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Br₃Dy DyBr ₃	Dysprosium tribromide Computational, vibrational spectroscopic, and ED studies of monomeric and dimeric DyBr ₃ <i>C.P. Groen, Z. Varga, M. Kolonits, K.A. Peterson, M. Hargittai</i> <i>Inorg. Chem.</i> 48 (2009) 4143-4153
Cl₂V VCl ₂	Vanadium dichloride Structures of VCl ₂ and VCl ₃ by ED and quantum chemical calculations <i>Z. Varga, B. Vest, P. Schwerdtfeger, M. Hargittai</i> <i>Inorg. Chem.</i> 49 (2010) 2816-2821
Cl₃Fe FeCl ₃ ,	Iron trichloride Quantum chemical calculations and ED study of monomeric and dimeric FeCl ₃ <i>Z. Varga, M. Kolonits, M. Hargittai</i> <i>Inorg. Chem.</i> 49 (2010) 1039-1045
Cl₃V VCl ₃	Vanadium trichloride Structures of VCl ₂ and VCl ₃ by ED and quantum chemical calculations <i>Z. Varga, B. Vest, P. Schwerdtfeger, M. Hargittai</i> <i>Inorg. Chem.</i> 49 (2010) 2816-2821
Cl₆Fe₂ Fe ₂ Cl ₆	Iron trichloride dimer Quantum chemical calculations and ED study of monomeric and dimeric FeCl ₃ <i>Z. Varga, M. Kolonits, M. Hargittai</i> <i>Inorg. Chem.</i> 49 (2010) 1039-1045
CrF₂ CrF ₂	Chromium difluoride Structure by ED and quantum chemical calculations <i>B. Vest, P. Schwerdtfeger, M. Kolonits, M. Hargittai</i> <i>Chem. Phys. Lett.</i> 468 (2009) 143-147
Dyl₃ Dyl ₃	Dysprosium triiodide Computational, vibrational spectroscopic, and ED studies of monomeric and dimeric Dyl ₃ <i>Z. Varga, C.P. Groen, M. Kolonits, M. Hargittai</i> Submitted
	Glenn T. Seaborg; discoveries; and the capital of knowledge

	<p><i>B. Hargittai, I. Hargittai</i> Struct. Chem. 20 (2009) 355-359</p>
	<p>Structures beyond crystals <i>I. Hargittai</i> J. Mol. Struct., DOI: 10.1016/j.molstruc.2010.02.009</p>
	<p>Ronald J. Gillespie; the VSEPR model; and molecular symmetry <i>I. Hargittai</i> Struct. Chem. 20 (2009) 155-159</p>
	<p>The tetranucleotide hypothesis: a centennial <i>I. Hargittai</i> Struct. Chem. 20 (2009) 753-756</p>
	<p>Neil Bartlett and the first noble-gas compound <i>I. Hargittai</i> Struct. Chem. 20 (2009) 953-959</p>
	<p>Linus Pauling's quest for the structure of proteins <i>I. Hargittai</i> Struct. Chem. 21 (2010) 1-7</p>
	<p>The Last Boat from Lisbon: Conversations with Peter D. Lax <i>I. Hargittai</i> Math. Intell., in production</p>
	<p>Lev V. Vilkov (1931-2010)—Scientist, Friend, Editorial Board member <i>I. Hargittai</i> Struct. Chem. 21 (2010), in production</p>
	<p>Pioneer of hyaluronan structural chemistry and other studies of polysaccharides: Torvard C. Laurent (1930-2009) <i>I. Hargittai</i> Struct. Chem. 21 (2010), in production</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, 2010, in production</p>
	<p>Book chapter Nobel Prize <i>I. Hargittai</i> in: Encyclopedia of Global Studies, SAGE Publications, 2011.</p>
	<p>The twentieth year of Structural Chemistry <i>I. Hargittai, A. Kovacs</i> Struct. Chem. 20 (2009) 1-10</p>
	<p>Further VSEPRing about molecular geometries <i>I. Hargittai, D. Menyhard</i> J. Mol. Struct., DOI: 10.1016/j.molstruc.2010.02.038</p>
	<p>Book chapter Electron Diffraction Theory and Methods <i>I. Hargittai, M. Hargittai</i> in: Encyclopedia of Spectroscopy and Spectrometry, 2nd Ed., Elsevier, 2010.</p>
	<p>Actanide 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), in press</p>
	<p>Group 12 dihalides Quantum chemical calculations <i>K. J. Donald, M. Hargittai, R. Hoffmann</i> Chem. Eur. J. 15 (2009) 158-177</p>

	Structural Effects in Molecular Metal Halides Review <i>M. Hargittai</i> Accounts Chem. Res. 42 (2009) 453-462
	Vibronic Interactions in Metal Halide Molecules Review <i>M. Hargittai</i> Struct. Chem. 20 (2009) 21-30
	Hermann Jahn and Rudolf Renner of the Jahn–Teller and Renner–Teller Effects <i>M. Hargittai, I. Hargittai</i> Struct. Chem. 20 (2009) 537-540
	Book Visual Symmetry <i>M. Hargittai, I. Hargittai</i> World Scientific Pub. (2009) 209
	Book Symmetry Through the Eyes of a Chemist, 3rd edition <i>M. Hargittai, I. Hargittai</i> Springer, 2009 (hardcover), 2010 (softcover), 520p.
	Book chapter Electron Diffraction Applications <i>M. Hargittai, I. Hargittai</i> in: Encyclopedia of Spectroscopy and Spectrometry, 2nd Ed., Elsevier, 2010.
	Book chapter Polyhedral molecular geometries <i>M. Hargittai, I. Hargittai</i> in: Shaping Space: A Polyhedral Approach, 2nd Ed., Birkhäuser, 2010, in press