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Br₂Fe FeBr ₂	Iron dibromide Iron dihalides: structures, vibrational frequencies, and thermodynamic properties of all iron dihalides from computation, an ED study of iron diiodide, and a reinvestigation of iron dibromide <i>Z. Varga, M. Kolonits, M. Hargittai</i> Struct. Chem., DOI: 10.1007/s11224-010-9713-8
Br₄Fe₂ Fe ₂ Br ₄	Iron dibromide dimer Iron dihalides: structures, vibrational frequencies, and thermodynamic properties of all iron dihalides from computation, an ED study of iron diiodide, and a reinvestigation of iron dibromide <i>Z. Varga, M. Kolonits, M. Hargittai</i> Struct. Chem., DOI: 10.1007/s11224-010-9713-8
Cl₂V VCl ₂	Vanadium dichloride Structures by ED and quantum chemical calculations <i>Z. Varga, B. Vest, P. Schwerdtfeger, M. Hargittai</i> Inorg. Chem. 49 (2010), 2816
Cl₃Fe FeCl ₃	Iron trichloride Quantum chemical calculations of all iron trihalides and ED study of monomeric and dimeric FeCl ₃ <i>Z. Varga, M. Kolonits, M. Hargittai</i> Inorg. Chem. 49 (2010), 1039
Cl₃V VCl ₃	Vanadium trichloride Structures by ED and quantum chemical calculations <i>Z. Varga, B. Vest, P. Schwerdtfeger, M. Hargittai</i>

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Cl₆Fe₂ Fe ₂ Cl ₆	Iron trichloride dimer Quantum chemical calculations of all iron trihalides and ED <i>Z. Varga, M. Kolonits, M. Hargittai</i> Inorg. Chem. 49 (2010), 1039
DyI₃ DyI ₃	Dysprosium triiodide Computational, vibrational spectroscopic, and ED study of monomeric and dimeric DyI ₃ <i>Z. Varga, C.P. Groen, M. Kolonits, M. Hargittai</i> Dalton Trans. 39 (2010), 6221
Dy₂I₆ Dy ₂ I ₆	Dysprosium triiodide dimer Computational, vibrational spectroscopic, and ED study of monomeric and dimeric DyI ₃ <i>Z. Varga, C.P. Groen, M. Kolonits, M. Hargittai</i> Dalton Trans. 39 (2010), 6221
FeI₂ FeI ₂	Iron diiodide Iron dihalides: structures, vibrational frequencies, and thermodynamic properties of all iron dihalides from computation and an ED study of iron diiodide <i>Z. Varga, M. Kolonits, M. Hargittai</i> Struct. Chem., DOI: 10.1007/s11224-010-9713-8
Fe₂I₄ Fe ₂ I ₄	Iron diiodide dimer Iron dihalides: structures, vibrational frequencies, and thermodynamic properties of all iron dihalides from computation and an ED study of iron diiodide <i>Z. Varga, M. Kolonits, M. Hargittai</i> Struct. Chem., DOI: 10.1007/s11224-010-9713-8
I₃La LaI ₃	Lanthanum triiodide On the thermal expansion of molecules <i>Z. Varga, M. Hargittai, L. S. Bartell</i> Struct. Chem., DOI: 10.1007/s11224-010-9699-2
	Benzene derivatives Comparison of the molecular structures of five benzene derivatives as determined independently by gas-phase electron diffraction in two different laboratories: a perspective <i>A. R. Campanelli, A. Domenicano, I. Hargittai</i> Struct. Chem. 21 (2010), 803
	Caesium halides Matrix-isolation FT-IR study of (CsBr)(n) and (CsI)(n) (n=1-3) <i>C. P. Groen, A. Kovacs</i> Vib. Spectrosc. 54 (2010), 30
	Structures beyond crystals <i>I. Hargittai</i> J. Mol. Struct. 21 (2010), 81
	Linus Pauling's quest for the structure of proteins <i>I. Hargittai</i> Struct. Chem. 21 (2010), 1

	<p>Pioneer of hyaluronan structural chemistry and other studies of polysaccharides: Torvard C. Laurent (1930-2009)</p> <p><i>I. Hargittai</i> Struct. Chem. 21 (2010), 471</p>
	<p>Lev V. Vilkov (1931-2010)—Scientist, Friend, Editorial Board member</p> <p><i>I. Hargittai</i> Struct. Chem. 21 (2010), 469</p>
	<p>The Human Genome Project-A triumph (also) of structural chemistry: On Victor McElheny's new book, Drawing the Map of Life</p> <p><i>I. Hargittai</i> Struct. Chem. 21 (2010), 667</p>
	<p>The Last Boat from Lisbon: Conversations with Peter D. Lax</p> <p><i>I. Hargittai</i> Math. Intell. 32 (2010), 24</p>
	<p>More than design science-design in science: Hommage a Gyorgy Kepes</p> <p><i>I. Hargittai</i> Struct. Chem. 21 (2010), 901</p>
	<p>Graphene 2010</p> <p><i>I. Hargittai</i> Struct. Chem. 22 (2011), in press</p>
	<p>Marie Sklodowska Curie and the Year of Chemistry</p> <p><i>I. Hargittai</i> Struct. Chem. 22 (2011), in press</p>
	<p>Geometry and models in chemistry</p> <p><i>I. Hargittai</i> Struct. Chem. 22 (2011), in press</p>
	<p>Aleksandr Mikhailovich Butlerov and chemical structure: Tribute to a scientist and to a 150-year old concept</p> <p><i>I. Hargittai</i> Struct. Chem. 22 (2011), in press</p>
	<p>Book Judging Edward Teller: A Closer Look at One of the Most Influential Scientists of the Twentieth Century <i>I. Hargittai</i> Prometheus Books, Inc.: New York, U.S.A., 2010. 575 pp.</p>
	<p>Book Drive and Curiosity <i>I. Hargittai</i> Prometheus Books, Inc., 2011</p>
	<p>Book chapter Nobel Prize <i>I. Hargittai</i> in: Encyclopedia of Global Studies, SAGE Publications, 2011.</p>
	<p>A life in structural chemistry: Hommage a Lev V. Vilkov <i>I. Hargittai, A. L. Vilkova</i></p>

	Struct. Chem. 22 (2011), in press
	Further VSEPRing about molecular geometries <i>I. Hargittai, D. Menyhard</i> J. Mol. Struct. 21 (2010), 136
	Book chapter Electron Diffraction Theory and Methods <i>I. Hargittai, M. Hargittai</i> in: Encyclopedia of Spectroscopy and Spectrometry, 2nd Ed., Elsevier, 2010. 461–465 pp.
	Actinide mono- and dioxides Quantum chemical calculations from Th to Cm <i>I. Infante, A. Kovacs, G. La Macchia, A. R. M. Shahi, J. K. Gibson, L. Gagliardi</i> J Phys Chem A, 114 (2010), 6007
	Book Symmetry through the Eyes of a Chemist. [Paperback]. Third, revised edition <i>M. Hargittai, I. Hargittai</i> Springer, 2010. xii + 520 pp.
	Book chapter Electron Diffraction Applications <i>M. Hargittai, I. Hargittai</i> in: Encyclopedia of Spectroscopy and Spectrometry, 2nd Ed., Elsevier, 2010. 456–460 pp.
	Book chapter Polyhedral molecular geometries <i>M. Hargittai, I. Hargittai</i> in: Shaping Space: A Polyhedral Approach, 2nd Ed., Birkhäuser, 2010, 172-188 pp.
	Paradigms and paradoxes: the conformation of the fundamental unit of hyaluronic acid <i>Z. Varga, I. Hargittai</i> Struct. Chem. 21 (2010), 1211