the Abbott Lecturer at the University of North Dakota, the Five College Lecturer, the Merck Lecturer at Rutgers, the Sherwin-Williams Lecturer at the University of Illinois, the Falk-Plaut Lecturer at Columbia, the G. N. Lewis Lecturer at the University of California at Berkeley, the Phi Lambda Upsilon Rho Chapter Lecturer at the University of Nebraska, the Liebig Lecturer at the University of Colorado, the Remsen Lecturer at Johns Hopkins, the Camille and Henry Dreyfus Distinguished Lecturer at Rice University, Carleton College, Bryn Mawr College, Dartmouth College, Franklin and Marshall College, University of Wisconsin, The Silliman Lecturer at Yale, the Stieglitz Lecturer at the University of Chicago, the John Stauffer Lecturer at the University of Southern California, Mack Memorial Award Lecturer at Ohio State University, Gerhard Schmidt Memorial Lecturer at the Weizmann Institute of Science, the Mobay Lecturer at the University of Pittsburgh, the Thomas A. Edison Memorial Lecturer at the Naval Laboratory, the first du Pont Lecturer at the du Pont de Nemours Company, Hill Memorial Lecturer at Duke University, Gooch-Stephens Lecturer at Baylor University, Boomer Lecturer at University of Alberta, Gilman Lecturer at Iowa State University, R. B. Woodward Visiting Professor at Harvard University, GAF Lecturer at Lehigh University, H. Martin Friedman Lecturer at Brooklyn College, Gregory Lecturer at Colgate University, Walter Kaskan Memorial Lecturer at SUNY Binghamton, the Dakin Memorial Lecturer at Adelphi, the Robbins Lecturer at Pomona College, the Arthur Birch Lecturer at Australian National University, the Chemistry Lecturer of the Royal Swedish Academy of Engineering Sciences, Timothy J. O'Leary Distinguished Scientist at Gonzaga University, Carl M. Stevens Lecturer at Washington State University, the Nyholm Lecturer of the Royal Society of Chemistry, the 11th Annual J. T. Baker Nobel Lecturer at Cambridge University, the Flygare Lecturer at the University of Illinois, the Frontiers in Science Lecturer at Ohio State University, the Kohnstamm Prize Lecturer at Columbia University, the Milton Kohn Lecturer at the University of New Mexico, the Ames Lecturer at the University of Edinburgh, the F.G.A. Stone Lecturer at the University of Bristol, the Baxter Lecturer at Northern Illinois University, the Reid and Polly Anderson Lecturer at Denison University, Seonam Lecturer at Seoul National University, President's Lecturer at Rice University, Maryland/Grace Distinguished Lecturer at the University of Maryland, Plant Lecturer at Hamilton College, Morgan Lecturer at Appalachian State University, Alix Mautner Lecturer at UCLA, Convocation Speaker at Berea College, Matsen Lecturer at the University of Texas, Arthur Sweeney Jr. Lecturer at Lehman College, DuPont Marshall Lecturer at the University of Pennsylvania, Dibner Library Lecturer at the Smithsonian Institution Libraries, Probst Lecturer at Southern Illinois University at Edwardsville, Kolthoff Lecturer at the University of Minnesota, Liao Ying-Ming Foundation Lecturer at Feng Chia University, Yuan Tse Lee Foundation for Excellence Lecturer at several Taiwanese universities, Laird Lecturer and Cecil H. And Ida Green Lecturer at the University of British Columbia, as well as numerous other lectureships.

In 1971 Dr. Hoffmann was elected a member of the American Academy of Arts and Sciences, and in 1972 a member of the National Academy of Sciences. He was an elected member of the council of the NAS, 1987-90. In 1978 he was elected to the International Academy of Quantum Molecular Sciences and in 1983 a Foreign Fellow of the Indian National Science Academy. In 1984 he was elected a Foreign Member of the Royal Society and a member of the American Philosophical Society, in 1985 a Foreign Member of the Royal

Swedish Academy of Sciences, in 1988 a Foreign Member of the Societas Scientarum Fennica and the Academy of Sciences of the USSR, in 1998 a Corresponding member of the Nordrhein-Westfälische Academy of Sciences, and in 2000 a member of the Deutsche Akademie der Naturforscher Leopoldina. In 1989 Dr. Hoffmann was elected an Honorary Member of the Royal Institution. He is an Honorary Fellow of the Royal Society of Chemistry. He is an Overseas Fellow of Churchill College, Cambridge, England, and a Foreign Member of the Academia Europaea.

In 1966-68 Dr. Hoffmann was the recipient of a Sloan Foundation Research Fellowship and in 1978 of a Guggenheim Fellowship. He has been a visiting professor at the College de France. In 1986-87 he served as the Tage Erlander Professor of the Swedish Research Council, lecturing at the Universities of Stockholm, Lund, Uppsala and Gothenburg.

Roald Hoffmann is a member of the American Chemical Society, and a Fellow of the American Physical Society. He has served on the Editorial Advisory Boards of Chemical Reviews, Accounts of Chemical Research, Nouveau Journal de Chimie, the Journal of the American Chemical Society, Langmuir, and Organometallics. From 1970 to 1974 he was a member of the Advisory Panel for Chemistry of the National Science Foundation. Dr. Hoffmann has been a consultant for Tennessee Eastman Company, Eastman Kodak Company, Eli Lilly Company, John Wiley and Sons, Inc., Allied Chemical Corporation, and the du Pont de Nemours Company. He is a Director of the National Patent and Development Corporation. Dr. Hoffmann was a member of the Smithsonian Council, and is a member of the Board of Overseers of the Chemical Heritage Foundation.

In 1986-88 Dr. Hoffmann participated in the production of a television course in introductory chemistry. "The World of Chemistry" is a series of 26 half-hour episodes developed at the University of Maryland and produced by Richard Thomas. The project has been funded by the Annenberg Foundation - Corporation for Public Broadcasting. Dr. Hoffmann is the Presenter for the series, which began to be aired on PBS in 1990. "The World of Chemistry" continues to be used in hundreds of US classrooms, and abroad.

Dr. Hoffmann's research interests are in the electronic structure of stable and unstable molecules across the periodic table, and of transition states in reactions. He applies a variety of quantum chemical computational methods as well as qualitative arguments to problems of structure and reactivity of both organic and inorganic molecules of medium size and to extended systems in one-, two-, and three dimensions.

His first major contribution was the development of the extended Hückel method (in collaboration with the Lipscomb group), a molecular orbital scheme which allowed the calculation of the approximate electronic structure of molecules, and which gave reasonable predictions of molecular conformations and simple potential surfaces. These calculations were instrumental in a renaissance of interest in  $\sigma$  electrons and their properties.

Roald Hoffmann's second major contribution was a two-pronged exploration of the electronic structure of transition states and intermediates in organic reactions. In a fruitful collaboration with R. B. Woodward of Harvard University, he applied simple but powerful arguments of symmetry and bonding to the analysis of concerted reactions. These considerations

have been of remarkable predictive value and have stimulated much productive experimental work. In the second approach Dr. Hoffmann analyzed with the aid of various semiempirical methods the molecular orbitals of most types of reactive intermediates in organic chemistry — carbonium ions, diradicals, methylenes, benzyne, etc. Important concepts such as through-bond coupling, and hyperconjugative orbital interaction came out of this work, as well as the general concept of frontier orbital control.

Dr. Hoffmann and his collaborators then explored the structure and reactivity of inorganic and organometallic molecules. Approximate molecular orbital calculations and symmetry-based arguments were applied by his group to explore the basic structural features of every kind of inorganic molecule, from complexes of small diatomics to clusters containing many transition metal atoms. A particularly useful theoretical device, the conceptual building up of complex molecules from  $ML_n$  fragments, has been used by the Hoffmann group to analyze cluster bonding and the equilibrium geometries and conformational preferences of olefin and polyene metal carbonyl complexes. A satisfactory understanding of the mode of binding of essentially every organic ligand to a metal-ligand aggregate is now available, and a beginning has been made on organometallic reactivity with the exploration of potential energy surfaces for ethylene insertion, reductive elimination and alkyl migrative insertion reactions. Several new structural types, such as the triple-decker and porphyrin sandwiches, were predicted, and have been synthesized.

On the more inorganic side, Dr. Hoffmann and his coworkers systematically explored the geometries, polytopal rearrangements and substitution site preferences of five, six, seven and eight coordination, the factors that influence whether certain ligands will bridge or not, the constraints on metal-metal bonding, and the geometry of uranyl and other actinide complexes.

An important conceptual advance from the Hoffmann group has been the isolobal analogy, a mapping onto each other of the most important fragments of organic and inorganic chemistry. The analogy is most useful for seeing structural similarities between organic and inorganic molecules, often unexpected ones. But it also serves as a guide to reactivity and synthesis. The isolobal analogy was the subject of Hoffmann's Nobel Lecture.

In recent times, Hoffmann has looked at the electronic structure of extended systems in one-, two-, and three dimensions. Frontier orbital arguments find an analogue in this work in densities of states and their partitioning. An especially useful tool, the COOP curve, has been introduced by the Hoffmann group. This is the solid state analogue of an overlap population, showing the way the bond strength depends on electron count. The group has studied molecules as diverse as the platinocyanides, Chevrel phases, transition metal carbides, displacive transitions in NiAs, MnP and NiP, new metallic forms of carbon, the making and breaking of bonds in the solid state and many other systems. One focus of the solid state work has been on surfaces, especially on the interaction of  $CH_4$ , acetylene and CO with specific metal faces. The group has been able to carry through unique comparisons of inorganic and surface reactions. More recently, the design of new networks, novel conducting materials, and possible superconductors has been the main focus of the Hoffmann group. His work has ranged between novel organic polymers, complex intermetallics with more than 1000 atoms per unit cell, and the building of a chemical intuition for matter under high pressure.

"Applied theoretical chemistry" is the way Roald Hoffmann likes to characterize the particular blend of computations stimulated by experiment and the construction of generalized models, of frameworks for understanding, that is his contribution to chemistry.

At Cornell University, Dr. Hoffmann has taught primarily undergraduates and indeed almost every year since 1966 has taught first-year general chemistry. He has also taught chemistry courses to non-scientists and graduate courses in bonding theory and quantum mechanics.

The following students have received their Ph.D. at Cornell under his direction: Chien-Chuen Wan, David Hayes, Jerrald Swenson, James Howell, Maynard M. L. Chen, David L. Thorn, B. E. R. Schilling, Charles N. Wilker, David M. Hoffman, Timothy R. Hughbanks, Sunil D. Wijeyesekera, Shen-shu Sung, Chong Zheng, Ralph A. Wheeler, Marja C. Zonneville, Yat-Ting Wong, Edith A. Chan, Jing Li, Zafiria Nomikou, Kimberly Lawler, Michael Bucknum, Qiang Liu, Hugh Genin, Grigori Vajenine, Gregory Landrum, Abds-Sami Malik, Erika Merschrod, Garegin Papoian, Wingfield Glassey, Ying Wang, Melania Oana, Mihaela Bojin, Daniel Frederickson, Pradeep Gutta.

Undergraduates working in his group have included over the years Warren Hehre, Roy R. Gould, Peter Rossky, Karen Goldberg, Robert Weber, Geoffrey Zeiss, Chris Zeiss, Leigh Ann Henderson, Mikhail Velikanov, Lori Rayburn, Jeffrey R. Long, Aliya Courtney, Pooja Pathak, Georgios Markopoulos, Tomasz Jarón.

Among his postdoctoral collaborators have been Patricia Clark, George Van Dine, Mircea Gheorghiu, Akira Imamura, Rolf Gleiter, Robert Bissell, S. Swaminathan, Donald Boyd, James Williams, Robert Davidson, Brian G. Odell, Charles C. Levin, Lawrence Libit, Victor Neagu, Wolf-Dieter Stohrer, Angelo Rossi, Alfred Anderson, Phillip Mollère, Hiroshi Fujimoto, C. Stephen Kim, Jack C. Thibeault, Notker Rösch, P. Jeffrey Hay, Mihai Elian, Alain Devaquet, Joseph W. Lauher, Richard H. Summerville, Daniel L. DuBois, Thomas A. Albright, Peter Hofmann, Prem Mehrota, Heinz Berke, Alain Dedieu, Myung-Hwan Whangbo, Armel Stockis, E. D. Jemmis, Sason Shaik, Richard Goddard, Odile Eisenstein, Kazuyuki Tatsumi, Pavel Kubacek, Zdenek Havlas, Christian Minot, Miklos Kertesz, Jean-Yves Saillard, Georges Trinquier, Boris Schubert, Richard Dronskowski, Yuri Slovokhotov, Ruslan Minyaev, Karl Anker Jørgensen, Jerome Silvestre, Santiago Alvarez, Douglas Keszler, William Bleam, Wolfgang Tremel, Dragan Vuckovic, Susan Jansen, Kenneth Merz, Jr., Jean-François Halet, Roy Johnston, Paul Sherwood, Christoph Janiak, Lalitha Subramanian, Meinolf Kersting, Christian Kollmar, Haibin Deng, Vladimir Pichko, Lars A. Bengtsson, Thomas R. Ward, William A. Shirley, Andrei L. Tchougreeff, Hans-Jürgen Meyer, Katrin Albert, Pere Alemany, Yuri Slovokhotov, Birgit Schiøtt, Davide Proserpio, Kazunari Yoshizawa, Gerhard Nuspl, F. Matthias Bickelhaupt, Udo Radius, Norman Goldberg, Huang Tang, Ruedi Rytz, Peter Kroll, Robert Konecny, Ralf Stowasser, Dong-Kyun Seo, Wojciech Grochala, Andrea Ienco, Pattath Pancharatna, M.M. Balakrishnarajan, Beate Flemmig, Gabriel Merino, Dean Tantillo, Peter Kroll, Marketa Munzarova, Kelling Donald, Jason D'Acchioli, Edyta Brzostowska.

Senior visitors to his group have included Nguyen Trong Anh, D. M. P. Mingos, Jeremy Burdett, Paul Dobosh, John Eisch, Clifford McGinn, Victor Tortorelli, Evgeny Shustorovich,

Robert Bach, Richard Harcourt, San-Yan Chu, Helga Dunken, Joel Bernstein, Yuansheng Jiang, Yitzhak Apeloig, Debbie Fu-tai Tuan, Daniel Zeroka, Reinhard Nesper, Jingling Huang, Maria José Calhorda, P. A. Cox, John Lowe, Mikhail Basilevsky, Peter Kazmaier, Vladimir Minkin, Gion Calzaferrì, Boris Simkin, Maria Matos, Hassan Rabaâ, Donald H. Galván, Sung Hong, Kee Hag Lee, Deborah Huntley, Carol Parish.

Roald Hoffmann is also a writer, carving out for himself a land between poetry, philosophy and science. His essays for American Scientist are part of a writing and speaking career. Hoffmann is also a poet. His interest in poetry was stimulated by Mark Van Doren at Columbia. In the eighties he joined an informal poetry group at Cornell, with A. R. Ammons, Phyllis Janowitz and David Burak. He also owes much to the instruction of Maxine Kumin and to two stays at the Djerassi Foundation in Woodside, California. Roald Hoffmann has been publishing poetry since 1984. His first book-length collection, The Metamict State, was published by the University of Central Florida Press (University Presses of Florida) in 1987. The same publisher issued a second collection, Gaps and Verges, in 1990; then Memory Effects (1999) was published by the Calhoun Press of Columbia College, Chicago. A third collection, Soliton (2002) was published by Truman State University Press, and most recently, a bilingual Spanish/English collection of his selected poems, Catalista (2002) was published by Huerga & Fierro Editores, Madrid.

In 1993 the Smithsonian Institution Press published Chemistry Imagined. A unique art/science/literature collaboration of Roald Hoffmann with artist Vivian Torrence reveals the creative and humanistic sparks that drive science in general and chemistry in particular. A series of thirty collages by Torrence paired with short essays, personal commentary, and poems by Hoffmann evokes the magic of chemistry, its historical roots, the richness of modern chemical activities, and the mysterious confluences of science and art. Showing the general reader how science permeates daily life, Hoffmann stress the social, cultural, literary, and psychological contexts of chemistry. With delicate, surreal images, Torrence explores the highly visual nature and the intellectual essence of chemistry, the way chemists think, and the way they formulate their questions. Chemistry Imagined has been translated into Chinese and Spanish.

In 1995, Columbia University Press published Hoffmann's The Same and Not the Same. This book points to the dualities that lie under the surface of chemistry, and that endow this seemingly quiet central science with tension, thus making it interesting both to its practitioners and the thoughtful observer. The Same and Not the Same has been translated into Korean, Spanish, Russian, Italian, German and Chinese (Taiwan and PRC versions), and received the 1997 Literaturpreis of the Verband der Chemischen Industrie. It has also been chosen by the Ministry of Cultural Affairs and Sports of the Republic of Korea as one of the best academic books of the year.

In 1997, W.H. Freeman published Old Wine, New Flasks; Reflections on Science and Jewish Tradition, by Roald Hoffmann and Shira Leibowitz Schmidt. This book looks in a nonconfrontational (and witty) way at how science and religion, dealing with the mundane, are both led to eternal and important questions of authority, purity, identity, the natural and the unnatural. Old Wine, New Flasks has been translated into Spanish.

A play, Oxygen, by Carl Djerassi and Roald Hoffmann premiered in the U.S. at the San Diego Repertory Theatre in 2001, and had productions at the Riverside Studios in London, and (in German) in Würzburg and Munich in fall 2001. The play has also been broadcast by BBC World Service and West German Radio, and has been published in English, German, French, Chinese, Korean, Brazilian Portuguese, Portuguese and Spanish. A second play by Roald Hoffmann, Should've, had its initial workshop production in Edmonton, Canada in 2006.

Unadvertised, a monthly cabaret Roald runs at the Cornelia Street Café in Greenwich Village, “Entertaining Science,” has become the hot cheap ticket in NYC.

Dr. Hoffmann was married in 1960, to Eva Börjesson from Lidingö, Sweden. He is the father of two children: Hillel Jan (born in 1963) and Ingrid Helena (born in 1965). His office address is Department of Chemistry & Chemical Biology, Cornell University, Baker Laboratory, Ithaca, New York 14853-1301; telephone 607-255-3419, fax 607-255-5707, his e-mail is [rh34@cornell.edu](mailto:rh34@cornell.edu).

Information on Roald Hoffmann’s literary publications may be found on his website [www.roaldhoffmann.com](http://www.roaldhoffmann.com).

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