Magdolna Hargittai

Curriculum Vitae

Hungarian Academy of Sciences

Materials Structure and Modeling Research Group at the Budapest University of Technology and Economics, Szt. Gellért tér 4, Budapest, H-1111, Hungary Office phone: 36-1-463-3407, Office fax: 36-1-463-4052

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Web page: http://www.amkcs.ch.bme.hu/HM/hm.html

Employment

Hungarian Academy of Sciences, Materials Structure and Modeling Research Group at the Budapest University of Technology and Economics, Research Professor of Chemistry, 2007 – present

Hungarian Academy of Sciences, Structural Chemistry Research Group at Eötvös University, Research Professor of Chemistry, 2004–2006; Science advisor, 1991-2004, Senior Research Scientist, 1978-1991; Research Scientist, 1969-1978

Visiting Positions

Matrix Biology Institute, Edgewater, NJ, U.S.A., Visiting Scolar, March-June 2009; March-June 2008; Jan-June 2007

MRC-Laboratory of Molecular Biology, Cambridge, England, Visiting Fellow, Jan-March, 2000. University of North Carolina at Wilmington, Visiting Scientist, 1996/97, Spring, 1998, Spring 1999 University of Hawaii, Honolulu, Visiting Scientist, Spring 1993 University of Hawaii, Honolulu, Visiting Scientist, Fall 1989 University of Connecticut, Storrs, Visiting Scientist, 1988/1989

University of Connecticut, Storrs, Visiting Scientist, 1983/1985

University of Texas, Austin, Visiting Scientist, 1969

Education

Hungarian Academy of Sciences, Doctor of Science, 1991 Hungarian Academy of Sciences, Ph.D. in chemistry, 1978 Eötvös University, Budapest, Dr. rer. nat., 1970 Eötvös University, Budapest, M.Sc., 1969

Membership in Learned Societies

Member of the Academia Europaea (London), 2006 Corresponding Member of the Hungarian Academy of Sciences, 2004

Honors and Awards

University of North Carolina at Wilmington, D.Sc. honoris causa, 2000 Szechenyi State Prize of Hungary (equivalent to the U.S. National Medal of Science), 1996 Keynote speaker, Smithsonian Institution, Washington, DC, 1996 Kaskan Lectureship, State University of New York at Binghamton, 1994 Academy prize for authors, Budapest, 1977 Academy prize for young scientists, Budapest, 1974

Publications

 Books: Monographs: 10 (20 including revisions and translations) Edited volumes: 11
Book chapters: 25
Scienctific papers: about 150 in peer-reviewed journals
Articles in non-scientific popular magazines: about 50

Book reviews: over 300

Monographs

- Symmetry through the Eyes of a Chemist (with I. Hargittai), VCH Weinheim, 1986; Paperback edition: VCH Publishers, New York, 1987 (Russian translation, MIR, Moscow, 1989). Second, revised edition, hardback and paperback: Plenum Press, New York, 1995. Third, revised edition, Springer, 2009
- Visual Symmetry (with I. Hargittai), World Scientific, 2009; Symmetry in Pictures (In Hungarian, with I. Hargittai), Galenus, Budapest, 2005
- Candid Science VI: Conversation with Famous Scientists (with I. Hargittai), Imperial College Press, London, 2006.
- Candid Science IV: Conversation with Famous Physicists (with I. Hargittai), Imperial College Press, London, 2004
- *In Our Own Image: Personal Symmetry in Discovery* (with I. Hargittai), Kluwer/Plenum, New York, 2000; in Hungarian, Vince Kiadó, Budapest, 2003
- Symmetry: A Unifying Concept (with I. Hargittai), Shelter Publications, Bolinas, California, 1994, Second Printing, Random House, New York, 1996. Abridged German version: Symmetrie: Eine neue Art, die Welt zu sehen, Rowohlt Taschenbuch Verlag, Reinbek, 1998.
- *Discover Symmetry* (in Hungarian, for children, with I. Hargittai), Tankönyvkiadó, Budapest, 1989, Revised Swedish edition, Natur och Kultur, Stockholm, 1998
- *The Molecular Geometries of Coordination Compounds in the Vapour Phase* (with I. Hargittai), Elsevier, Amsterdam, New York, 1977 (Russian translation, MIR, Moscow, 1976)

Edited books

Candid Science III: More Conversation with Famous Chemists, Imperial College Press, London, 2003

Candid Science II: Conversation with Famous Biomedical Scientists, Imperial College Press, London, 2002.

Candid Science: Conversation with Famous Chemists, Imperial College Press, London, 2000.

- Advances in Molecular Structure Research, (with I. Hargittai), JAI Press, Greenwich, Connecticut, Volume 1, 1995; Volume 2, 1996; Volume 3, 1997; Volume 4, 1998; Volume 5, 1999, Volume 6, 2000.
- Stereochemical Applications of Gas-Phase Electron Diffraction (with I. Hargittai), Vol. A: The Electron Diffraction Technique. Vol. B: Structural Information for Selected Classes of Compounds. VCH Publishers, New York, 1988.

Selected Refereed Journal Articles

for full references of the past ten years see: http://www.amkcs.ch.bme.hu/HM/hm.html

Hargittai, M. Structural Effects in Molecular Metal Halides, Acc. Chem. Res. 2009, 42(3), 453-462.

Vest, B.; Schwerdtfeger, P.; Kolonits, M.; Hargittai, M. Chromium Difluoride: Probing the Limits of Structure Determination, *Chem. Phys. Lett.* 2009, 468, 143-147.

Groen, C.P.; Varga, Z.; Kolonits, M.; Peterson, K.A.; Hargittai, M. Does the 4*f* Electron Configuration Affect Molecular Geometries? Inorg. Chem. 2009, 48, 4143-4153.

Donald, K. J.; Hargittai, M.; Hoffmann, R. Group 12 Dihalides: Structural Predilections from Gases to Solids, *Chem. Eur.J.* 2009, 15, 158-177.

Lanza, G.; Varga, Z.; Kolonits, M.; Hargittai, M. On the effect of 4*f* electrons on the structural characteristics of lanthanide trihalides: Computational and electron diffraction study of dysprosium trichloride, *J. Chem. Phys.* 2008, 128, 074301-14.

Vest, B.; Varga, Z.; Hargittai, M.; Hermann, A.; Schwerdtfeger, P. The Elusive Structure of CrCl₂ – A Combined Computational and Gas Phase Electron Diffraction Study, *Chem. Eur. J.* 2008, 14, 5130-5143.

Hargittai, M. Symmetry, Crystallography, and Art Applied Physics B, 2007, A89, 889-898.

Varga, Z.; Lanza, G.; Minichino, C.; Hargittai, M. Quasilinear Molecule par Excellence, SrCl2: Structure from High-Temperature Gas-Phase Electron Diffraction and Quantum Chemical Calculations; Computed Structures of SrCl2-Argon Complexes, *Chem. Eur. J.* 2006, 12, 8345-8357.

Hargittai, M. On the Structure of the FeF₃ Molecule, J. Chem. Phys. 2005, 123, 196101-196102.

Müller-Rösing, H.C.; Schulz, A.; Hargittai, M. Structure and Bonding in Silver Halides. A Quantum Chemical Study of the Monomers: Ag2X, AgX, AgX2, and AgX3 (X = F, CI, Br, I), *J. Am. Chem. Soc.* 2005, 127, 8133-8145.

Hargittai, M.; Schwerdtfeger, P.; Réffy, B.; Brown R. The Molecular Structure of Different Species of Cuprous Chloride from Gas-Phase Electron Diffraction and Quantum Chemical Calculation, *Chem. Eur. J.* 2003, 9, 327-333.

Hargittai, I.; Hargittai, M. Experiments, Calculation, Computation: in a Shifting Balance, J. Mol. Struct. (Theochem), 2002, 592, 1.

Hargittai, M. Metal Halide Molecular Structures, Chem. Rev. 2000, 100, 2233

Hargittai, M.; Schulz, A.; Réffy, B.; Kolonits, M. Molecular Structure, Bonding and Jahn-Teller Effect in Gold Chlorides: Quntum Chemical Study of AuCl₃, Au₂Cl₆, AuCl₄, AuCl, and Au₂Cl₂ and Electron Diffraction Study of Au₂Cl₆, *J. Am. Chem. Soc.* 2001, 123, 1449-1458

Réffy, B.; Kolonits, M.; Schulz, A.; Klapötke, T.M.; Hargittai, M. Intriguing Gold Trifluoride – Molecular Structure of Monomers and Dimers: An Electron Diffraction and Quantum Chemical Study, *J. Am. Chem.* Soc., 2000, 122, 3127-3134

Hargittai, M.; Réffy, B.; Kolonits, M.; Marsden, C.J.; Heully, J.-L. The Structure of the Free MnF₃ Molecule – A Beautiful Example of the Jahn-Teller Effect, *J. Am. Chem. Soc.*, 1997, 119, 9042-9048

Invited Lectureships to International Meetings

Gordon Conference on Matrix-Isolated Species, Oxford, England, 2009 17th Conference on Current Trends in Computational Chemistry, Jackson, MS, 2008 15th Conference on Current Trends in Computational Chemistry, Jackson, MS, 2006 International Symmetry Festival, Budapest, 2006 2nd Not Strictly Inorganic Chemistry Conference, Prullans, Spain, 2006 2nd International School on Structural Archaelogy, Erice, Sicily, 2006 Gordon Conference on High Temperature Materials and Processes, Waterville, ME, 2004 11th Conference on Current Trends in Computational Chemistry, Jackson, MS, 2002 9th European Symposium on Gas Electron Diffraction, Blaubeuren, Germany, 2001 32nd International School of Crystallography, Erice, Sicily, 2001 Conference on High-Temperature Materials Chemistry, Jülich, Germany, 2000 8th European Symposium on Gas Electron Diffraction, Blaubeuren, Germany, 1999 7th Conference on Current Trends in Computational Chemistry, Vicksburg, MS, 1998 17th Austin Symposium on Molecular Structure, Austin, TX, 1998 2nd UNCW Symposium on Chemistry and Biochemistry, Wilmington, NC, 1998 "Nexus" Mathematics and Architecture Meeting, Florence, Italy, 1996 4th Conference on Current Trends in Computational Chemistry, Vicksburg, MS, 1995 15th Austin Symposium on Molecular Structure, Austin, TX, 1994 Fifth European Meeting of Gas Electron Diffraction, Blaubeuren, Germany, 1993 NATO Adv. Res. Workshop: Structures and Conformations of Nonrigid Molecules, Ulm, 1992 Gordon Conference on High-Temperature Chemistry, 1992 School on Inorganic Structural Chemistry, Budapest, 1992 Fourth European Meeting of Gas Electron Diffraction, Firbush Point, Scotland, 1991

Visits, Invited Lectures

University of Oslo, University of Trondheim, University of Leiden, University of Rome, CNR Structural Chemistry Laboratory (Montelibretti), University of Moscow, Soviet Academy of Sciences (Moscow), University of Debrecen, University of Ulm, University of L'Aquila, Rocasolano Institute of Physical Chemistry (Madrid), University of Granada, CISE Tecnologie Innovative (Milan), University of Brescia, Netherlands Energy Research Foundation ECN (Petten), University of Paul Sabatier (Toulouse), Technion, Israel Institute of Technology (Haifa), Moravian College (Bethlehem, PA), University of North Carolina (Wilmington, NC), University of Arkansas (Fayetteville, AR) Jackson State University (Jackson, MS), University of Michigan (Ann Arbor), Ludwig-Maximilians University of Munich, University of Auckland (New Zealand), New Zealand Institute of Chemistry (Auckland, NZ), Medical Research Council – Laboratory of Molecular Biology (Cambridge, UK), University of Rome, University of Wisconsin (Madison), University of Minnesota (Minneapolis), University of Stockholm, Czech Academy of Sciences (Prague), Princeton University (Princeton, NJ), University of Maryland at Baltimore County (Baltimore), Moravian College (Bethlehem, PA), University of Michigan (Ann Arbor), Northwestern University (Evanston, IL), Stanford University (Stanford, CA), Tokyo University, Ochanomisu University (Japan), University of Rome, University of Barcelona, University of L'Aquila (Italy), Technion, Israel Institute of Technology (Haifa), Weizmann Institute (Rehovot, Israel), New York University, New York, City College, New York; Lawrence Livermore National Laboratory, Livermore, CA;

Professional Service

Founding Member, Association of Hungarian Women Scientists, Budapest, 2008-present
Member, Board of Janos Bolyai Research Fellowship Program, Budapest, 2007-present
Member, Ad-hoc Committee on Interdisciplinarity, Hungarian Academy of Sciences, 2006
Member, Ad-hoc Committee on How to Elect Members of the Academy, Hungarian Academy of
Sciences, 2005

Member, PhD School of the Chemistry Institute, Eotvos University, 2004-present Member, Committee of Physical and Inorganic Chemistry of the Hungarian Academy of Sciences, 2004-present

Editor, Advances in Molecular Structure Research (JAI Press, Stamford, Connecticut), 1995-2000

Book Review Editor, Structural Chemistry (Plenum Press, New York), 1990-present Member, Working Committe on the Structure of Matter and Molecules, HAS, 1991-present Member, Working Committe on Inorganic and Metalorganic Chemistry, HAS, 1991-1993 Member, Working Committe on Coordination Chemistry, HAS, 1981-1991

Member, The New York Academy of Sciences, 1987

Member, Institute of Materials Science, University of Connecticut, 1983/1985, 1988/89

Outreach Programs

Columnist, Természet Világa (The World of Nature), on Women in Science, 2007-present

Lectures on symmetry, on the connection of art and science, on famous scientists, especially on prominent women scientists

Lectures on Women in Science

Among others at the Universities of Stockholm; Rome, L'Aquila, Michigan (Ann Arbor), Maryland (at Baltimore County), Princeton, Stanford; St. Francis University (PA, USA), Moravian College, (PA, USA}, Chech Academy of Sciences, Prague; Ochanomizu University, Tokyo; Technion, Haifa; Weizmann Institute, Rehovot, City College, New York; University of Barcelona.

Main lecturer at a meeting on Women in Science organized by the Japanese Cabinet, Tokyo, 2005

Invited after dinner talks at different international conferences Conferences on Women in Science

Research Interest

Structural chemistry; coordination compounds; metal halides; high-temperature chemistry; gasphase electron diffraction; combined use of experimental techniques (electron diffraction, vibrational spectroscopy, mass spectrometry) and theoretical chemistry; gas-solid structural differences, models of molecular geometry; general problems of symmetry.

Symmetry as a bridge between the sciences and the humanities

The personal aspects of science, famous scientists and science history, women scientists