A Bibliography of Publications of Frank E. Harris

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Abstract

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References

Harris:1950:MGM

[1] Frank E. Harris and Leonard K. Nash. Microeffusiometry of gaseous mixtures. *Analytical Chemistry (Washington, DC, USA)*, 22(12):1552–1556, December 1, 1950. CODEN ANCHAM. ISSN 0003-2700 (print), 1520-6882 (electronic).

Harris:1951:DTW

[2] Frank E. Harris and Leonard K. Nash. Determination of traces of water vapor in gases. *Analytical Chemistry (Washington, DC, USA)*, 23(5):736–739, May 1951. CODEN ANCHAM. ISSN 0003-2700 (print), 1520-6882 (electronic).

Lundin:1952:VPAa

[3] R. E. Lundin, Frank E. Harris, and Leonard K. Nash. The vapor phase association of butyric and heptanoic acids. *Journal of the American Chemical Society*, 74(3):743–745, February 1, 1952. CODEN JACSAT. ISSN 0002-7863 (print), 1520-5126 (electronic), 1943-2984.

Lundin:1952:VPAb

[4] R. E. Lundin, Frank E. Harris, and Leonard K. Nash. The vapor phase association of trifluoroacetic acid. *Journal of the American Chemical Society*, 74(18):4654–4656, September 1, 1952. CODEN JACSAT. ISSN 0002-7863 (print), 1520-5126 (electronic), 1943-2984.

Harris:1953:DPP

[5] Frank E. Harris and Berni J. Alder. Dielectric polarization in polar substances. *Journal of Chemical Physics*, 21(6):1031–1038, June 1, 1953. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/21/6/10.1063/1.1699105`.

Harris:1953:DPSa

[6] Frank E. Harris and Berni J. Alder. Dielectric polarization and self ionization in carboxylic acids. *Journal of Chemical Physics*, 21(7):1306–1307,

July 1, 1953. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://scitation.aip.org/content/aip/journal/jcp/21/7/10.1063/1.1699201.

Harris:1953:DPSb

[7] Frank E. Harris, Ernest W. Haycock, and Berni J. Alder. Dielectric polarization and structure of polar liquids under pressure. *Journal of Chemical Physics*, 21(11):1943–1948, November 1, 1953. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://scitation.aip.org/content/aip/journal/jcp/21/11/10.1063/1.1698722.

Harris:1953:IPD

[8] Frank E. Harris and Berni J. Alder. Intermolecular potentials from dielectric polarization in polar gases. *Journal of Chemical Physics*, 21(8):1351–1357, August 1, 1953. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://scitation.aip.org/content/aip/journal/jcp/21/8/10.1063/1.1699219.

Harris:1953:PDD

[9] Frank E. Harris, Ernest W. Haycock, and Berni J. Alder. Pressure dependence of the dielectric constant of water and the volume contraction of water and n-butanol upon addition of electrolyte. *Journal of Physical Chemistry*, 57(9):978–979, September 1953. CODEN JPCHAX. ISSN 0022-3654 (print), 1541-5740 (electronic).

Harris:1953:RRP

[10] Frank E. Harris and Berni J. Alder. Restricted rotation in polar gases near the critical point. *Nature*, 172(4382):774, October 24, 1953. CODEN NATUAS. ISSN 0028-0836 (print), 1476-4687 (electronic). URL http://www.nature.com/nature/journal/v172/n4382/pdf/172774a0.pdf.

Harris:1954:CMPa

[11] Frank E. Harris and Stuart A. Rice. A chain model for polyelectrolytes. *Abstracts of Papers of the American Chemical Society*, 126(??):17S–17S, ???? 1954. CODEN ACSRAL. ISSN 0065-7727.

Harris:1954:CMPb

[12] Frank E. Harris and Stuart A. Rice. A chain model for polyelectrolytes. I. *Journal of Physical Chemistry*, 58(9):725–732, 1954. CODEN JPCHAX. ISSN 0022-3654 (print), 1541-5740 (electronic). URL http://pubs.acs.org/doi/abs/10.1021/j150519a010.

Harris:1954:DCLa

[13] Frank E. Harris and Chester T. O'Konski. The dielectric constant of liquid trifluoroacetic acid. *Abstracts of Papers of the American Chemical Society*, 125(??):25Q–25Q, ???? 1954. CODEN ACSRAL. ISSN 0065-7727.

Harris:1954:DCLb

[14] Frank E. Harris and Chester T. O'Konski. The dielectric constant of liquid trifluoroacetic acid. *Journal of the American Chemical Society*, 76(17): 4317–4318, 1954. CODEN JACSAT. ISSN 0002-7863 (print), 1520-5126 (electronic), 1943-2984. URL `http://pubs.acs.org/doi/abs/10.1021/ja01646a019`.

Harris:1954:DPA

[15] Frank Ephraim Harris. *Dielectric Properties of Aqueous Solutions at Microwave Frequencies*. Ph.D. dissertation, Department of Chemistry and Chemical Engineering, University of California, Berkeley, Berkeley, CA, USA, January 1954. iii + 98 pp. URL `http://search.proquest.com/docview/302005505`.

Harris:1954:SMD

[16] Frank E. Harris and Berni J. Alder. Statistical mechanical derivation of Onsager's equation for dielectric polarization. *Journal of Chemical Physics*, 22(11):1806–1808, November 1, 1954. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/22/11/10.1063/1.1739924`.

Harris:1954:TFS

[17] Frank E. Harris and Berni J. Alder. Thermodynamic functions for self-ionization in carboxylic acids. *Transactions of the Faraday Society*, 50 (??):13–16, ???? 1954. CODEN TFSOA4. ISSN 0014-7672.

Rice:1954:CMP

[18] Stuart A. Rice and Frank E. Harris. A chain model for polyelectrolytes. II. *Journal of Physical Chemistry*, 58(9):733–739, September 1954. CODEN JPCHAX. ISSN 0022-3654 (print), 1541-5740 (electronic). URL `http://pubs.acs.org/doi/abs/10.1021/j150519a011`.

Cotton:1955:TCF

[19] F. Albert Cotton and Frank E. Harris. The thermodynamics of chelate formation. I. Experimental determination of enthalpies and entropies in diamine-metal ion systems. *Journal of Physical Chemistry*, 59(12):1203–1208, December 1955. CODEN JPCHAX. ISSN 0022-3654 (print),

1541-5740 (electronic). URL http://pubs.acs.org/doi/abs/10.1021/j150534a006.

Harris:1955:BRB

[20] F. E. Harris. Book review: "*Molecular Theory of Gases and Liquids*", by J. O. Hirschfelder, C. F. Curtiss & R. B. Bird. Wiley, New York, 1954. xxvi + 1219 pp., $20.00. *Journal of Polymer Science*, 17(83):116, May 1955. CODEN JPSCAU. ISSN 0022-3832 (print), 1542-6238 (electronic). URL http://onlinelibrary.wiley.com/doi/10.1002/pol.1955.120178311/abstract.

Harris:1955:CFA

[21] Frank E. Harris. Contributions of fluctuations and anisotropy to dielectric polarization in polar substances. *Journal of Chemical Physics*, 23(9):1663–1672, September 1, 1955. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://scitation.aip.org/content/aip/journal/jcp/23/9/10.1063/1.1742407.

Harris:1955:EDM

[22] Frank E. Harris. Equilibrium distribution of molecular weights in non-cyclic polymerizations. *Journal of Polymer Science*, 18(89):351–357, November 1955. CODEN JPSCAU. ISSN 0022-3832 (print), 1542-6238 (electronic). URL http://adsabs.harvard.edu/abs/1955JPoSc..18..351H.

Harris:1955:MHP

[23] Frank E. Harris and Chester T. O'Konski. Measurement of high permittivity dielectrics at microwave frequencies. *Review of Scientific Instruments*, 26(5):482–485, 1955. CODEN RSINAK. ISSN 0034-6748 (print), 1089-7623 (electronic). URL http://scitation.aip.org/content/aip/journal/rsi/26/5/10.1063/1.1771331.

Harris:1955:NIG

[24] Frank E. Harris. Note on imperfect gas theory. *Journal of Chemical Physics*, 23(10):1965, October 1, 1955. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://scitation.aip.org/content/aip/journal/jcp/23/10/10.1063/1.1740625.

Harris:1955:RCM

[25] Frank E. Harris and Stuart A. Rice. The random chain model for polyelectrolytes. *Journal of Polymer Science*, 15(79):151–156, January 1955. CODEN JPSCAU. ISSN 0022-3832 (print), 1542-6238 (electronic). URL http://adsabs.harvard.edu/abs/1955JPoSc..15..151H.

Harris:1955:RFM

[26] Frank E. Harris. Ring formation and molecular weight distributions in branched chain polymers. I. *Journal of Chemical Physics*, 23(8):1518–1525, August 1, 1955. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/23/8/10.1063/1.1742340`.

Harris:1955:RLE

[27] Frank E. Harris and Leonard K. Nash. A Raoult's law experiment for the general chemistry course: Manometry without a manometer. *Journal of Chemical Education*, 32(11):575–577, 1955. CODEN JCEDA8. ISSN 0021-9584 (print), 1938-1328 (electronic). URL `http://pubs.acs.org/doi/abs/10.1021/ed032p575`.

Cotton:1956:TCF

[28] F. Albert Cotton and Frank E. Harris. The thermodynamics of chelate formation. II. A Monte Carlo study of the distribution of configuration in short chains. *Journal of Physical Chemistry*, 60(10):1451–1454, 1956. CODEN JPCHAX. ISSN 0022-3654 (print), 1541-5740 (electronic). URL `http://pubs.acs.org/doi/abs/10.1021/j150544a030`.

Harris:1956:CMP

[29] Frank E. Harris and Stuart A. Rice. Chain model for polyelectrolytes. IV. Skeletal distribution effects in equimolar polyampholytes. *Journal of Chemical Physics*, 24(2):336–344, February 1, 1956. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/24/2/10.1063/1.1742472`.

Harris:1956:DMDa

[30] Frank E. Harris and Stephen G. Brush. Dipole moments and dielectric polarization in solutions. *Abstracts of Papers of the American Chemical Society*, 129(??):21Q–21Q, ???? 1956. CODEN ACSRAL. ISSN 0065-7727.

Harris:1956:DMDb

[31] Frank E. Harris and Stephen G. Brush. Dipole moments and dielectric polarization in solutions. *Journal of the American Chemical Society*, 78(7):1280–1287, 1956. CODEN JACSAT. ISSN 0002-7863 (print), 1520-5126 (electronic), 1943-2984. URL `http://pubs.acs.org/doi/abs/10.1021/ja01588a004`.

Harris:1956:ECT

[32] Frank E. Harris and Stuart A. Rice. Electrostatic contributions to thermodynamic functions of systems containing polymeric ions. *Journal of Chemical Physics*, 25(5):955–964, November 1, 1956. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/25/5/10.1063/1.1743150`.

Harris:1956:MIE

[33] Frank E. Harris and Stuart A. Rice. Model for ion exchange resins. *Journal of Chemical Physics*, 24(6):1258, June 1, 1956. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/24/6/10.1063/1.1742759`.

Rice:1956:CMP

[34] Stuart A. Rice and Frank E. Harris. Chain model for polyelectrolytes. III. Equimolar polyampholytes of regularly alternating structure. *Journal of Chemical Physics*, 24(2):326–335, February 1, 1956. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/24/2/10.1063/1.1742471`.

Rice:1956:PGIa

[35] Stuart A. Rice and Frank E. Harris. Polyelectrolyte gels and ion exchange reactions. *Abstracts of Papers of the American Chemical Society*, 129(??): 20Q–20Q, ???? 1956. CODEN ACSRAL. ISSN 0065-7727.

Rice:1956:PGIb

[36] Stuart A. Rice and Frank E. Harris. Polyelectrolyte gels and ion exchange reactions. *Zeitschrift für Physikalische Chemie [Neue Folge, 1954–1990, Frankfurt am Main]*, 8(3–4):207–239, August 1956. CODEN ZPCFAX. ISSN 0942-9352. URL `http://www.degruyter.com/view/j/zpch.1956.8.issue-3_4/zpch.1956.8.3_4.207/zpch.1956.8.3_4.207.xml`.

Harris:1957:DPA

[37] Frank E. Harris and Chester T. O'Konski. Dielectric properties of aqueous ionic solutions at microwave frequencies. *Journal of Physical Chemistry*, 61(3):310–319, 1957. CODEN JPCHAX. ISSN 0022-3654 (print), 1541-5740 (electronic). URL `http://pubs.acs.org/doi/abs/10.1021/j150549a009`.

Harris:1957:ELC

[38] F. E. Harris. Energy level calculations for small diatomic molecules. *Spectrochimica Acta*, 10(??):232–??, ???? 1957. CODEN ???? ISSN 0038-6987.

Harris:1957:MIB

[39] Frank E. Harris and Stuart A. Rice. A model for ion binding and exchange in polyelectrolyte solutions and gels. *Journal of Physical Chemistry*, 61(10):1360–1364, 1957. CODEN JPCHAX. ISSN 0022-3654 (print), 1541-5740 (electronic). URL `http://pubs.acs.org/doi/abs/10.1021/j150556a023`.

Harris:1957:MOG

[40] Frank E. Harris. Molecular orbitals for the ground state of the H_2 molecule. *Journal of Chemical Physics*, 27(3):812–813, September 1, 1957. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/27/3/10.1063/1.1743838`.

Harris:1957:TEI

[41] Frank E. Harris. Tables of the exponential integral $\mathrm{Ei}(x)$. *Mathematical Tables and Other Aids to Computation*, 11(57):9–16, January 1957. CODEN MTTCAS. ISSN 0891-6837.

OKonski:1957:EFE

[42] Chester T. O'Konski and Frank E. Harris. Electric free energy and the deformation of droplets in electrically conducting systems. *Journal of Physical Chemistry*, 61(9):1172–1174, 1957. CODEN JPCHAX. ISSN 0022-3654 (print), 1541-5740 (electronic). URL `http://pubs.acs.org/doi/abs/10.1021/j150555a009`.

Rice:1958:CPB

[43] Stuart A. Rice and Frank E. Harris. Comments on the paper "*Potentiometric Titration, Association Phenomena, and Interaction of Neighboring Groups in Polyelectrolytes*". *Journal of Chemical Physics*, 28(5):988–989, May 1, 1958. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://adsabs.harvard.edu/abs/1958JChPh..28..988R`; `http://scitation.aip.org/content/aip/journal/jcp/28/5/10.1063/1.1744319`. See [345].

Harris:1959:VBC

[44] Gilda Maki Harris and Frank E. Harris. Valence bond calculation of the barrier to internal rotation in molecules. *Journal of Chemical Physics*, 31(6):1450–1453, December 1, 1959. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/31/6/10.1063/1.1730633`.

Harris:1960:MOS

[45] Frank E. Harris. Molecular orbital studies of diatomic molecules. I. Method of computation for single configurations of heteronuclear systems. *Journal of Chemical Physics*, 32(1):3–18, January 1, 1960. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/32/1/10.1063/1.1700944`.

Harris:1962:BRB

[46] Frank E. Harris and Richard H. Eastman. Book review: *Molecular Orbital Theory for Organic Chemists*. Andrew Streitwieser, Jr. Wiley, New York, 1961. xvi + 489 pp. Illus. $14.50. *Science*, 136(3511):143, April 13, 1962. CODEN SCIEAS. ISSN 0036-8075 (print), 1095-9203 (electronic). URL `http://adsabs.harvard.edu/abs/1962Sci...136..143S`.

Harris:1963:DNE

[47] Frank E. Harris, Robert K. Nesbet, Per-Olov Löwdin, and Ernest R. Davidson. Discussion on "Natural Expansions and Properties of the Chemical Bond". *Reviews of Modern Physics*, 35(3):629–630, July 1963. CODEN RMPHAT. ISSN 0034-6861 (print), 1538-4527 (electronic), 1539-0756. URL `http://link.aps.org/doi/10.1103/RevModPhys.35.629`; `http://rmp.aps.org/abstract/RMP/v35/i3/p629_1`.

Harris:1963:GWF

[48] Frank E. Harris. Gaussian wave functions for polyatomic molecules. *Reviews of Modern Physics*, 35(3):558–569, July 1963. CODEN RMPHAT. ISSN 0034-6861 (print), 1538-4527 (electronic), 1539-0756. URL `http://link.aps.org/doi/10.1103/RevModPhys.35.558`; `http://rmp.aps.org/abstract/RMP/v35/i3/p558_1`.

Harris:1963:MOS

[49] Frank E. Harris and Howard S. Taylor. Molecular orbital studies of diatomic molecules. III. The ground state of the hydrogen molecule. *Journal of Chemical Physics*, 38(11):2591–2596, June 1, 1963. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/38/11/10.1063/1.1733556`.

Harris:1963:NUS

[50] Frank E. Harris. *Numbers and Units for Science*. Addison-Wesley, Reading, MA, USA, 1963. xi + 305 pp. LCCN QC88 .H38.

Harris:1963:PCI

[51] Frank E. Harris. *Principles of chemistry: Instructor's manual, part 1 (for books 1, 2, and 3)*. Addison-Wesley, Reading, MA, USA, 1963. ???? pp. LCCN D33 .H28.

Harris:1963:PCP

[52] Frank E. Harris. *Principles of chemistry: a programmed text*. Addison-Wesley, Reading, MA, USA, 1963–1965. ???? pp. LCCN D33 .H28.

Michels:1963:MOS

[53] H. Harvey Michels and Frank E. Harris. Molecular orbital studies of excited states of HeH. *Journal of Chemical Physics*, 39(6): 1464–1469, September 1963. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://adsabs.harvard.edu/abs/1963JChPh..39.1464M`; `http://scitation.aip.org/content/aip/journal/jcp/39/6/10.1063/1.1734465`.

Taylor:1963:MOS

[54] Howard S. Taylor and Frank E. Harris. Molecular orbital studies of diatomic molecules. II. Method of computation for multi-configurations of heteronuclear and homonuclear systems. *Molecular Physics*, 6(2):183–192, 1963. CODEN MOPHAM. ISSN 0026-8976 (print), 1362-3028 (electronic). URL `http://adsabs.harvard.edu/abs/1963MolPh...6..183T`.

Taylor:1963:PCF

[55] Howard S. Taylor and Frank E. Harris. Potential curve for the $^2\Sigma_u^+$ state of H_2. *Journal of Chemical Physics*, 39(4):1012–1016, August 1963. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://adsabs.harvard.edu/abs/1963JChPh..39.1012T`; `http://scitation.aip.org/content/aip/journal/jcp/39/4/10.1063/1.1734350`.

Harris:1964:QMS

[56] Frank E. Harris and Howard S. Taylor. A quantum-mechanical study of the LiH molecule in the ground state. *Physica*, 30(1):105–112, January 1964. CODEN PHYSAG. ISSN 0031-8914 (print), 1873-1767 (electronic). URL `http://adsabs.harvard.edu/abs/1964Phy....30..105H`; `http://www.sciencedirect.com/science/article/pii/0031891464902058`.

Rein:1964:PTR

[57] Robert Rein and Frank E. Harris. Proton tunneling in radiation-induced mutation. *Science*, 146(3644):649–650, October 30, 1964. CODEN SCIEAS. ISSN 0036-8075 (print), 1095-9203 (electronic). URL

http://adsabs.harvard.edu/abs/1964Sci...146..649R; http://www.sciencemag.org/content/146/3644/649.

Rein:1964:SHB

[58] Robert Rein and Frank E. Harris. Studies of hydrogen bonded systems. I. The electronic structure and the double well potential of the N–H$\cdots$N hydrogen bond of the guanine–cytosine base pair. *Journal of Chemical Physics*, 41(11):3393–3401, December 1, 1964. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://scitation.aip.org/content/aip/journal/jcp/41/11/10.1063/1.1725737.

Taylor:1964:QMS

[59] Howard S. Taylor and Frank E. Harris. A quantum mechanical study of the He, H^-, He–He and He–H systems. *Molecular Physics*, 7(3):287–295, 1964. CODEN MOPHAM. ISSN 0026-8976 (print), 1362-3028 (electronic). URL http://adsabs.harvard.edu/abs/1964MolPh...7..287T.

Harris:1965:DFS

[60] Frank E. Harris. Discussion following Slater's paper. *Journal of Chemical Physics*, 43(10):S17, November 15, 1965. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). See [346].

Harris:1965:EMI

[61] Frank E. Harris and H. Harvey Michels. Evaluation of multicenter integrals occurring in molecular quantum mechanics. *Journal of Chemical Physics*, 42(9):3325–3326, May 1965. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://adsabs.harvard.edu/abs/1965JChPh..42.3325H; http://scitation.aip.org/content/aip/journal/jcp/42/9/10.1063/1.1696419.

Harris:1965:IPS

[62] Frank E. Harris, David A. Micha, and Herbert A. Pohl. The interaction potential surface for H_3. *Arkiv för fysik*, 30(??):259–266, December 13–17, 1965. CODEN AFYSA7. ISSN 0365-2440.

Harris:1965:MIQ

[63] Frank E. Harris and H. Harvey Michels. Multicenter integrals in quantum mechanics. I. Expansion of Slater-type orbitals about a new origin. *Journal of Chemical Physics*, 43(10):S165–S169, July 1965. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://adsabs.harvard.edu/abs/1965JChPh..43..165H; http://scitation.aip.org/content/aip/journal/jcp/43/10/10.1063/1.1701480.

Harris:1965:SSM

[64] Frank E. Harris and Herbert A. Pohl. Split-shell molecular orbitals for sigma bonded systems: Hydrogen halides. *Journal of Chemical Physics*, 42 (10):3648–3651, May 15, 1965. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/42/10/10.1063/1.1695775`.

Rein:1965:SHBa

[65] Robert Rein and Frank E. Harris. Studies of hydrogen bonded systems. II. Tunneling and tautomeric equilibria in the N–H$\cdots$N hydrogen bond of the guanine–cytosine base pair. *Journal of Chemical Physics*, 42(6): 2177–2180, March 15, 1965. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/42/6/10.1063/1.1696263`.

Rein:1965:SHBb

[66] Robert Rein and Frank E. Harris. Studies of hydrogen bonded systems. III. Potential energy surface, tunneling, and tautomeric equilibria in the N–H$\cdots$N and O$\cdots$H–N bonds of the guanine–cytosine base pair. *Journal of Chemical Physics*, 43(12):4415–4421, December 15, 1965. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/43/12/10.1063/1.1696707`.

Harris:1966:AMI

[67] Frank E. Harris and Robert Rein. Approximation of molecular integrals. *Nature*, 212(5067):1232, December 10, 1966. CODEN NATUAS. ISSN 0028-0836 (print), 1476-4687 (electronic). URL `http://www.nature.com/nature/journal/v212/n5067/pdf/2121232a0.pdf`.

Harris:1966:CSD

[68] Frank E. Harris. On the calculation of spin densities. *Molecular Physics*, 11(3):243–256, January 1966. CODEN MOPHAM. ISSN 0026-8976 (print), 1362-3028 (electronic). URL `http://adsabs.harvard.edu/abs/1966MolPh..11..243H`.

Harris:1966:E

[69] Frank E. Harris and Robert Rein. Erratum. *Theoretica Chimica Acta*, 6 (5):452, January 1966. CODEN TCHAAM. ISSN 0040-5744. URL `http://link.springer.com/article/10.1007/BF00528472`. See [70].

Harris:1966:IAM

[70] Frank E. Harris and Robert Rein. Integral approximations for molecular orbital theory. *Theoretica Chimica Acta*, 6(1):73–82, January 1966. CODEN TCHAAM. ISSN 0040-5744. URL `http://link.springer.com/article/10.1007/BF00528293`. See erratum [69].

Harris:1966:MIQ

[71] Frank E. Harris and H. Harvey Michels. Multicenter integrals in quantum mechanics. II. Evaluation of electron-repulsion integrals for Slater-type orbitals. *Journal of Chemical Physics*, 45(1):116–123, July 1, 1966. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://adsabs.harvard.edu/abs/1966JChPh..45..116H`.

Harris:1966:PCH

[72] Frank E. Harris. Potential curve for HeH^+. *Journal of Chemical Physics*, 44(9):3636–3637, May 1, 1966. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/44/9/10.1063/1.1727277`.

Rein:1966:IEH

[73] Robert Rein, Nubuo Fukuda, Htain Win, George A. Clarke, and Frank E. Harris. Iterative extended Hückel theory. *Journal of Chemical Physics*, 45(12):4743–4744, December 15, 1966. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/45/12/10.1063/1.1727568`.

Rein:1966:SHB

[74] Robert Rein and Frank E. Harris. Studies of hydrogen bonded systems. IV. Radiation induced tunneling and tautomeric equilibria in the guanine–cytosine base pair. *Journal of Chemical Physics*, 45(5):1797–1799, September 1, 1966. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/45/5/10.1063/1.1727832`.

Harris:1967:EAS

[75] Frank E. Harris. Expansion approach to scattering. *Physical Review Letters*, 19(4):173–175, July 24, 1967. CODEN PRLTAO. ISSN 0031-9007 (print), 1079-7114 (electronic), 1092-0145. URL `http://link.aps.org/doi/10.1103/PhysRevLett.19.173`.

Harris:1967:EMI

[76] Frank E. Harris and H. Harvey Michels. *The Evaluation of Molecular Integrals for Slater-Type Orbitals*, pages 205–266. Volume 13 of Prigogine

[407], 1967. ISBN 0-470-14015-1. URL http://onlinelibrary.wiley.com/book/10.1002/9780470140154.

Harris:1967:MES

[77] Frank E. Harris. Matrix elements of spin interaction operators. *Journal of Chemical Physics*, 47(3):1047–1061, August 1, 1967. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://scitation.aip.org/content/aip/journal/jcp/47/3/10.1063/1.1711988.

Harris:1967:MOT

[78] Frank E. Harris. Molecular orbital theory. *Advances in Quantum Chemistry*, 3:61–127, 1967. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327608600878.

Harris:1967:OSO

[79] Frank E. Harris. Open-shell orthogonal molecular orbital theory. *Journal of Chemical Physics*, 46(7):2769–2776, April 1, 1967. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://scitation.aip.org/content/aip/journal/jcp/46/7/10.1063/1.1841112.

Harris:1967:OSV

[80] Frank E. Harris and H. Harvey Michels. Open-shell valence configuration-interaction studies of diatomic and polyatomic molecules. *International Journal of Quantum Chemistry*, 1(S1):329–338, January 16–21, 1967. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory.

Michels:1967:EAL

[81] H. Harvey Michels and Frank E. Harris. Expansion approach to low-energy electron-hydrogen-atom scattering. *Physical Review Letters*, 19(16):885–886, October 16, 1967. CODEN PRLTAO. ISSN 0031-9007 (print), 1079-7114 (electronic), 1092-0145. URL http://adsabs.harvard.edu/abs/1967PhRvL..19..885M.

Schaefer:1967:CIU

[82] Henry F. Schaefer III and Frank E. Harris. Configuration interaction using open-shell spin-projected functions. *Chemical Physics Letters*, 1(9):407–408, November 1967. CODEN CHPLBC. ISSN 0009-2614 (print), 1873-4448 (electronic). URL http://adsabs.harvard.edu/abs/1967CPL....1..407S; http://www.sciencedirect.com/science/article/pii/0009261467800496.

Harris:1968:DMS

[83] F. E. Harris and H. H. Michels. Diatomic molecule studies beyond the Hartree–Fock approximation. *Bulletin of the American Physical Society*, 13(??):191–??, ???? 1968. CODEN BAPSA6. ISSN 0003-0503.

Harris:1968:SCM

[84] Frank E. Harris. Self consistent methods in Hückel theory. *Journal of Chemical Physics*, 48(9):4027–4028, May 1, 1968. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/48/9/10.1063/1.1669730`.

Kaldor:1968:SEC

[85] Uzi Kaldor, Henry F. Schaefer III, and Frank E. Harris. Spin-extended and configuration-interaction studies of first-row atoms. *International Journal of Quantum Chemistry*, 2(S2):13–20, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

Michels:1968:CIS

[86] H. Harvey Michels and Frank E. Harris. Configuration interaction study of the linear H_3 system. *Journal of Chemical Physics*, 48(5):2371–2372, March 1, 1968. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/48/5/10.1063/1.1669440`.

Michels:1968:EDH

[87] H. Harvey Michels, Frank E. Harris, and James C. Browne. Electron detachment in $H^- + F$ and $H + F^-$ collisions. *Journal of Chemical Physics*, 48(6):2821–2822, March 1968. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://adsabs.harvard.edu/abs/1968JChPh..48.2821M`; `http://scitation.aip.org/content/aip/journal/jcp/48/6/10.1063/1.1669523`.

Michels:1968:IPL

[88] H. H. Michels and F. E. Harris. Interaction potentials for the low-lying states of HeNe+. *Bulletin of the American Physical Society*, 13(??):192–??, ???? 1968. CODEN BAPSA6. ISSN 0003-0503.

Michels:1968:VCI

[89] H. Harvey Michels and Frank E. Harris. Valence configuration interaction calculations for atomic scattering. *International Journal of Quantum*

Chemistry, 2(S2):21–27, January 15–20, 1968. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

Rein:1968:IEH

[90] Robert Rein, Nobuo Fukuda, George A. Clarke, and Frank E. Harris. Iterative extended Hückel study of nucleic acid bases. *Journal of Theoretical Biology*, 21(1):88–96, October 1968. CODEN JTBIAP. ISSN 0022-5193 (print), 1095-8541 (electronic). URL `http://www.sciencedirect.com/science/article/pii/0022519368900611`.

Rein:1968:MOS

[91] Robert Rein, George A. Clarke, and Frank E. Harris. Molecular orbital study of the hydrogen bonding of water. *Journal of Molecular Structure*, 2(2):103–109, August 1968. CODEN JMOSB4. ISSN 0022-2860 (print), 1872-8014 (electronic). URL `http://adsabs.harvard.edu/abs/1968JMoSt...2..103R`; `http://www.sciencedirect.com/science/article/pii/0022286068870322`.

Schaefer:1968:AHS

[92] Henry F. Schaefer III, Richard A. Klemm, and Frank E. Harris. Atomic hyperfine structure. I. Polarization wave functions for the ground states of B, C, N, O, and F. *Physical Review*, 176(1):49–58, December 5, 1968. CODEN PHRVAO. ISSN 0031-899X (print), 1536-6065 (electronic). URL `http://link.aps.org/doi/10.1103/PhysRev.176.49`.

Schaefer:1968:CEA

[93] Henry F. Schaefer III and Frank E. Harris. Calculation of the electron affinity of boron. *Physical Review*, 170(1):108–115, June 5, 1968. CODEN PHRVAO. ISSN 0031-899X (print), 1536-6065 (electronic). URL `http://link.aps.org/doi/10.1103/PhysRev.170.108`.

Schaefer:1968:CUA

[94] Henry F. Schaefer III and Frank E. Harris. Construction and use of atomic *L–S* eigenfunctions. *Journal of Computational Physics*, 3(2):217–225, October 1968. CODEN JCTPAH. ISSN 0021-9991 (print), 1090-2716 (electronic). URL `http://www.sciencedirect.com/science/article/pii/0021999168900193`.

Schaefer:1968:ESA

[95] Henry F. Schaefer III and Frank E. Harris. Electronic structure of atomic boron. *Physical Review*, 167(1):67–73, March 5, 1968. CODEN PHRVAO.

ISSN 0031-899X (print), 1536-6065 (electronic). URL http://link.aps.org/doi/10.1103/PhysRev.167.67.

Schaefer:1968:ICL

[96] Henry F. Schaefer III and Frank E. Harris. Ab initio calculations on 62 low lying states of the O_2 molecule. *Journal of Chemical Physics*, 48 (11):4946–4955, June 1, 1968. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://scitation.aip.org/content/aip/journal/jcp/48/11/10.1063/1.1668161.

Schaefer:1968:MDS

[97] Henry F. Schaefer III and Frank E. Harris. Metastability of the ^{1}D state of the nitrogen negative ion. *Physical Review Letters*, 21(23):1561–1563, December 2, 1968. CODEN PRLTAO. ISSN 0031-9007 (print), 1079-7114 (electronic), 1092-0145. URL http://link.aps.org/doi/10.1103/PhysRevLett.21.1561.

Schaefer:1968:MSN

[98] Henry F. Schaefer III and Frank E. Harris. Metastability of the ^{1}D state of the nitrogen negative ion. *Physical Review Letters*, 21(23):1561–1563, December 2, 1968. CODEN PRLTAO. ISSN 0031-9007 (print), 1079-7114 (electronic), 1092-0145. URL http://adsabs.harvard.edu/abs/1968PhRvL..21.1561S; http://www.sciencedirect.com/science/article/pii/0022286068870322.

Harris:1969:CCE

[99] Frank E. Harris and Hendrik J. Monkhorst. Complete calculations of the electronic energies of solids. *Physical Review Letters*, 23(18):1026–1030, November 3, 1969. CODEN PRLTAO. ISSN 0031-9007 (print), 1079-7114 (electronic), 1092-0145. URL http://link.aps.org/doi/10.1103/PhysRevLett.23.1026.

Harris:1969:CCI

[100] Frank E. Harris and H. Harvey Michels. Comparison of configuration-interaction methods for F_2. *International Journal of Quantum Chemistry*, 4(S3b):461–467, January 13–18, 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Quantum Biology and Quantum Pharmacology.

Harris:1969:ETI

[101] Frank E. Harris and H. Harvey Michels. Expansion technique for inelastic scattering. *Physical Review Letters*, 22(20):1036–1039, May 19, 1969.

CODEN PRLTAO. ISSN 0031-9007 (print), 1079-7114 (electronic), 1092-0145. URL http://link.aps.org/doi/10.1103/PhysRevLett.22.1036.

Harris:1969:IEA

[102] Frank E. Harris and H. Harvey Michels. Integrals for electron-atom scattering calculations. *Journal of Computational Physics*, 4(4):579–593, December 1969. CODEN JCTPAH. ISSN 0021-9991 (print), 1090-2716 (electronic). URL http://www.sciencedirect.com/science/article/pii/0021999169900229.

Harris:1969:LSM

[103] Frank E. Harris and Hendrik J. Monkhorst. Lattice sums and Madelung constants. *Chemical Physics Letters*, 4(4):181–182, November 1, 1969. CODEN CHPLBC. ISSN 0009-2614 (print), 1873-4448 (electronic). URL http://adsabs.harvard.edu/abs/1969CPL.....4..181H; http://www.sciencedirect.com/science/article/pii/000926146980093X.

Harris:1969:QMC

[104] F. E. Harris. Quantum mechanics in the chemistry curriculum. *Abstracts of Papers of the American Chemical Society*, 158(??):CHED–21, ???? 1969. CODEN ACSRAL. ISSN 0065-7727.

Harris:1969:REC

[105] Frank E. Harris. Rapid evaluation of Coulomb integrals. *Journal of Chemical Physics*, 51(11):4770–4778, December 1, 1969. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://scitation.aip.org/content/aip/journal/jcp/51/11/10.1063/1.1671865.

Kaldor:1969:SOS

[106] Uzi Kaldor and Frank E. Harris. Spin-optimized self-consistent field wave functions. *Physical Review*, 183(1):1–7, July 5, 1969. CODEN PHRVAO. ISSN 0031-899X (print), 1536-6065 (electronic). URL http://link.aps.org/doi/10.1103/PhysRev.183.1.

Michels:1969:CCS

[107] H. Harvey Michels, Frank E. Harris, and R. M. Scolsky. Calculation of cross-sections for electron–helium collisions. *Physics Letters A*, 28 (7):467–468, January 13, 1969. CODEN PYLAAG. ISSN 0375-9601 (print), 1873-2429 (electronic). URL http://adsabs.harvard.edu/abs/1969PhLA...28..467M; http://www.sciencedirect.com/science/article/pii/037596016990629X.

Michels:1969:OET

[108] H. Harvey Michels and Frank E. Harris. An optimum expansion technique for inelastic scattering. In Anonymous, editor, *6th International Conference on the Physics of Electronic and Atomic Collisions, VI ICPEAC. Abstracts of papers from the 6th International Conference, held at MIT, Cambridge, Massachusetts from July 28–August 2, 1969*, pages 384–?? MIT Press, Cambridge, MA, USA, 1969. ISSN 0538-6268. LCCN QC721 .I573. URL `http://adsabs.harvard.edu/abs/1969peac.conf..384M`.

Michels:1969:PES

[109] H. Harvey Michels and Frank E. Harris. Predissociation effects in the A $^2\Sigma^+$ state of the OH radical. *Chemical Physics Letters*, 3(6):441–442, June 1969. CODEN CHPLBC. ISSN 0009-2614 (print), 1873-4448 (electronic). URL `http://adsabs.harvard.edu/abs/1969CPL.....3..441M`; `http://www.sciencedirect.com/science/article/pii/0009261469801612`.

Michels:1969:VCI

[110] H. Harvey Michels and Frank E. Harris. Valence configuration interaction calculations for atomic scattering. *International Journal of Quantum Chemistry*, 3(5):751, September 1969. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Monkhorst:1969:MIG

[111] Hendrik J. Monkhorst and Frank E. Harris. Multicenter integrals via Gaussian expansion of Slater-orbital products. *Chemical Physics Letters*, 3(7):537–539, August 1969. CODEN CHPLBC. ISSN 0009-2614 (print), 1873-4448 (electronic). URL `http://adsabs.harvard.edu/abs/1969CPL.....3..537M`; `http://www.sciencedirect.com/science/article/pii/0009261469850566`.

Schaefer:1969:AHS

[112] Henry F. Schaefer III, Richard A. Klemm, and Frank E. Harris. Atomic hyperfine structure. II. First-order wave functions for the ground states of B, C, N, O, and F. *Physical Review*, 181(1):137–143, May 5, 1969. CODEN PHRVAO. ISSN 0031-899X (print), 1536-6065 (electronic). URL `http://link.aps.org/doi/10.1103/PhysRev.181.137`.

Schaefer:1969:FOW

[113] Henry F. Schaefer III, Richard A. Klemm, and Frank E. Harris. First-order wavefunctions, orbital correlation energies, and electron affinities of first row atoms. *Journal of Chemical Physics*, 51(10):4643–4650, November

15, 1969. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://scitation.aip.org/content/aip/journal/jcp/51/10/10.1063/1.1671837.

Smith:1969:PES

[114] Vedene H. Smith, Jr. and Frank E. Harris. Projection of exact spin eigenfunctions. *Journal of Mathematical Physics*, 10(4):771–778, April 1969. CODEN JMAPAQ. ISSN 0022-2488 (print), 1089-7658 (electronic), 1527-2427. URL http://jmp.aip.org/resource/1/jmapaq/v10/i4/p771_s1.

Harris:1970:ANM

[115] Frank E. Harris and Hendrik J. Monkhorst. Application of new Madelung summation method to close packed alkali halide structures. *Journal of Chemical Physics*, 52(8):4310–4311, April 15, 1970. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://scitation.aip.org/content/aip/journal/jcp/52/8/10.1063/1.1673644.

Harris:1970:ESS

[116] Frank E. Harris and Hendrik J. Monkhorst. Electronic-structure studies of solids. I. Fourier representation method for Madelung sums. *Physical Review B: Solid State*, 2(11):4400–4405, December 1, 1970. CODEN PLRBAQ. ISSN 0556-2805. URL http://link.aps.org/doi/10.1103/PhysRevB.2.4400. See erratum [145].

Harris:1970:IQM

[117] F. E. Harris. Ab-initio quantum-mechanical calculations for atomic and molecular processes. *Bulletin of the American Physical Society*, 15(??): 1525–??, ???? 1970. CODEN BAPSA6. ISSN 0003-0503.

Harris:1970:SAC

[118] Frank E. Harris. Systematics of atomic correlation energies. *Journal de physique (Paris)*, 31(11–12):C4–111–C4–115, November/December 1970. CODEN JOPQAG. ISSN 0302-0738. URL http://hal.archives-ouvertes.fr/docs/00/21/38/74/PDF/ajp-jphyscol197031C419.pdf; http://www.journaldephysique.org/articles/jphyscol/abs/1970/04/jphyscol197031C419/jphyscol197031C419.html.

Harris:1970:THF

[119] F. E. Harris and H. J. Monkhorst. Toward Hartree–Fock calculations for simple crystals. *Bulletin of the American Physical Society*, 15(??):890–??, ???? 1970. CODEN BAPSA6. ISSN 0003-0503.

Michels:1970:ECE

[120] H. H. Michels, H. J. Kolker, J. W. Viers, and F. E. Harris. Expansion calculations of electron–hydrogen scattering. *Bulletin of the American Physical Society*, 15(??):1523–??, ???? 1970. CODEN BAPSA6. ISSN 0003-0503.

Michels:1970:MOS

[121] H. Harvey Michels, Frank E. Harris, and J. B. Addison. Molecular orbital studies of the stability of CH_5^+ and BH_5. *International Journal of Quantum Chemistry*, 5(S4):149–151, January 19–24, 1970. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory and Quantum Biology.

Rein:1970:IEH

[122] Robert Rein, George A. Clarke, and Frank E. Harris. Iterative extended Hückel studies of electronic structure with application to heterocyclic compounds. In Bergmann and Pullman [408], pages 86–117. ISSN 0075-3696. LCCN QD331 .A75.

Schaefer:1970:CAP

[123] Henry F. Schaefer III, Donald R. McLaughlin, Frank E. Harris, and Berni J. Alder. Calculation of the attractive He pair potential. *Physical Review Letters*, 25(15):988–990, October 12, 1970. CODEN PRLTAO. ISSN 0031-9007 (print), 1079-7114 (electronic), 1092-0145. URL `http://link.aps.org/doi/10.1103/PhysRevLett.25.988`.

Viers:1970:PCE

[124] Jimmy W. Viers, Frank E. Harris, and Henry F. Schaefer III. Pair correlations and the electronic structure of neon. *Physical Review A (Atomic, Molecular, and Optical Physics)*, 1(1):24–27, January 1, 1970. CODEN PLRAAN. ISSN 1050-2947 (print), 1094-1622, 1538-4446, 1538-4519. URL `http://link.aps.org/doi/10.1103/PhysRevA.1.24`.

Harris:1971:EHFa

[125] Frank E. Harris, Lalit Kumar, and Hendrik J. Monkhorst. "Exact" Hartree–Fock results for atomic hydrogen crystals. *International Journal of Quantum Chemistry*, 5(S5):527–531, January 18–23, 1971. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular and Solid-State Theory and Quantum Biology.

Harris:1971:EHFb

[126] Frank E. Harris and Hendrik J. Monkhorst. 'Exact' Hartree–Fock calculations for atomic-hydrogen crystal. *Solid State Communications*, 9 (17):1449–1453, September 1, 1971. CODEN SSCOA4. ISSN 0038-1098 (print), 1879-2766 (electronic). URL `http://adsabs.harvard.edu/abs/1971SSCom...9.1449H`; `http://www.sciencedirect.com/science/article/pii/0038109871901542`.

Harris:1971:EME

[127] Frank E. Harris and H. Harvey Michels. Expansion methods for electron atom scattering. In Alder et al. [409], pages 143–210. ISBN 0-12-460810-8. ISSN 0076-6860. LCCN QA401 .M514 v.10. URL `http://www.sciencedirect.com/science/article/pii/B9780124608108500099`.

Harris:1971:QMB

[128] Frank E. Harris and Robert Rein. Quantum mechanics in biochemistry. In Thewlis et al. [412], pages 351–354. ISBN 0-08-006359-4. LCCN ????

Harris:1971:SRA

[129] Frank E. Harris and H. Harvey Michels. Scattering resonances in algebraic expansion methods. In Branscomb et al. [410], pages 84–?? ISBN 0-7204-0234-4, 0-7204-0235-2 (vol. 1), 0-7204-0236-0 (vol. 2). LCCN QC721 I618 1971; QC794.6.C6. URL `http://adsabs.harvard.edu/abs/1971peac.conf...84H`.

Harris:1971:THF

[130] Frank E. Harris and Hendrik J. Monkhorst. Toward Hartree–Fock calculations for simple crystals. In Marcus et al. [411], pages 517–541. ISBN 1-4684-1892-0 (print), 1-4684-1890-4 (e-book). URL `http://link.springer.com/chapter/10.1007/978-1-4684-1890-3_44`.

Herbelin:1971:BZD

[131] John M. Herbelin and Frank E. Harris. Balanced zero-differential-overlap approximations in nonempirical molecular orbital calculations. *Journal of the American Chemical Society*, 93(10):2565–2566, 1971. CODEN JACSAT. ISSN 0002-7863 (print), 1520-5126 (electronic), 1943-2984. URL `http://pubs.acs.org/doi/abs/10.1021/ja00739a051`.

Matsen:1971:CST

[132] F. A. Matsen, Harrison Shull, Peter Lykos, and Frank Harris. Computational support for theoretical chemistry: report of a conference held at the

National Institutes of Health Bethesda, Maryland, May 8–9, 1970. Report, National Academy of Sciences, Washington, DC, USA, 1971. vii + 51 pp. URL `https://books.google.com/books?id=ZUArAAAAYAAJ&pg=PR3`. See also the sequel report [151].

Michels:1971:APC

[133] H. Harvey Michels and Frank E. Harris. Adiabatic potential curves for the system O + O^-. In Branscomb et al. [410], pages 1170–?? ISBN 0-7204-0234-4, 0-7204-0235-2 (vol. 1), 0-7204-0236-0 (vol. 2). LCCN QC721 I618 1971; QC794.6.C6. URL `http://adsabs.harvard.edu/abs/1971peac.conf.1170M`.

Harris:1972:FRM

[134] Frank E. Harris. Fourier representation methods for electronic structures of linear polymers. *Journal of Chemical Physics*, 56(9):4422–4425, May 1, 1972. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/56/9/10.1063/1.1677884`.

Harris:1972:HFP

[135] Frank E. Harris, Lalit Kumar, and Hendrik J. Monkhorst. The Hartree–Fock problem for lithium crystals: a preliminary report. *J Phys*, 33(C3): 99–101, ???? 1972.

Harris:1972:QC

[136] Frank E. Harris. Quantum chemistry. *Annual Review of Physical Chemistry*, 23:415–438, October 1972. CODEN ARPLAP. ISSN 0066-426X (print), 1545-1593 (electronic). URL `http://adsabs.harvard.edu/abs/1972ARPC...23..415H`; `http://www.annualreviews.org/doi/abs/10.1146/annurev.pc.23.100172.002215`.

Monkhorst:1972:ACF

[137] Hendrik J. Monkhorst and Frank E. Harris. Accurate calculation of Fourier transform of two-center Slater orbital products. *International Journal of Quantum Chemistry*, 6(4):601–607, July 1972. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:1973:ALM

[138] Frank E. Harris. Approximations for large-molecule calculations. In Herman et al. [413], pages 81–86. ISBN 1-4684-2015-1 (print), 1-4684-2013-5 (e-book). LCCN QD450-882. URL `http://link.springer.com/chapter/10.1007/978-1-4684-2013-5_10`.

Harris:1973:CSP

[139] Frank E. Harris. Construction of spin-projected matrix elements. In Smith and McRae [414], pages 112–129. ISBN 0-471-80140-2. LCCN QD462.A1 B68 1972. Proceedings of the Boulder Quantum Theory Symposium and Research Workshop, held at the University of Colorado, Boulder, CO, USA, June 1972.

Harris:1973:ESS

[140] Frank E. Harris, Lalit Kumar, and Hendrik J. Monkhorst. Electronic-structure studies of solids. II. "Exact" Hartree–Fock calculations for cubic atomic-hydrogen crystals. *Physical Review B: Solid State*, 7(6):2850–2866, March 15, 1973. CODEN PLRBAQ. ISSN 0556-2805. URL `http://link.aps.org/doi/10.1103/PhysRevB.7.2850`.

Trautwein:1973:ISC

[141] Alfred Trautwein, J. R. Regnard, Frank E. Harris, and Yutaka Maeda. Isomer-shift calibrations using multivalent states of ^{57}Fe in $KMgF_3$. *Physical Review B: Solid State*, 7(3):947–951, February 1, 1973. CODEN PLRBAQ. ISSN 0556-2805. URL `http://link.aps.org/doi/10.1103/PhysRevB.7.947`.

Trautwein:1973:MOSa

[142] Alfred Trautwein and Frank E. Harris. Molecular-orbital study of Mössbauer results on iron dissolved in solid noble gases. *Physical Review B: Solid State*, 7(11):4755–4757, June 1, 1973. CODEN PLRBAQ. ISSN 0556-2805. URL `http://link.aps.org/doi/10.1103/PhysRevB.7.4755`.

Trautwein:1973:MOSb

[143] Alfred Trautwein and Frank E. Harris. Molecular orbital structure, Mössbauer isomer shift, and quadrupole splitting in iron complexes. *Theoretica Chimica Acta*, 30(1):45–58, March 1973. CODEN TCHAAM. ISSN 0040-5744. URL `http://link.springer.com/article/10.1007/BF00527634`.

Harris:1974:CAE

[144] F. E. Harris. Chemists approach to electronic-structure calculations on crystalline solids. *Abstracts of Papers of the American Chemical Society*, 167(??):PHYS–35, ???? 1974. CODEN ACSRAL. ISSN 0065-7727.

Harris:1974:EES

[145] Frank E. Harris and Hendrik J. Monkhorst. Erratum: "*Electronic-structure studies of solids. I. Fourier representation method for Madelung*

sums". *Physical Review B: Solid State*, 9(9):3946, May 1, 1974. CODEN PLRBAQ. ISSN 0556-2805. URL `http://link.aps.org/doi/10.1103/PhysRevB.9.3946.3`. See [116].

Harris:1974:MCN

[146] F. E. Harris. Meeting computing needs in chemistry. *Abstracts of Papers of the American Chemical Society*, 168(??):COMP–3, ???? 1974. CODEN ACSRAL. ISSN 0065-7727.

Kumar:1974:ESS

[147] Lalit Kumar, Hendrik J. Monkhorst, and Frank E. Harris. Electronic-structure studies of solids. III. Hartree–Fock band functions and energies for cubic lithium crystals. *Physical Review B: Solid State*, 9(10):4084–4095, May 15, 1974. CODEN PLRBAQ. ISSN 0556-2805. URL `http://link.aps.org/doi/10.1103/PhysRevB.9.4084`.

Trautwein:1974:IEM

[148] Alfred Trautwein, Frank E. Harris, and Istvan Dézsi. Interpretation of experimental Mössbauer quadrupole splittings of iron pentacyanide complexes using molecular orbital theory. *Theoretica Chimica Acta*, 35(3): 231–236, September 1974. CODEN TCHAAM. ISSN 0040-5744. URL `http://link.springer.com/article/10.1007/BF00546907`.

Trautwein:1974:IEQ

[149] Alfred Trautwein, Reiner Reschke, Reinhart Zimmermann, Istvan Dézsi, and Frank E. Harris. Interpretation of experimental quadrupole splitting of iron-containing complexes using molecular orbital theory. *Journal de physique (Paris)*, 35(C6):235–239, December 1974. CODEN JOPQAG. ISSN 0302-0738. URL `http://jphyscol.journaldephysique.org/articles/jphyscol/abs/1974/06/jphyscol197435C630/jphyscol197435C630.html`.

Trautwein:1974:MMO

[150] Alfred Trautwein, Yutaka Maeda, Frank E. Harris, and Helmuth Formanek. Mössbauer and molecular orbital study of the myoglobin-CO complex. *Theoretica Chimica Acta*, 36(1):67–76, March 1974. CODEN TCHAAM. ISSN 0040-5744. URL `http://link.springer.com/article/10.1007/BF00549150`.

Wiberg:1974:SNC

[151] Kenneth B. Wiberg, Lawrence S. Bartell, Jacob Bigeleisen, Robert B. K. Dewar, Frank E. Harris, F. A. Matsen, Harrison Shull, and Lawrence C. Snyder. A study of a national center for computation in chemistry. Report,

National Academy of Sciences, Washington, DC, USA, 1974. ix + 79 pp. URL `https://books.google.com/books?id=qTYrAAAAYAAJ`. This is a sequel to an earlier report [132].

Harris:1975:ESC

[152] Frank E. Harris. Electronic structure calculations on crystals and polymers. In André et al. [415], pages 453–477. ISBN 1-4757-0321-X (print), 1-4757-0319-8 (e-book). LCCN QD380.N371974. URL `http://link.springer.com/chapter/10.1007/978-1-4757-0319-1_12`.

Harris:1975:HFS

[153] Frank E. Harris. Hartree–Fock studies of electronic structures of crystalline solids. In Eyring and Henderson [416], pages 147–218. CODEN THCHDM. ISBN 0-323-15958-3, 0-12-681901-7 (e-book). ISSN 0305-9995. LCCN ???? URL `http://www.sciencedirect.com/science/article/pii/B9780126819014500118`.

Harris:1975:RAP

[154] Frank E. Harris and Richard H. Ault. Remote-access programming system for electronic-structure calculations. *Abstracts of Papers of the American Chemical Society*, ??(169):30, ???? 1975. CODEN ACSRAL. ISSN 0065-7727.

Kreber:1975:MMB

[155] E. Kreber, Ulrich Gonser, Alfred Trautwein, and Frank E. Harris. Mössbauer measurements of bipyramidal lattice site in $BaFe_{12}O_{19}$. *The Journal of Physics and Chemistry of Solids*, 36(4):263–265, ???? 1975. CODEN JPCSAW. ISSN 0022-3697 (print), 1879-2553 (electronic). URL `http://www.sciencedirect.com/science/article/pii/0022369775900190`.

Ramaker:1975:EEC

[156] David E. Ramaker, Lalit Kumar, and Frank E. Harris. Exact-exchange crystal Hartree–Fock calculations of molecular and metallic hydrogen and their transitions. *Physical Review Letters*, 34(13):812–814, March 31, 1975. CODEN PRLTAO. ISSN 0031-9007 (print), 1079-7114 (electronic), 1092-0145. URL `http://link.aps.org/doi/10.1103/PhysRevLett.34.812`.

Trautwein:1975:CED

[157] Alfred Trautwein and Frank E. Harris. Calculated electron densities and experimental isomer shifts of Fe-57 in deoxy- and CO-compounds of myoglobin and hemoglobin. *Theoretica Chimica Acta*, 38(1):65–69, March 1975. CODEN TCHAAM. ISSN 0040-5744.

Trautwein:1975:MOM

[158] Alfred Trautwein, E. Kreber, Ulrich Gonser, and Frank E. Harris. Molecular orbital and Mössbauer study of iron–oxygen compounds. *The Journal of Physics and Chemistry of Solids*, 36(4):325–328, April 1975. CODEN JPCSAW. ISSN 0022-3697 (print), 1879-2553 (electronic). URL `http://www.sciencedirect.com/science/article/pii/0022369775900311`.

Trautwein:1975:MSQ

[159] Alfred Trautwein, Reinhart Zimmermann, and Frank E. Harris. Molecular-structure, quadrupole splitting, and magnetic-susceptibility of iron in deoxygenated myoglobin and hemoglobin. *Theoretica Chimica Acta*, 37(2):89–104, June 1975. CODEN TCHAAM. ISSN 0040-5744.

Trautwein:1975:RED

[160] Alfred Trautwein, Frank E. Harris, Arthur J. Freeman, and Jean-Paul Desclaux. Relativistic electron densities and isomer shifts of ^{57}Fe in iron-oxygen and iron-fluorine clusters and of iron in solid noble gases. *Physical Review B: Solid State*, 11(11):4101–4105, June 1, 1975. CODEN PLRBAQ. ISSN 0556-2805. URL `http://link.aps.org/doi/10.1103/PhysRevB.11.4101`.

Zimmermann:1975:EMS

[161] Reinhart Zimmermann, Alfred Trautwein, and Frank E. Harris. Electronic and magnetic structure of α-$FeSO_4$. *Physical Review B: Solid State*, 12 (9):3902–3907, November 1, 1975. CODEN PLRBAQ. ISSN 0556-2805. URL `http://link.aps.org/doi/10.1103/PhysRevB.12.3902`.

Harris:1976:TDC

[162] Frank E. Harris. Technique development for complete electronic-structure calculations in crystalline solids. Technical report, Department of Physics, University of Utah, Salt Lake City, UT, USA, March 1976. URL `http://adsabs.harvard.edu/abs/1976utah.rept.....H`. Final Report, 1 Nov. 1970–31 Oct. 1975.

Trautwein:1976:SIF

[163] Alfred Trautwein, Reiner Reschke, Istvan Dézsi, and Frank E. Harris. Spectroscopic investigation of ferrocene and related derivatives. *Journal de physique (Paris)*, 37(12(C-6)):463–470, December 1976. CODEN JOPQAG. ISSN 0302-0738. URL `http://jphyscol.journaldephysique.org/articles/jphyscol/abs/1976/06/jphyscol197637C691/jphyscol197637C691.html`. International Conference on the Applications of the Mössbauer Effect = Conférence

internationale sur les applications de l'effet Mössbauer, Corfu, Greece, September 13–17, 1976.

Harris:1977:CAT

[164] Frank E. Harris. Convergence acceleration technique for lattice sums arising in electronic-structure studies of crystalline solids. *Journal of Mathematical Physics*, 18(12):2377–2381, December 1977. CODEN JMAPAQ. ISSN 0022-2488 (print), 1089-7658 (electronic), 1527-2427. URL `http://jmp.aip.org/resource/1/jmapaq/v18/i12/p2377_s1`.

Harris:1977:CCM

[165] Frank E. Harris. Coupled-cluster method for excitation energies. *International Journal of Quantum Chemistry*, 12(S11):403–411, January 16–22, 1977. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory, Collision Phenomena, and Computational Methods.

Harris:1977:IME

[166] Frank E. Harris. *Ab Initio* methods for electronic structures of crystalline solids. In Phariseau and Scheire [417], pages 274–320. ISBN 0-306-35724-0, 1-4684-2813-6 (print), 1-4684-2811-X (e-book). LCCN QC176.8.E4 N34 1976. URL `http://link.springer.com/chapter/10.1007/978-1-4684-2811-7_4`.

Harris:1977:SSM

[167] Frank E. Harris and Joseph Delhalle. Structure and stability of metallic hydrogen. *Physical Review Letters*, 39(21):1340–1342, November 21, 1977. CODEN PRLTAO. ISSN 0031-9007 (print), 1079-7114 (electronic), 1092-0145. URL `http://link.aps.org/doi/10.1103/PhysRevLett.39.1340`.

Reschke:1977:ESP

[168] Reiner Reschke, Alfred Trautwein, and Frank E. Harris. Electronic structure, pressure- and temperature-dependent charge densities, and electric field gradients in FeF_2. *Physical Review B: Solid State*, 15 (5):2708–2717, March 1, 1977. CODEN PLRBAQ. ISSN 0556-2805. URL `http://adsabs.harvard.edu/abs/1977PhRvB..15.2708R`; `http://prb.aps.org/abstract/PRB/v15/i5/p2708_1`.

Delhalle:1978:EST

[169] Joseph Delhalle, S. Delhalle, and Frank E. Harris. Evaluation of some trigonometric series occurring in infinite chain polymer calculations. *Inter-*

national Journal of Quantum Chemistry, 13(2):239–254, February 1978. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Delhalle:1978:FRM

[170] Joseph Delhalle and Frank E. Harris. Fourier representation method for electronic structures of linear polymers. II. Linear chain of hydrogen atoms. *Theoretica Chimica Acta*, 48(2):127–141, June 1978. CODEN TCHAAM. ISSN 0040-5744.

Harris:1978:FRM

[171] Frank E. Harris. Fourier representation methods in electronic structure studies of crystals and polymers. In André et al. [418], pages 117–135. ISBN 94-009-9814-7 (print), 94-009-9812-0 (e-book). URL `http://link.springer.com/chapter/10.1007/978-94-009-9812-4_7`.

Harris:1978:HLM

[172] Frank E. Harris. Hartree-like methods in electronic structure theory. *International Journal of Quantum Chemistry*, 13(2):189–198, February 1978. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:1979:EN

[173] Frank E. Harris and Nelson H. F. Beebe. Editors' note. In *Proceedings of the conference Software Standards in Chemistry, Held at the University of Utah, July 25–27, 1979* [419], pages ix–x. URL `http://escholarship.org/uc/item/19b1d4sw`.

Harris:1979:HFF

[174] Frank E. Harris, Hendrik J. Monkhorst, and William A. Schwalm. Hartree–Fock formalism for the calculation of total energies and charge densities of thin films. *Journal of Vacuum Science Technology*, 16 (5):1318–1322, September 1979. CODEN JVSTAL. ISSN 0022-5355. URL `http://scitation.aip.org/content/avs/journal/jvst/16/5/10.1116/1.570149`.

Randic:1979:RHE

[175] Milan Randić and Frank E. Harris. Reduction of hybrid electron repulsion integrals to overlap integrals. *Croatica Chemica Acta*, 52(4):347–352, ???? 1979. CODEN CCACAA. ISSN 0011-1643 (print), 1334-417X (electronic).

Reschke:1979:ESEa

[176] Reiner Reschke, Alfred Trautwein, Frank E. Harris, and Sadgopal K. Date. Electronic structure and electric field gradient tensor in potassium ferricyanide. *Journal de physique (Paris)*, 40(C2):280–282,

March 1979. CODEN JOPQAG. ISSN 0302-0738. URL http://jphyscol.journaldephysique.org/articles/jphyscol/abs/1979/02/jphyscol197940C299/jphyscol197940C299.html.

Reschke:1979:ESEb

[177] Reiner Reschke, Alfred Trautwein, Frank E. Harris, and Sadgopal K. Date. Electronic structure, electron density, electric field gradient-, magnetic susceptibility- and G-tensor of $K_3Fe(CN)_6$. *Journal of Magnetism and Magnetic Materials*, 12(2):176–186, June/July 1979. CODEN JMMMDC. ISSN 0304-8853 (print), 1873-4766 (electronic). URL http://adsabs.harvard.edu/abs/1979JMMM...12..176R; http://www.sciencedirect.com/science/article/pii/0304885379900131.

Harris:1980:CCM

[178] Frank E. Harris. The coupled-cluster method. In Harris et al. [420], pages 422–439. Two volumes.

Harris:1980:DMB

[179] Frank E. Harris. Diagrams and many-body perturbation theory. In Harris et al. [420], pages 336–393. Two volumes.

Harris:1980:FMM

[180] Frank E. Harris, Alfred Trautwein, and Joseph Delhalle. The FAKE method of molecular orbital calculation. *International Journal of Quantum Chemistry*, 18(S14):355–361, March 10–20, 1980. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-State Theory, Collision Phenomena, Quantum Statistics, and Computational Methods.

Harris:1980:FMO

[181] Frank E. Harris, Alfred Trautwein, and Joseph Delhalle. FAKE molecular-orbital calculations. *Chemical Physics Letters*, 72(2):315–318, June 1, 1980. CODEN CHPLBC. ISSN 0009-2614 (print), 1873-4448 (electronic). URL http://adsabs.harvard.edu/abs/1980CPL....72..315H; http://www.sciencedirect.com/science/article/pii/0009261480802995.

Harris:1980:XM

[182] Frank E. Harris. The x-α method. In Harris et al. [420], pages 293–302. Two volumes.

Harris:1981:CCM

[183] Frank E. Harris. Coupled cluster method for electron correlation. In ????, editor, *Proceedings of Workshop on Effective Potentials for Real Materials*, page ?? IBM, Poughkeepsie, NY, USA, 1981. ISBN ???? LCCN ????

Harris:1981:CTA

[184] Frank E. Harris, Bogumił Jeziorski, and Hendrik J. Monkhorst. Contraction theorem for the algebraic reduction of (anti)commutators involving operator strings. *Physical Review A (3)*, 23(4):1632–1638, April 1, 1981. CODEN PLRAAN. ISSN 0556-2791. URL `http://link.aps.org/doi/10.1103/PhysRevA.23.1632`.

Harris:1981:M

[185] Frank E. Harris. Molecules. In Lerner and Trigg [421], pages 745–749. ISBN 0-201-04313-0. LCCN QC5 .E545 1981. Foreword by Walter Sullivan.

Harris:1981:TFS

[186] Frank E. Harris. Thin films, surfaces and interfaces: A Fourier-transform theory of their electronic structure. Technical report, Department of Physics, University of Utah, Salt Lake City, UT, USA, May 1981. URL `http://adsabs.harvard.edu/abs/1981utah.rept.....H`. Final Report, 1 May 1977–30 Apr. 1980.

Monkhorst:1981:RSO

[187] Hendrik J. Monkhorst, Bogumił Jeziorski, and Frank E. Harris. Recursive scheme for order-by-order many-body perturbation theory. *Physical Review A (3)*, 23(4):1639–1644, April 1, 1981. CODEN PLRAAN. ISSN 0556-2791. URL `http://link.aps.org/doi/10.1103/PhysRevA.23.1639`.

Harris:1982:AFS

[188] Frank E. Harris. Auxiliary functions for STO molecular integrals: Si, Ci and Ei. In Weatherford and Jones [422], pages 135–140. ISBN 94-009-7923-1 (print), 94-009-7921-5 (e-book). URL `http://link.springer.com/chapter/10.1007/978-94-009-7921-5_13`.

Harris:1983:EGM

[189] Frank E. Harris. Evaluation of GTO molecular integrals. *International Journal of Quantum Chemistry*, 23(4):1469–1478, April 1983. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Delhalle:1984:ECA

[190] Joseph Delhalle, Joseph G. Fripiat, and Frank E. Harris. Evaluation of computational aspects of a modified CS–LCAO–SCF–CO strategy for electronic structure calculations of extended model chains. *International Journal of Quantum Chemistry*, 26(S18):141–152, March 1–15, 1984. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Atomic, Molecular and Solid-State Theory, and Computational Quantum Chemistry.

Lauer:1984:ESC

[191] S. Lauer, Alfred X. Trautwein, and Frank E. Harris. Electronic-structure calculations, photoelectron spectra, optical spectra, and Mössbauer parameters for the pyrites MS_2 (M = Fe, Co, Ni, Cu, Zn). *Physical Review B: Condensed Matter and Materials Physics*, 29(12):6774–6783, June 15, 1984. CODEN PRBMDO. ISSN 1098-0121. URL `http://adsabs.harvard.edu/abs/1984PhRvB..29.6774L`; `http://prb.aps.org/abstract/PRB/v29/i12/p6774_1`.

Delhalle:1985:ACS

[192] Joseph Delhalle and Frank E. Harris. An alternative computational strategy for direct space Hartree–Fock calculations on extended model chains. *International Journal of Quantum Chemistry*, 27(2):219–229, February 1985. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Delhalle:1985:FRM

[193] Joseph Delhalle and Frank E. Harris. Fourier-representation method for electronic structure of chainlike systems: Restricted Hartree–Fock equations and applications to the $(H)_x$ chain in a basis of Gaussian functions. *Physical Review B: Condensed Matter and Materials Physics*, 31 (10):6755–6765, May 15, 1985. CODEN PRBMDO. ISSN 1098-0121. URL `http://link.aps.org/doi/10.1103/PhysRevB.31.6755`.

Trautwein:1985:AFM

[194] Alfred X. Trautwein, S. Lauer, Joseph Delhalle, and Frank E. Harris. Application of the FAKE molecular orbital method to diatomic molecules XY (X, Y = H, F, Cl, Br, I). *Theoretica Chimica Acta*, 67(3):175–185, April 1985. CODEN TCHAAM. ISSN 0040-5744.

Harris:1987:CLM

[195] Frank E. Harris and Antonios G. Koures. A closer look at the multiple scattering X-alpha (MS-X-alpha) method. *Abstracts of Papers of the American Chemical Society*, 193(??):137–PHYS, April 1987. CODEN ACSRAL. ISSN 0065-7727.

Koures:1988:NMN

[196] Antonios G. Koures and Frank E. Harris. New method for numerical integration of the radial electronic Schrödinger equation. *Journal of Chemical Physics*, 89(12):7344–7348, December 15, 1988. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/89/12/10.1063/1.455265`.

Harris:1992:ADM

[197] Frank E. Harris, Hendrik J. (Hendrik Jan) Monkhorst, and David L. Freeman. *Algebraic and diagrammatic methods in many-fermion theory*. Oxford University Press, Walton Street, Oxford OX2 6DP, UK, 1992. ISBN 0-19-506130-6. vii + 403 pp. LCCN QD455.3.M3 H37 1992. URL `http://www.loc.gov/catdir/enhancements/fy0637/89016016-d.html`; `http://www.loc.gov/catdir/enhancements/fy0637/89016016-t.html`.

Harris:1993:CCM

[198] Frank E. Harris. Coupled-cluster method for quantum lattices: Application to square $S = 1/2$ Heisenberg antiferromagnets. *Physical Review B: Condensed Matter and Materials Physics*, 47(13):7903–7909, April 1, 1993. CODEN PRBMDO. ISSN 1098-0121. URL `http://link.aps.org/doi/10.1103/PhysRevB.47.7903`.

Trinajstic:1994:NNS

[199] Nenad Trinajstić, Zlatko Mihalić, and Frank E. Harris. A note on the number of spanning trees in buckminsterfullerene. *International Journal of Quantum Chemistry*, 52(S28):525–528, February 12–19, 1994. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods.

Harris:1995:CSP

[200] Frank E. Harris and Antonios G. Koures. Critical study of plane-wave density-functional methods for extended systems. *International Journal of Quantum Chemistry*, 56(S29):235–239, February 25, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods.

Koures:1995:LCH

[201] Vasilios G. Koures and Frank E. Harris. Light cone Hamiltonian in quantum chemistry: Gaussian basis representation for quantum electrodynamics. *International Journal of Quantum Chemistry*, 56(S29):277–282,

February 25, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods.

Koures:1996:ICE

[202] Antonios G. Koures and Frank E. Harris. Improved correlation energy functional. *International Journal of Quantum Chemistry*, 59(1): 3–6, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60522`.

Koures:1996:SCQa

[203] Vasilios G. Koures and Frank E. Harris. Sinc collocation in quantum chemistry: Solving the planar Coulomb Schrödinger equation. *International Journal of Quantum Chemistry. Quantum Chemistry Symposium*, S30(7):99–106, ???? 1996. CODEN IJQSDI. ISSN 0161-3642.

Koures:1996:SCQb

[204] Vasilios G. Koures and Frank E. Harris. Sinc collocation in quantum chemistry: Solving the planar Coulomb Schrödinger equation. *International Journal of Quantum Chemistry*, 60(7):1311–1318, ???? 1996. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=60688`. 1996 Sanibel Symposia.

Harris:1997:AET

[205] Frank E. Harris. Analytic evaluation of three-electron atomic integrals with Slater wave functions. *Physical Review A (Atomic, Molecular, and Optical Physics)*, 55(3):1820–1831, March 1, 1997. CODEN PLRAAN. ISSN 1050-2947 (print), 1094-1622, 1538-4446, 1538-4519. URL `http://link.aps.org/doi/10.1103/PhysRevA.55.1820`.

Harris:1997:NAC

[206] Frank E. Harris. New approach to calculation of the leaky aquifer function. *International Journal of Quantum Chemistry*, 63(5):913–916, ???? 1997. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=42641`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=42641&PLACEBO=IE.pdf`.

Harris:1998:ARD

[207] Frank E. Harris. Algebraic reduction in discrete light-cone quantized electrodynamics using Maple V. Technical report, Department of Physics,

University of Utah and Quantum Theory Project, Departments of Physics and Chemistry, University of Florida, Salt Lake City, UT 84112, USA and Gainesville, FL 32611, USA, November 1998. Submitted to Computer Physics Communications.

Harris:1998:CGC

[208] Frank E. Harris. Computer generation of coupled-cluster equations. Technical report, Department of Physics, University of Utah and Quantum Theory Project, Departments of Physics and Chemistry, University of Florida, Salt Lake City, UT 84112, USA and Gainesville, FL 32611, USA, November 1998. Appear in International Journal of Quantum Chemistry [212]. A Maple V program is available at `http://courses.chem.utah.edu/facultyandstaff/harrisf/harrisf.html#software`.

Harris:1998:ESS

[209] Frank E. Harris. Ewald summations in systems with two-dimensional periodicity. *International Journal of Quantum Chemistry*, 68(6):385–404, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=29957`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=29957&PLACEBO=IE.pdf`.

Harris:1998:MAL

[210] Frank E. Harris. More about the leaky aquifer function. *International Journal of Quantum Chemistry*, 70(4–5):623–626, ???? 1998. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract?ID=75040`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=75040&PLACEBO=IE.pdf`.

Randic:1998:GSD

[211] Milan Randić, L. M. DeAlba, and Frank E. Harris. Graphs with the same detour matrix. *Croatica Chemica Acta*, 71(1):53–68, ???? 1998. CODEN CCACAA. ISSN 0011-1643 (print), 1334-417X (electronic).

Harris:1999:CGC

[212] Frank E. Harris. Computer generation of coupled-cluster equations. *International Journal of Quantum Chemistry*, 75(4–5):593–597, November 15, 1999. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/66004954/START`; `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=66004954&PLACEBO=IE.pdf`.

Flamant:2000:EES

[213] Isabelle Flamant, Joseph G. Fripiat, Joseph Delhalle, and Frank E. Harris. Efficient electronic structure calculations for systems of one-dimensional periodicity with the restricted Hartree–Fock linear combination of atomic orbitals method implemented in Fourier space. *Theoretical Chemistry Accounts*, 104(5):350–357, ???? 2000. CODEN TCACFW. ISSN 1432-881X (print), 1432-2234 (electronic).

Fripiat:2000:CAP

[214] Joseph G. Fripiat, Isabelle Flamant, Frank E. Harris, and Joseph Delhalle. Computational aspects of polymer band structure calculations by the Fourier space restricted Hartree–Fock method. *International Journal of Quantum Chemistry*, 80(4–5):856–862, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/73505378/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/73505378/FILE?TPL=ftx_start; http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=73505378&PLACEBO=IE.pdf`.

Harris:2000:ARD

[215] Frank E. Harris. Algebraic reduction in discrete light-cone quantized electrodynamics using Maple V. *Computer Physics Communications*, 132(1–2):21–29, October 15, 2000. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465500001338`.

Harris:2000:SBE

[216] Frank E. Harris. Spherical Bessel expansions of sine, cosine, and exponential integrals. *Applied Numerical Mathematics: Transactions of IMACS*, 34(1):95–98, June 2000. CODEN ANMAEL. ISSN 0168-9274 (print), 1873-5460 (electronic). URL `http://www.elsevier.nl/gej-ng/29/17/21/62/27/32/abstract.html; http://www.elsevier.nl/gej-ng/29/17/21/62/27/32/article.pdf; http://www.sciencedirect.com/science/article/pii/S0168927499000318`.

Harris:2001:KFL

[217] Frank E. Harris. On Kryachko's formula for the leaky aquifer function. *International Journal of Quantum Chemistry*, 81(5):332–334, ???? 2001. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/76507286/START; http://www3.interscience.wiley.com/cgi-bin/fulltext/76507286/FILE?TPL=ftx_start; http:`

//www3.interscience.wiley.com/cgi-bin/fulltext?ID=76507286&PLACEBO=IE.pdf.

Delhalle:2002:ECE

[218] Joseph Delhalle, Joseph G. Fripiat, and Frank E. Harris. Exchange contributions in the electronic structure of systems with 1D-periodicity: Importance and computation. *International Journal of Quantum Chemistry*, 90(2):587–593, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Delhalle:2002:VPF

[219] Joseph Delhalle, Joseph G. Fripiat, and Frank E. Harris. Virtues and potentialities of the Fourier transform method for electronic structure calculations of 1-D periodic systems at the Hartree–Fock level and beyond. *International Journal of Quantum Chemistry*, 90(4-5):1326–1333, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2002:AET

[220] Frank E. Harris. Analytic evaluation of two-center STO electron repulsion integrals via ellipsoidal expansion. *International Journal of Quantum Chemistry*, 88(6):701–734, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2002:AQI

[221] Frank E. Harris. Analytic quadratic integration over the two-dimensional Brillouin zone. *Journal of Physics: Condensed Matter*, 14(3):621–630, January 28, 2002. CODEN JCOMEL. ISSN 0953-8984 (print), 1361-648X (electronic). URL http://adsabs.harvard.edu/abs/2002JPCM...14..621H; http://iopscience.iop.org/0953-8984/14/3/329/.

Harris:2002:CBA

[222] Frank E. Harris. Cumulant-based approximations to reduced density matrices. *International Journal of Quantum Chemistry*, 90(1):105–113, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2002:CBS

[223] Frank E. Harris. Comments on "*Ewald summation technique for one-dimensional charge distributions*". *Computer Physics Communications*, 146(2):271–273, July 1, 2002. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465502004526. See [351, 352].

Harris:2002:SSI

[224] Frank E. Harris and Ryan T. Chancey. Simulated surface-impact collisions of fullerenes. In *APS Meeting Abstracts [American Physical Society, Annual APS March Meeting, March 18–22, 2002 Indiana Convention Center; Indianapolis, Indiana]*, page 11014. American Physical Society, Ridge, NY 11961, USA, March 2002. URL `http://adsabs.harvard.edu/abs/2002APS..MARW11014H`; `http://flux.aps.org/meetings/YR02/MAR02/baps/abs/S7710014.html`. Abstract #W11.014.

Tang:2002:ODC

[225] Qi-Heng Tang, Keith Runge, Hai-Ping Cheng, and Frank E. Harris. Orientation dependence in C60 surface-impact collisions. *Journal of Physical Chemistry A*, 106(6):893–896, 2002. CODEN JPCAFH. ISSN 1089-5639 (print), 1520-5215 (electronic). URL `http://pubs.acs.org/doi/abs/10.1021/jp012951k`.

Chancey:2003:FF

[226] Ryan T. Chancey, Lene B. Oddershede, Frank E. Harris, and John R. Sabin. Fragmentation of fullerenes. *Physical Review A (Atomic, Molecular, and Optical Physics)*, 67(4):043203, April 22, 2003. CODEN PLRAAN. ISSN 1050-2947 (print), 1094-1622, 1538-4446, 1538-4519. URL `http://link.aps.org/doi/10.1103/PhysRevA.67.043203`.

Gautschi:2003:EEI

[227] Walter Gautschi, Frank E. Harris, and Nico M. Temme. Expansions of the exponential integral in incomplete gamma functions. *Applied Mathematics Letters*, 16(7):1095–1099, October 2003. CODEN AMLEEL. ISSN 0893-9659 (print), 1873-5452 (electronic).

Harris:2003:CAR

[228] Frank E. Harris. Cumulant approximations to reduced density matrices. In *APS Meeting Abstracts [American Physical Society, Annual APS March Meeting 2003, March 3–7, 2003, Austin, Texas]*, page 19010. American Physical Society, Ridge, NY 11961, USA, March 2003. URL `http://adsabs.harvard.edu/abs/2003APS..MARW19010H`; `http://flux.aps.org/meetings/YR03/MAR03/baps/abs/S8190010.html`. Abstract #W19.010.

Harris:2003:CBC

[229] Frank E. Harris. Comment: "*On the computation of molecular auxiliary functions A_n and B_n*". *Pramana: Journal of Physics*, 61(4):C779–C780, October 2003. CODEN PRAMCI. ISSN 0304-4289 (print), 0973-7111

(electronic). URL `http://adsabs.harvard.edu/abs/2003Prama..61..779H; http://link.springer.com/article/10.1007/BF02706128`. See [350] and response [353].

Harris:2003:CBT

[230] Frank E. Harris. Comment on "*Computation of Two-Center Coulomb Integrals over Slater-Type Orbitals Using Elliptical Coordinates*". *International Journal of Quantum Chemistry*, 93(5):332–334, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [354].

Harris:2003:EVE

[231] Frank E. Harris, Alexei M. Frolov, and Vedene H. Smith, Jr. Exponential variational expansion in relative coordinates for highly accurate bound state calculations in four-body systems. *Journal of Chemical Physics*, 119(17):8833–8841, November 1, 2003. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/119/17/10.1063/1.1613943`.

Harris:2003:RIS

[232] Frank E. Harris and Joseph Delhalle. Rigorous ab initio studies of periodic systems: approaches to electron correlation. Workshop report, CECAM, Paris, France (??), 2003. 36 pp.

Oddershede:2003:FAF

[233] Lene B. Oddershede, Ryan T. Chancey, Frank E. Harris, and John R. Sabin. Fragmentering af fullerener. (Danish) [Fragmentation of fullerenes]. *Kvant*, 14(2):3–7, ???? 2003. CODEN KVANEU. ISSN 0905-8893.

Harris:2004:CAS

[234] Frank E. Harris, Alexei M. Frolov, and Vedene H. Smith, Jr. Comment on Analysis of some integrals arising in the atomic four-electron problem [J. Chem. Phys. **99**, 3622 (1993)]. *Journal of Chemical Physics*, 120(6): 3040–3041, February 8, 2004. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/120/6/10.1063/1.1638993`.

Harris:2004:CBV

[235] Frank E. Harris, Alexei M. Frolov, and Vedene H. Smith, Jr. Comment on "*Analytic value of the atomic three-electron correlation integral with Slater wave functions*". *Physical Review A (Atomic, Molecular, and Optical Physics)*, 69(5):056501, May 28, 2004. CODEN PLRAAN. ISSN 1050-2947 (print), 1094-1622, 1538-4446, 1538-4519. URL `http://adsabs.harvard.edu/abs/2004PhRvA..69e6501H;`

http://link.aps.org/doi/10.1103/PhysRevA.69.056501. See [347, 355, 356].

Harris:2004:CMC

[236] Frank E. Harris. Current methods for Coulomb few-body problems. *Advances in Quantum Chemistry*, 47:129–155, 2004. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327604470087.

Harris:2004:CUS

[237] Frank E. Harris. Conventional and unconventional symbolic computation in chemistry. *Abstracts of Papers of the American Chemical Society*, 228 (??):U534–U535, August 2004. CODEN ACSRAL. ISSN 0065-7727.

Harris:2004:EEM

[238] Frank E. Harris. Efficient evaluation of the molecular auxiliary function B_n by downward recursion. *International Journal of Quantum Chemistry*, 100(2):142–145, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2004:ER

[239] Frank E. Harris. Expansion(s) of r_{12}^{-2}. *International Journal of Quantum Chemistry*, 97(5):908–913, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2004:HAE

[240] Frank E. Harris, Alexei M. Frolov, and Vedene H. Smith, Jr. Highly accurate evaluation of atomic three-electron integrals of lowest orders. *Journal of Chemical Physics*, 120(21):9974–9983, June 1, 2004. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://scitation.aip.org/content/aip/journal/jcp/120/21/10.1063/1.1735537.

Harris:2004:IEC

[241] Frank E. Harris. Integrals for exponentially correlated four-body systems of general angular symmetry. In Brändas and Kryachko [423], pages 115–127. ISBN 90-481-6687-X (print), 94-017-0448-1 (e-book). URL http://link.springer.com/chapter/10.1007/978-94-017-0448-9_7.

Harris:2004:MCF

[242] Frank E. Harris. Methods for Coulomb few-body problems. In *APS Meeting Abstracts [American Physical Society, March Meeting 2004, March 22–26, 2004, Palais des Congrès de Montréal, Montréal, Québec,*

Canada], page 38006. American Physical Society, Ridge, NY 11961, USA, March 2004. URL http://adsabs.harvard.edu/abs/2004APS..MARV38006H; http://flux.aps.org/meetings/YR04/MAR04/baps/abs/S7980006.html. Abstract #V38.006.

Harris:2004:NMO

[243] Frank E. Harris, Alexei M. Frolov, and Vedene H. Smith, Jr. New methods for old Coulomb few-body problems. *International Journal of Quantum Chemistry*, 100(6):1086–1091, ???? 2004. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comment [265].

Harris:2004:SNT

[244] Frank E. Harris, Alexei M. Frolov, and Vedene H. Smith, Jr. Singular and nonsingular three-body integrals for exponential wave functions. *Journal of Chemical Physics*, 121(13):6323–6333, October 1, 2004. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://scitation.aip.org/content/aip/journal/jcp/121/13/10.1063/1.1786912.

Harris:2005:ASH

[245] Frank E. Harris. Angular symmetry and Hylleraas coordinates in four-body problems. *Advances in Quantum Chemistry*, 50:61–75, 2005. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327605500042.

Harris:2005:CBR

[246] Frank E. Harris. Comment on "*Exponential representation in the Coulomb three-body problem*". See [358]. Submitted [where??]. Was this paper dropped after the publication of the corrigendum [357]?, 2005.

Harris:2005:CEB

[247] Frank E. Harris, Vedene H. Smith, Jr., and Alexei M. Frolov. Correlated exponential-basis integrals with logarithmic integrands. *Molecular Physics*, 103(15–16):2047–2054, August 2005. CODEN MOPHAM. ISSN 0026-8976 (print), 1362-3028 (electronic). URL http://adsabs.harvard.edu/abs/2005MolPh.103.2047H.

Harris:2005:CWL

[248] F. E. Harris. Compact wavefunctions for He-like systems. *Bulletin of the American Physical Society*, ??(??):DB.00002, ???? 2005. CODEN BAPSA6. ISSN 0003-0503. URL http://adsabs.harvard.edu/abs/2005APS..SES.DB002H; http://meetings.aps.org/link/BAPS.2005.SES.DB.2; http://meetings.aps.org/Meeting/SES05/

Session/DB.2. 2005 72nd Annual Meeting of the Southeastern Section of the APS Thursday Saturday, November 10–12, 2005; Gainesville, FL, USA.

Harris:2005:GET

[249] Frank E. Harris. Gegenbauer expansions for three-electron integrals. *International Journal of Quantum Chemistry*, 102(5):940–947, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2005:HCWa

[250] Frank E. Harris. Highly compact wavefuntions for He-like systems. In *APS March Meeting Abstracts: [American Physical Society, APS March Meeting, March 21–25, 2005, Los Angeles, CA]*, page 1053. American Physical Society, Ridge, NY 11961, USA, March 2005. URL http://adsabs.harvard.edu/abs/2005APS..MAR.R1053H; http://meetings.aps.org/Meeting/MAR05/Event/27924. Abstract #R1.053.

Harris:2005:HCWb

[251] Frank E. Harris and Vedene H. Smith, Jr. Highly compact wave functions for He-like systems. *Journal of Physical Chemistry A*, 109(50): 11413–11416, 2005. CODEN JPCAFH. ISSN 1089-5639 (print), 1520-5215 (electronic). URL http://pubs.acs.org/doi/abs/10.1021/jp0531098. PMID: 16354029.

Harris:2005:HCWc

[252] Frank E. Harris and Vedene H. Smith, Jr. Highly compact wavefunctions for two-electron systems. *Advances in Quantum Chemistry*, 48: 407–419, 2005. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327605480211.

Harris:2005:IET

[253] Frank E. Harris. Improving the efficiency of table-driven CI. *International Journal of Quantum Chemistry*, 105(1):34–36, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2005:MPC

[254] F. E. Harris. Molecular properties from compact few-electron wavefunctions. In ????, editor, *Pacifichem 2005 conference proceedings*, page ?? ????, ????, 2005.

Harris:2005:RRM

[255] Frank E. Harris. Recurrence relations for matrix elements of few-body correlated wave functions. *International Journal of Quantum Chemistry*,

105(6):857–865, ???? 2005. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2005:SIT

[256] Frank E. Harris, Alexei M. Frolov, and Vedene H. Smith, Jr. Singular integrals and their application to a hypervirial theorem. *Physical Review A (Atomic, Molecular, and Optical Physics)*, 72(1):012511, July 27, 2005. CODEN PLRAAN. ISSN 1050-2947 (print), 1094-1622, 1538-4446, 1538-4519. URL `http://link.aps.org/doi/10.1103/PhysRevA.72.012511`.

Trickey:2005:ADF

[257] S. B. Trickey, V. V. Karasiev, and F. E. Harris. Approximate density functionals for molecular dynamics simulations of material properties. In Peter Politzer, Jane Murray, and Erkki Brändas, editors, *Special issue: proceedings from the Fifth Congress of the International Society for Theoretical Chemical Physical (ISTCP-V): held at New Orleans, USA, July 20–26, 2005*, page ?? Wiley, New York, NY, USA, 2005.

Fripiat:2006:FRM

[258] Joseph G. Fripiat, Joseph Delhalle, and Frank E. Harris. Fourier representation methods for Møller–Plesset perturbation theory in one-dimensionally periodic systems. *Chemical Physics Letters*, 422(1–3):11–14, April 28, 2006. CODEN CHPLBC. ISSN 0009-2614 (print), 1873-4448 (electronic). URL `http://adsabs.harvard.edu/abs/2006CPL...422...11F`; `http://www.sciencedirect.com/science/article/pii/S0009261406002363`.

Harris:2006:CSF

[259] Frank E. Harris. Current studies of few-electron systems. In Simos and Maroulis [425], pages 1035–?? CODEN LSCCAR. ISBN 90-04-15542-2 (set). ISSN 1573-4196. LCCN Q183.9 .I524 2006.

Harris:2006:DFB

[260] Frank E. Harris. Dilogarithms and four-body atomic Coulomb interaction integrals for fully correlated exponential wavefunctions. In *American Mathematical Society 2006 Spring Central Sectional Meeting Notre Dame, IN, April 8–9, 2006, Meeting # 1016*, page ?? American Mathematical Society, Providence, RI, USA, 2006. URL `http://www.ams.org/meetings/sectional/1016-33-181.pdf`; `http://www.ams.org/meetings/sectional/2130_program_ss5.html`. Abstract 1016-33-181.

Harris:2006:ECW

[261] Frank E. Harris. Explicitly correlated wavefunctions for few-body problems. In *APS Meeting Abstracts: [American Physical Society, APS March Meeting, March 13–17, 2006, Baltimore, MD, USA]*, page 43003. American Physical Society, Ridge, NY 11961, USA, March 2006. URL `http://adsabs.harvard.edu/abs/2006APS..MARV43003H`; `http://meetings.aps.org/Meeting/MAR06/Event/45096`. Abstract #V43.003.

Harris:2006:IFC

[262] Frank E. Harris and Hendrik J. Monkhorst. Integrals for fully correlated Gaussians in relative coordinates. *International Journal of Quantum Chemistry*, 106(1):54–64, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2006:ISI

[263] Frank E. Harris. Introduction: [to special issue on Mathematical Methods and Symbolic Calculation in Chemistry and Chemical Biology]. *International Journal of Quantum Chemistry*, 106(1):1–2, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2006:NIE

[264] Frank E. Harris, Joseph G. Fripiat, and Joseph Delhalle. Numerical integration of exchange energy in the two-dimensional Brillouin zone. *Journal of Physics: Condensed Matter*, 18(23):5493–5501, June 14, 2006. CODEN JCOMEL. ISSN 0953-8984 (print), 1361-648X (electronic). URL `http://adsabs.harvard.edu/abs/2006JPCM...18.5493H`; `http://iopscience.iop.org/0953-8984/18/23/019/`.

Harris:2006:RCN

[265] Frank E. Harris, Alexei M. Frolov, and Vedene H. Smith, Jr. Re: Comment on "*New methods for old Coulomb few-body problems*". *International Journal of Quantum Chemistry*, 106(2):552–553, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [243].

Harris:2006:RRF

[266] Frank E. Harris and Hendrik J. Monkhorst. Recurrence relations for fully correlated Gaussians with odd powers of interparticle coordinates. *International Journal of Quantum Chemistry*, 106(15):3186–3189, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2006:SGS

[267] Frank E. Harris and Vedene H. Smith, Jr. Systematics of the ground states of the He isoelectronic series. In King et al. [424], pages 127–137. ISBN 83-231-1901-5. LCCN QC16.W93 P76 2005.

Karasiev:2006:BOI

[268] V. V. Karasiev, Samuel B. Trickey, and Frank E. Harris. Born–Oppenheimer interatomic forces from simple, local kinetic energy density functionals. *Journal of Computer-Aided Materials Design*, 13(1–3):111–129, October 2006. CODEN JCODES. ISSN 0928-1045 (print), 1573-4900 (electronic). URL `http://adsabs.harvard.edu/abs/2006JCMD...13..111K`; `http://link.springer.com/article/10.1007/s10820-006-9019-8`.

Karasiev:2006:DFM

[269] V. V. Karasiev, Samuel B. Trickey, and Frank E. Harris. Density fitting and model densities. Submitted [where??]., 2006.

Karasiev:2006:FAF

[270] V. V. Karasiev, Samuel B. Trickey, and Frank E. Harris. Faster approximate force calculations via quasi-spin density exchange-correlation functionals. *Chemical Physics*, 330(1–2):216–223, November 8, 2006. CODEN CMPHC2. ISSN 0301-0104 (print), 1873-4421 (electronic). URL `http://adsabs.harvard.edu/abs/2006CP....330..216K`; `http://www.sciencedirect.com/science/article/pii/S0301010406004605`.

Karasiev:2006:FMD

[271] V. V. Karasiev, Samuel B. Trickey, and Frank E. Harris. Fitting of molecular densities by compact, atom-centered expansion. In *APS Meeting Abstracts: [American Physical Society, APS March Meeting, March 13–17, 2006, Baltimore, MD, USA]*, page 27008. American Physical Society, Ridge, NY 11961, USA, March 2006. URL `http://adsabs.harvard.edu/abs/2006APS..MARP27008K`; `http://meetings.aps.org/Meeting/MAR06/Event/43158`. Abstract #P27.008.

Karwowski:2006:RDE

[272] J. Karwowski, G. Pestka, M. Stanke, and Frank E. Harris. Representation of the Dirac equation and the variational principle. *International Journal of Quantum Chemistry*, 106(15):3129–3139, ???? 2006. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Taylor:2006:GMQ

[273] DeCarlos E. Taylor, V. V. Karasiev, Keith Runge, Samuel B. Trickey, and Frank E. Harris. Graded methods for quantum mechanical force generation in molecular dynamics simulations. In Simos and Maroulis [425], pages 532–?? CODEN LSCCAR. ISBN 90-04-15542-2 (set). ISSN 1573-4196. LCCN Q183.9 .I524 2006.

Trickey:2006:PBOa

[274] Samuel B. Trickey, V. V. Karasiev, and Frank E. Harris. Prediction of Born–Oppenheimer interatomic forces using orbital-free density functional theory with approximate kinetic energy functionals. In *APS Meeting Abstracts: [American Physical Society, APS March Meeting, March 13–17, 2006, Baltimore, MD, USA]*, page 27007. American Physical Society, Ridge, NY 11961, USA, March 2006. URL `http://adsabs.harvard.edu/abs/2006APS..MARP27007T`; `http://meetings.aps.org/Meeting/MAR06/Event/43157`. Abstract #P27.007.

Trickey:2006:PBOb

[275] Samuel B. Trickey, V. V. Karasiev, and Frank E. Harris. Prediction of Born–Oppenheimer interatomic forces using orbital-free density functional theory with approximate kinetic energy functionals. *Bulletin of the American Physical Society*, 51(??):1008–??, ???? 2006. CODEN BAPSA6. ISSN 0003-0503. URL `http://meetings.aps.org/link/BAPS.2006.MAR.P27.7`; `http://meetings.aps.org/Meeting/MAR06/Event/43157`.

Albert:2007:SSE

[276] Victor V. Albert, John R. Sabin, and Frank E. Harris. Simulated structure and energetics of endohedral complexes of noble gas atoms in buckminsterfullerene. *International Journal of Quantum Chemistry*, 107(15): 3061–3066, ???? 2007. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fripiat:2007:FRM

[277] Joseph G. Fripiat, Joseph Delhalle, and Frank E. Harris. Fourier representation methods for Møller–Plesset perturbation theory in one-dimensionally periodic systems. In Simos and Maroulis [427], pages 179–182. ISBN 0-7354-0476-3 (set), 0-7354-0477-1 (vol. 1), 0-7354-0478-X (vol. 2). LCCN Q183.9 2007. URL `http://scitation.aip.org/content/aip/proceeding/aipcp/10.1063/1.2836033`. Two volumes.

Harris:2007:CNT

[278] Frank E. Harris. Comment on "*Numerical treatment of two-center overlap integrals*". *Journal of Molecular Modeling*, 13(9):949–950, ???? 2007.

CODEN JMMOFK. ISSN 0948-5023 (print), 1610-2940 (electronic). See [359].

Harris:2007:CWL

[279] Frank E. Harris. Correlated wavefunction for the Li atom. In *APS Meeting Abstracts: [American Physical Society, APS March Meeting, March 5–9, 2007]*, page 32012. American Physical Society, Ridge, NY 11961, USA, March 2007. URL `http://adsabs.harvard.edu/abs/2007APS..MARY32012H`. Abstract #Y32.012.

Harris:2007:DCT

[280] Frank E. Harris and John R. Sabin. On a dynamic career: a tribute to Nils Yngve Öhrn. In Simos and Maroulis [427], pages 138–146. ISBN 0-7354-0476-3 (set), 0-7354-0477-1 (vol. 1), 0-7354-0478-X (vol. 2). LCCN Q183.9 2007. URL `http://scitation.aip.org/content/aip/proceeding/aipcp/10.1063/1.2836013`. Two volumes.

Harris:2007:HCW

[281] Frank E. Harris. Highly compact wavefunctions for four-body systems. In Maroulis and Simos [426], pages 448–459. ISBN 0-7354-0476-3 (set), 0-7354-0477-1 (vol. 1). ISSN 0094-243X (print), 1551-7616 (electronic), 1935-0465. LCCN Q183.9.I524 2007. URL `http://scitation.aip.org/content/aip/proceeding/aipcp/10.1063/1.2827027`.

Harris:2007:NYO

[282] Frank E. Harris and John R. Sabin. The Nils Yngve Öhrn Symposium. In Simos and Maroulis [427], page 137. ISBN 0-7354-0476-3 (set), 0-7354-0477-1 (vol. 1), 0-7354-0478-X (vol. 2). LCCN Q183.9 2007. URL `http://scitation.aip.org/content/aip/proceeding/aipcp/10.1063/1.2836010`. Two volumes.

Karasiev:2007:RAD

[283] V. V. Karasiev, R. S. Jones, Samuel B. Trickey, and Frank E. Harris. Recent advances in developing orbital-free kinetic energy functionals. In Paz and Hernández [428], pages 25–54. ISBN 81-7895-446-X. LCCN QD462 .N48 2009. URL `http://www.ressign.com/UserBookDetail.aspx?bkid=1006`.

Runge:2007:GSA

[284] Keith Runge, DeCarlos E. Taylor, V. V. Karasiev, Samuel B. Trickey, and Frank E. Harris. Graded-sequence-of-approximations: Quantum mechanical forces for molecular dynamics. In *APS Meeting Abstracts:*

[American Physical Society, APS March Meeting, March 5–9, 2007], page 21010. American Physical Society, Ridge, NY 11961, USA, March 2007. URL `http://adsabs.harvard.edu/abs/2007APS..MARN21010R`. Abstract #N21.010.

Taylor:2007:GMR

[285] DeCarlos E. Taylor, V. V. Karasiev, Keith Runge, Samuel B. Trickey, and Frank E. Harris. Graded methods for rapid generation of quantum mechanical forces in molecular dynamics simulations. *Computational Materials Science*, 39(3):705–708, ???? 2007. CODEN CMMSEM. ISSN 0927-0256 (print), 1879-0801 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0927025606002734`.

Albert:2008:SXC

[286] Victor V. Albert, John R. Sabin, and Frank E. Harris. Simulations of Xe@C_{60} collisions with graphitic films. *International Journal of Quantum Chemistry*, 108(15):3010–3015, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2008:IBG

[287] Frank E. Harris. Incomplete Bessel, generalized incomplete gamma, or leaky aquifer functions. *Journal of Computational and Applied Mathematics*, 215(1):260–269, 2008. CODEN JCAMDI. ISSN 0377-0427 (print), 1879-1778 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0377042707002014`.

Pinchon:2008:NEL

[288] Didier Pinchon, Philip E. Hoggan, and Frank E. Harris. A new expansion of the leaky aquifer function. *International Journal of Quantum Chemistry*, 108(15):3042–3046, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Trickey:2008:OFK

[289] Samuel B. Trickey, V. V. Karasiev, R. S. Jones, and Frank E. Harris. Orbital-free kinetic energy density functionals of GGA type with positive-definite, finite Pauli potentials. In *APS Meeting Abstracts: [American Physical Society, 2008 APS March Meeting, March 10–14, 2008]*, page 13010. American Physical Society, Ridge, NY 11961, USA, March 2008. URL `http://adsabs.harvard.edu/abs/2008APS..MARL13010T`. Abstract #L13.010.

Albert:2009:FPE

[290] Victor V. Albert, Nicolais L. Guevara, John R. Sabin, and Frank E. Harris. Few-parameter exponentially correlated wavefunctions for the ground state of lithium. *International Journal of Quantum Chemistry*, 109(15): 3791–3797, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guevara:2009:AFP

[291] Nicolais L. Guevara, Frank E. Harris, and Alexander V. Turbiner. An accurate few-parameter ground state wave function for the lithium atom. *International Journal of Quantum Chemistry*, 109(13):3036–3040, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2009:BAM

[292] Frank E. Harris. Bill Adams Memorial Session. *International Journal of Quantum Chemistry*, 109(15):3840, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2009:CBS

[293] Frank E. Harris, V. V. Karasiev, R. S. Jones, and Samuel B. Trickey. Constraint-based, single-point approximate kinetic energy functionals. In *APS Meeting Abstracts: [American Physical Society, 2009 APS March Meeting, March 16–20, 2009]*, page 13002. American Physical Society, Ridge, NY 11961, USA, March 2009. URL `http://adsabs.harvard.edu/abs/2009APS..MARX13002H`. Abstract #X13.002.

Harris:2009:ECE

[294] Frank E. Harris. Energy computation for exponentially correlated four-body wavefunctions. In Piecuch et al. [429], pages 61–70. ISBN 90-481-2595-2 (print), 90-481-2596-0 (e-book). URL `http://adsabs.harvard.edu/abs/2009atam.book...61H`; `http://link.springer.com/chapter/10.1007/978-90-481-2596-8_4`.

Harris:2009:MIB

[295] Frank E. Harris and Joseph G. Fripiat. Methods for incomplete Bessel function evaluation. *International Journal of Quantum Chemistry*, 109(8): 1728–1740, February 4, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Harris:2009:RFF

[296] Frank E. Harris. Recurrence formulas for fully exponentially correlated four-body wave functions. *Physical Review A (Atomic, Molecular, and Optical Physics)*, 79(3):032517, March 24, 2009. CODEN PLRAAN. ISSN 1050-2947 (print), 1094-1622, 1538-4446, 1538-4519. URL `http://link.aps.org/doi/10.1103/PhysRevA.79.032517`.

Karasiev:2009:PCB

[297] V. V. Karasiev, R. S. Jones, Samuel B. Trickey, and Frank E. Harris. Properties of constraint-based single-point approximate kinetic energy functionals. *Physical Review B: Condensed Matter and Materials Physics*, 80(24):245120, December 15, 2009. CODEN PRBMDO. ISSN 1098-0121. URL `http://link.aps.org/doi/10.1103/PhysRevB.80.245120`. See erratum [329].

Albert:2010:FF

[298] Victor V. Albert, Ryan T. Chancey, Lene B. Oddershede, Frank E. Harris, and John R. Sabin. Fragmentation of fullerenes. In Sattler [430], chapter 26, pages 26:1–26:?? ISBN 1-4200-7554-3. LCCN QC173.4 M5. URL `http://www.crcpress.com/product/isbn/9781420075403`.

Fripiat:2010:ETF

[299] Joseph G. Fripiat, Joseph Delhalle, Isabelle Flamant, and Frank E. Harris. Ewald-type formulas for Gaussian-basis Bloch states in one-dimensionally periodic systems. *Journal of Chemical Physics*, 132(4):044108, January 28, 2010. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/132/4/10.1063/1.3298913`.

Harris:2011:RCT

[300] Frank E. Harris and Travis Sjostrom. Reference calculation of temperature-dependent behavior of confined many-electron systems. In *APS Meeting Abstracts: [American Physical Society, APS March Meeting 2011, March 21–25, 2011]*, page 15013. American Physical Society, Ridge, NY 11961, USA, March 2011. URL `http://adsabs.harvard.edu/abs/2011APS..MARD15013H`. Abstract #D15.013.

Sjostrom:2011:TDB

[301] Travis Sjostrom, Frank E. Harris, and Samuel B. Trickey. Temperature-dependent behavior of confined many-electron systems in the Hartree–Fock approximation. In *APS Meeting Abstracts: [American Physical Society, 53rd Annual Meeting of the APS Division of Plasma Physics,*

November 14-18, 2011], page 10003. American Physical Society, Ridge, NY 11961, USA, November 2011. URL `http://adsabs.harvard.edu/abs/2011APS..DPPY10003S`. Abstract #YM1.000.

Fripiat:2012:ETF

[302] Joseph G. Fripiat and Frank E. Harris. Ewald-type formulas for Gaussian-basis studies of one-dimensionally periodic systems. *Theoretical Chemistry Accounts*, 131(8):1257:1–1257:??, August 2012. CODEN TCACFW. ISSN 1432-881X (print), 1432-2234 (electronic).

Sjostrom:2012:CFT

[303] Travis Sjostrom, Samuel B. Trickey, and Frank E. Harris. Comparison of finite temperature Hartree–Fock and density functional theory for confined systems. In *APS Meeting Abstracts: [American Physical Society, APS March Meeting 2012, February 27–March 2, 2012]*, page 25002. American Physical Society, Ridge, NY 11961, USA, February 2012. URL `http://adsabs.harvard.edu/abs/2012APS..MARL25002S`. Abstract #L25.002.

Sjostrom:2012:TDB

[304] Travis Sjostrom, Frank E. Harris, and Samuel B. Trickey. Temperature-dependent behavior of confined many-electron systems in the Hartree–Fock approximation. *Physical Review B: Condensed Matter and Materials Physics*, 85(4):045125, January 15, 2012. CODEN PRBMDO. ISSN 1098-0121. URL `http://link.aps.org/doi/10.1103/PhysRevB.85.045125`.

Arfken:2013:AM

[305] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Angular momentum. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 16, pages 773–814. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL `http://www.sciencedirect.com/science/article/pii/B9780123846549000165`.

Arfken:2013:BF

[306] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Bessel functions. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 14, pages 643–713. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL `http://www.sciencedirect.com/science/article/pii/B9780123846549000141`.

Arfken:2013:CV

[307] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Calculus of variations. In *Mathematical Methods for Physicists:*

a Comprehensive Guide [431], chapter 22, pages 1081–1124. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL `http://www.sciencedirect.com/science/article/pii/B9780123846549000220`.

Arfken:2013:CVT

[308] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Complex variable theory. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 11, pages 469–550. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL `http://www.sciencedirect.com/science/article/pii/B9780123846549000116`.

Arfken:2013:DM

[309] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Determinants and matrices. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 2, pages 83–121. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL `http://www.sciencedirect.com/science/article/pii/B9780123846549000025`.

Arfken:2013:EP

[310] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Eigenvalue problems. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 6, pages 299–328. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL `http://www.sciencedirect.com/science/article/pii/B9780123846549000062`.

Arfken:2013:FS

[311] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Fourier series. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 19, pages 935–962. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL `http://www.sciencedirect.com/science/article/pii/B9780123846549000190`.

Arfken:2013:FTA

[312] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Further topics in analysis. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 12, pages 551–598. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL `http://www.sciencedirect.com/science/article/pii/B9780123846549000128`.

Arfken:2013:GFa

[313] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Green's functions. In *Mathematical Methods for Physicists: a*

Comprehensive Guide [431], chapter 10, pages 447–467. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL http://www.sciencedirect.com/science/article/pii/B9780123846549000104.

Arfken:2013:GFb

[314] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Gamma function. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 13, pages 599–641. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL http://www.sciencedirect.com/science/article/pii/B978012384654900013X.

Arfken:2013:GT

[315] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Group theory. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 17, pages 815–870. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL http://www.sciencedirect.com/science/article/pii/B9780123846549000177.

Arfken:2013:IE

[316] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Integral equations. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 21, pages 1047–1079. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL http://www.sciencedirect.com/science/article/pii/B9780123846549000219.

Arfken:2013:IT

[317] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Integral transforms. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 20, pages 963–1046. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL http://www.sciencedirect.com/science/article/pii/B9780123846549000207.

Arfken:2013:LF

[318] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Legendre functions. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 15, pages 715–772. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL http://www.sciencedirect.com/science/article/pii/B9780123846549000153.

Arfken:2013:MP

[319] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Mathematical preliminaries. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 1, pages iii–xvi; 1–82. ISBN

0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL http://www.sciencedirect.com/science/article/pii/B9780123846549000013.

Arfken:2013:MSF

[320] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. More special functions. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 18, pages 871–933. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL http://www.sciencedirect.com/science/article/pii/B9780123846549000189.

Arfken:2013:ODE

[321] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Ordinary differential equations. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 7, pages 329–380. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL http://www.sciencedirect.com/science/article/pii/B9780123846549000074.

Arfken:2013:PDE

[322] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Partial differential equations. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 9, pages 401–445. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL http://www.sciencedirect.com/science/article/pii/B9780123846549000098.

Arfken:2013:PS

[323] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Probability and statistics. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 23, pages 1125–1179. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL http://www.sciencedirect.com/science/article/pii/B9780123846549000232.

Arfken:2013:SLT

[324] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Sturm–Liouville theory. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 8, pages 381–399. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL http://www.sciencedirect.com/science/article/pii/B9780123846549000086.

Arfken:2013:TDF

[325] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Tensors and differential forms. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 4, pages 205–249. ISBN

0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL http://www.sciencedirect.com/science/article/pii/B9780123846549000049.

Arfken:2013:VA

[326] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Vector analysis. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 3, pages 123–203. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL http://www.sciencedirect.com/science/article/pii/B9780123846549000037.

Arfken:2013:VS

[327] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. Vector spaces. In *Mathematical Methods for Physicists: a Comprehensive Guide* [431], chapter 5, pages 251–297. ISBN 0-12-384654-4 (hardcover). LCCN QA37.3 .A74 2013. URL http://www.sciencedirect.com/science/article/pii/B9780123846549000050.

Harris:2013:FCW

[328] Frank E. Harris and Victor V. Albert. Fully correlated wavefunctions for three- and four-body systems. *Advances in Quantum Chemistry*, 67:3–18, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/B9780124115446000017.

Karasiev:2013:EPC

[329] V. V. Karasiev, R. S. Jones, Samuel B. Trickey, and Frank E. Harris. Erratum: "*Properties of constraint-based single-point approximate kinetic energy functionals*" [Phys. Rev. B **80**, 245120 (2009)]. *Physical Review B: Condensed Matter and Materials Physics*, 87(23):239903, June 15, 2013. CODEN PRBMDO. ISSN 1098-0121. URL http://link.aps.org/doi/10.1103/PhysRevB.87.239903. See [297].

Fripiat:2014:ETF

[330] Joseph G. Fripiat and Frank E. Harris. Ewald-type formulas for Gaussian-basis studies of one-dimensionally periodic systems. In Champagne et al. [432], pages 181–187. ISBN 3-642-41314-5 (print), 3-642-41315-3 (e-book). URL http://link.springer.com/chapter/10.1007/978-3-642-41315-5_15.

Fripiat:2014:FSR

[331] Joseph G. Fripiat and Frank E. Harris. The Fourier space restricted Hartree–Fock method for the electronic structure calculation of linear poly(tetrafluoroethylene). *Science China: Chemistry*, 57(10):1355–

1362, October 2014. CODEN SCCCCS. ISSN 1674-7291 (print), 1869-1870 (electronic). URL http://link.springer.com/article/10.1007/s11426-014-5104-0.

Harris:2014:ATF

[332] Frank E. Harris. Atomic three- and four-body recurrence formulas and related summations. *Theoretical Chemistry Accounts*, 133(5):1475:1–1475:7, May 2014. CODEN TCACFW. ISSN 1432-881X (print), 1432-2234 (electronic). URL http://link.springer.com/article/10.1007/s00214-014-1475-8. Shavitt Memorial Festschrift Collection.

Harris:2014:MMU

[333] Frank E. Harris. *Mathematics for physical science and engineering: symbolic computing applications in Maple and Mathematica*. Academic Press, New York, NY, USA, 2014. ISBN 0-12-801000-2 (hardcover), 0-12-801049-5 (e-book). xiv + 768 pp. LCCN QA37.3 .H36 2014. URL http://www.sciencedirect.com/science/book/9780128010006.

Karasiev:2014:IFT

[334] Valentin V. Karasiev, Travis Sjostrom, Debajit Chakraborty, James W. Dufty, Keith Runge, Frank E. Harris, and S. B. Trickey. Innovations in finite-temperature density functionals. In Graziani et al. [433], pages 61–85. ISBN 3-319-04912-7. ISSN 1439-7358. LCCN QA71-90. URL http://link.springer.com/chapter/10.1007/978-3-319-04912-0_3/.

Harris:2015:CCW

[335] Frank E. Harris. Comment on "Compact wave functions for four-electron atomic systems". *Physical Review A (Atomic, Molecular, and Optical Physics)*, 91(2):026501:1–026501:2, February 2015. CODEN PLRAAN. ISSN 1050-2947 (print), 1094-1622, 1538-4446, 1538-4519. URL http://journals.aps.org/pra/abstract/10.1103/PhysRevA.91.026501.

Harris:2015:FEC

[336] Frank E. Harris. Fully exponentially correlated wavefunctions for small atoms. *AIP Conference Proceedings*, 1642(1):205–208, 2015. CODEN APCPCS. ISSN 0094-243X (print), 1551-7616 (electronic), 1935-0465. URL http://scitation.aip.org/content/aip/proceeding/aipcp/10.1063/1.4906653.

Harris:2015:IMBa

[337] Frank E. Harris. *Instructor's Manual for* Mathematical Methods for Physicists: a Comprehensive Guide. Elsevier Academic Press, Amsterdam, The Netherlands, 2015. ???? pp.

Harris:2015:IMBb

[338] Frank E. Harris. *Instructor's Manual for* Mathematics for physical science and engineering: symbolic computing applications in Maple and Mathematica. Elsevier Academic Press, Amsterdam, The Netherlands, 2015. ???? pp.

Harris:2015:PSP

[339] Frank E. Harris. Polarizability of stereoregular polymers. *Journal of Chemical Physics*, 143(10):104111, September 2015. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/143/10/10.1063/1.4930846`.

Harris:2016:EKE

[340] Frank E. Harris. Erratum: "Kinetic-energy matrix elements for atomic Hylleraas–CI wave functions [J. Chem. Phys. **144**, 204110 (2016)]. *Journal of Chemical Physics*, 145(12):129901, September 2016. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). See [341].

Harris:2016:KEM

[341] Frank E. Harris. Kinetic-energy matrix elements for atomic Hylleraas–CI wave functions. *Journal of Chemical Physics*, 144(20):204110:1–204110:8, May 28, 2016. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). See erratum [340].

Harris:2017:ECW

[342] Frank E. Harris. Exponentially correlated wave functions for four-body systems. *Advances in Quantum Chemistry*, 73:81–102, 2017. CODEN AQCHA9. ISSN 0065-3276. URL `http://www.sciencedirect.com/science/article/pii/S0065327615000568`.

Harris:2018:AES

[343] Frank E. Harris. Atomic electronic structure computations with Hylleraas-CI wave functions. *Advances in Quantum Chemistry*, 76:187–210, 2018. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327617300345`.

Harris:2018:MEE

[344] Frank E. Harris. Matrix elements for explicitly-correlated atomic wave functions. In Wang et al. [436], pages 29–41. ISBN 3-319-74581-6, 3-319-74582-4 (e-book). LCCN QD462.A1 F76 2015. URL `http://public.eblib.com/choice/publicfullrecord.aspx?p=5398073`.

Lifson:1957:PTA

[345] Shneior Lifson. Potentiometric titration, association phenomena, and interaction of neighboring groups in polyelectrolytes. *Journal of Chemical Physics*, 26(6):727–734, June 1, 1957. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://scitation.aip.org/content/aip/journal/jcp/26/4/10.1063/1.1743393`. See comments [43].

Slater:1965:MOH

[346] John C. Slater. Molecular orbital and Heitler–London methods (with discussion). *Journal of Chemical Physics*, 43(10):S11–S17, November 15, 1965. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL `http://jcp.aip.org/resource/1/jcpsa6/v43/i10/pS11_s1`. See discussion [60].

Remiddi:1991:AVA

[347] Ettore Remiddi. Analytic value of the atomic three-electron correlation integral with Slater wave functions. *Physical Review A (Atomic, Molecular, and Optical Physics)*, 44(9):5492–5502, November 1991. CODEN PLRAAN. ISSN 1050-2947 (print), 1094-1622, 1538-4446, 1538-4519. URL `http://link.aps.org/doi/10.1103/PhysRevA.44.5492`. See comments [355, 356, 235].

Jorgensen:1992:BRB

[348] Poul Jørgensen. Book review: *Review of algebraic and diagrammatic methods in many-fermion theory*. By Frank E. Harris, Hendrik J. Monkhorst, and David L. Freeman, Oxford University Press, Inc., New York, 1992. *International Journal of Quantum Chemistry*, 44(6):1069, December 5, 1992. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [].

Negadi:2000:PPT

[349] Tidjani Négadi. On the planar periodic table. *International Journal of Quantum Chemistry*, 78(4):206–211, ???? 2000. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL `http://www3.interscience.wiley.com/cgi-bin/abstract/72000074/START;` `http://www3.interscience.wiley.com/cgi-bin/fulltext/72000074/FILE?TPL=ftx_start;` `http://www3.interscience.wiley.com/cgi-bin/fulltext?ID=72000074&PLACEBO=IE.pdf`.

Guseinov:2001:CMA

[350] I. I. Guseinov, B. A. Mamedov, M. Kara, and M. Orbay. On the computation of molecular auxiliary functions A_n and B_n. *Pramana: Journal of Physics*, 56(5):691–696, May 2001. CODEN PRAMCI. ISSN 0304-4289 (print), 0973-7111 (electronic). URL `http://link.springer.com/article/10.1007/s12043-001-0093-x`. See comment [229] and response [353].

Langridge:2001:EST

[351] D. J. Langridge, J. F. Hart, and S. Crampin. Ewald summation technique for one-dimensional charge distributions. *Computer Physics Communications*, 134(1):78–85, February 1, 2001. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465500001922`. See comments and reply [223, 352].

Langridge:2002:RCB

[352] D. J. Langridge, J. F. Hart, and S. Crampin. Reply to comment on "*Ewald summation technique for one-dimensional charge distributions*". *Computer Physics Communications*, 146(2):274–275, July 1, 2002. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465502004538`. See [351, 223].

Guseinov:2003:RCB

[353] I. I. Guseinov. Response to the comment: "*On the computation of molecular auxiliary functions A_n and B_n*". *Pramana: Journal of Physics*, 61(4): C781–C783, October 2003. CODEN PRAMCI. ISSN 0304-4289 (print), 0973-7111 (electronic). URL `http://link.springer.com/article/10.1007/BF02706129`. See [350, 229].

Ozmen:2003:CTC

[354] Ayhan Özmen, Asli Karakaş, Ülfet Atav, and Yusuf Yakar. Computation of two-center Coulomb integrals over Slater-type orbitals using elliptical coordinates. *International Journal of Quantum Chemistry*, 91(1):13–19, ???? 2003. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comment [230].

Sims:2003:CBV

[355] James S. Sims and Stanley A. Hagstrom. Comment on "*Analytic value of the atomic three-electron correlation integral with Slater wave functions*". *Physical Review A (Atomic, Molecular, and Optical Physics)*, 68

(1):016501, July 2003. CODEN PLRAAN. ISSN 1050-2947 (print), 1094-1622, 1538-4446, 1538-4519. URL `http://link.aps.org/doi/10.1103/PhysRevA.68.016501`. See [235, 347, 356].

Sims:2003:ECB

[356] James S. Sims and Stanley A. Hagstrom. Erratum: Comment on "*Analytic value of the atomic three-electron correlation integral with Slater wave functions*" [Phys. Rev. A **68**, 016501 (2003)]. *Physical Review A (Atomic, Molecular, and Optical Physics)*, 68(5):059903, November 2003. CODEN PLRAAN. ISSN 1050-2947 (print), 1094-1622, 1538-4446, 1538-4519. URL `http://link.aps.org/doi/10.1103/PhysRevA.68.059903`. See [235, 347, 355].

Frolov:2004:CBR

[357] Alexei M. Frolov and Vedene H. Smith, Jr. Corrigendum: "*Exponential representation in the Coulomb three-body problem*". *Journal of Physics B: Atomic, Molecular and Optical Physics*, 37(19):4037, October 14, 2004. CODEN JPAPEH. ISSN 0953-4075 (print), 1361-6455 (electronic). URL `http://iopscience.iop.org/0953-4075/37/19/C01`. See [358]. From the concluding paragraph: "We are indebted to Professors Frank E. Harris and Paul C. Abbott for calling to our attention the errors in the matrix elements and the lack of appropriate citations regarding removal of the $\cos\theta_{klm}$ integrals.".

Frolov:2004:ERC

[358] Alexei M. Frolov and Vedene H. Smith, Jr. Exponential representation in the Coulomb three-body problem. *Journal of Physics B: Atomic, Molecular and Optical Physics*, 37(14):2917–2932, July 28, 2004. CODEN JPAPEH. ISSN 0953-4075 (print), 1361-6455 (electronic). URL `http://iopscience.iop.org/0953-4075/37/14/006`; `http://stacks.iop.org/JPhysB/37/2917`. See corrigendum [357].

Safouhi:2006:NTT

[359] Hassan Safouhi. Numerical treatment of two-center overlap integrals. *Journal of Molecular Modeling*, 12(2):213–220, January 2006. CODEN JMMOFK. ISSN 0948-5023 (print), 1610-2940 (electronic). URL `http://link.springer.com/article/10.1007/s00894-005-0020-z`. See comment [278].

Bolcer:2007:DCC

[360] John D. Bolcer and Robert B. Hermann. The development of computational chemistry in the United States. In *Reviews in Computational Chemistry*, volume 5, pages 1–63. Wiley, New York, NY, USA, January

2007. ISSN 1069-3599 (print), 1934-5372 (electronic). LCCN QD39.3.E46 R48. URL `http://onlinelibrary.wiley.com/bookseries/10.1002/SERIES6143`.

Anonymous:2009:FHL

[361] Anonymous. Frank E. Harris: List of publications. *International Journal of Quantum Chemistry*, 109(13):2803–2816, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2009:SPA

[362] Anonymous. A short photo album of Frank Harris. *International Journal of Quantum Chemistry*, 109(13):2802, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maiti:2009:DDF

[363] Buddhadev Maiti, Patrick M. McLaurin, Raymond Sadeghi, S. Ajith Perera, and Jorge A. Morales. Dynamics for the dynamic Frank Harris: Exploring $H^+ + CF_4$ at $E_{lab} = 20$ and 30 eV. *International Journal of Quantum Chemistry*, 109(13):3026–3035, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Monkhorst:2009:MAF

[364] Hendrik J. Monkhorst. My association with Frank Harris: An arc of forty-four years. *International Journal of Quantum Chemistry*, 109(13): 2821–2825, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sabin:2009:FHF

[365] John R. Sabin and N. Yngve Öhrn. Frank E. Harris: The first 80 years. *International Journal of Quantum Chemistry*, 109(13):2801, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Taylor:2009:FHB

[366] Howard S. Taylor. Frank Harris: The Berkeley years—A personal memoir. *International Journal of Quantum Chemistry*, 109(13):2817–2820, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Trickey:2009:CKS

[367] Samuel B. Trickey, V. V. Karasiev, and R. S. Jones. Conditions on the Kohn–Sham kinetic energy and associated density. *International Journal of Quantum Chemistry*, 109(13):2943–2952, November 5, 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). URL

http://adsabs.harvard.edu/abs/2009IJQC..109.2943T; http://onlinelibrary.wiley.com/doi/10.1002/qua.22312/abstract.

Cabrera-Trujillo:2015:P

[368] Remigio Cabrera-Trujillo and John R. Sabin. Preface. *Advances in Quantum Chemistry*, 71:xi–xii, 2015. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327615000477.

Cardenuto:2015:CTE

[369] Marcelo Hidalgo Cardenuto, Kaline Coutinho, Benedito J. C. Cabral, and Sylvio Canuto. Chapter thirteen — electronic properties in supercritical fluids: the absorption spectrum of *p*-nitroaniline in supercritical water. *Advances in Quantum Chemistry*, 71:323–339, 2015. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327615000131.

Chakraborty:2015:CTS

[370] Debajit Chakraborty, James Dufty, and Valentin V. Karasiev. Chapter two — system-size dependence in grand canonical and canonical ensembles. *Advances in Quantum Chemistry*, 71:11–27, 2015. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S006532761500009X.

Cruz:2015:CFH

[371] Salvador A. Cruz and Eugenio Ley-Koo. Chapter five — the hydrogen H_2^+ and HeH^{2+} molecular ions confined in dihedral angles. *Advances in Quantum Chemistry*, 71:69–113, 2015. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327615000088.

Dominguez-Gutierrez:2015:CFM

[372] Fco. Javier Domínguez-Gutiérrez, Predrag S. Krstić, and Remigio Cabrera-Trujillo. Chapter fifteen — multiresolution approach for laser-modified collisions of atoms and ions. *Advances in Quantum Chemistry*, 71:353–371, 2015. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327615000155.

Fripiat:2015:CSF

[373] Joseph G. Fripiat, Benoît Champagne, and Frank E. Harris. Chapter seven — the Fourier space restricted Hartree–Fock method for the electronic structure calculation of one-dimensionally periodic systems. *Advances in Quantum Chemistry*, 71:153–194, 2015. CODEN AQCHA9. ISSN

0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327615000106.

Kaijser:2015:COF

[374] Per Kaijser. Chapter one — Frank Harris, a master of mountains. *Advances in Quantum Chemistry*, 71:1–9, 2015. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327615000039.

Karasiev:2015:CNF

[375] Valentin V. Karasiev and Samuel B. Trickey. Chapter nine — frank discussion of the status of ground-state orbital-free DFT. *Advances in Quantum Chemistry*, 71:221–245, 2015. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327615000052.

Koures:2015:CTS

[376] Vasilios G. Koures. Chapter ten — statistical inference with minimum relative entropy: a robust numerical algorithm employing sinc quadrature. *Advances in Quantum Chemistry*, 71:247–263, 2015. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S006532761500012X.

Mejia-Rodriguez:2015:CFH

[377] Daniel Mejía-Rodríguez, Xiaomin Huang, Jorge M. del Campo, and Andreas M. Köster. Chapter four — hybrid functionals with variationally fitted exact exchange. *Advances in Quantum Chemistry*, 71:41–67, 2015. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327615000167.

Mendez-Fragoso:2015:CFH

[378] Ricardo Méndez-Fragoso and Remigio Cabrera-Trujillo. Chapter fourteen — on a hyperbolic solution to the nonlinear Schrödinger equation for a square well potential coupled to a contact impurity at the delocalization threshold. *Advances in Quantum Chemistry*, 71:341–352, 2015. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327615000143.

Mendez-Fragoso:2015:CSA

[379] Ricardo Méndez-Fragoso and Eugenio Ley-Koo. Chapter six — angular momentum theory in bases of Lamé spheroconal harmonics. *Advances in Quantum Chemistry*, 71:115–152, 2015. CODEN AQCHA9. ISSN

0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327615000040.

Micha:2015:CEG

[380] David A. Micha. Chapter eight — generalized response theory for a photoexcited many-atom system. *Advances in Quantum Chemistry*, 71: 195–220, 2015. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327615000118.

Roman-Ancheyta:2015:CTA

[381] Ricardo Román-Ancheyta and José Récamier. Chapter twelve — approximate coherent states for nonlinear systems. *Advances in Quantum Chemistry*, 71:299–322, 2015. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327615000076.

Sauer:2015:CTM

[382] Stephan P. A. Sauer, Jens Oddershede, and John R. Sabin. Chapter three — the mean excitation energy of atomic ions. *Advances in Quantum Chemistry*, 71:29–40, 2015. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327615000027.

Stenger:2015:CEC

[383] Frank Stenger, Gerd Baumann, and Vasilios G. Koures. Chapter eleven — computational methods for chemistry and physics, and Schrödinger in $3 + 1^1$. *Advances in Quantum Chemistry*, 71:265–298, 2015. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327615000064.

Bonchev:1977:ITD

[384] D. Bonchev and Nenad Trinajstić. Information theory, distance matrix, and molecular branching. *Journal of Chemical Physics*, 67(10):4517–4533, November 15, 1977. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://scitation.aip.org/content/aip/journal/jcp/67/10/10.1063/1.434593.

Freeman:1977:CCE

[385] David L. Freeman. Coupled-cluster expansion applied to the electron gas: Inclusion of ring and exchange effects. *Physical Review B: Solid State*, 15 (12):5512–5521, June 15, 1977. CODEN PLRBAQ. ISSN 0556-2805. URL http://prb.aps.org/abstract/PRB/v15/i12/p5512_1.

Gutman:1977:FCS

[386] I. Gutman and Nenad Trinajstić. Factors contributing to the stability of conjugated heterocycles containing a single heteroatom. *Chemical Physics Letters*, 46(3):591–593, March 15, 1977. CODEN CHPLBC. ISSN 0009-2614 (print), 1873-4448 (electronic). URL `http://www.sciencedirect.com/science/article/pii/000926147780660X`.

Kumar:1977:ESS

[387] Lalit Kumar, Hendrik J. Monkhorst, and Jens Oddershede. Electronic-structure studies of solids. V. Rigorous Hartree–Fock treatment of metallic hydrogen using a plane-wave basis. *International Journal of Quantum Chemistry*, 12(1):145–160, July 1977. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Monkhorst:1977:CPC

[388] Hendrik J. Monkhorst. Calculation of properties with the coupled-cluster method. *International Journal of Quantum Chemistry*, 12(S11):421–432, January 16–22, 1977. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory, Collision Phenomena, and Computational Methods.

Pack:1977:SPB

[389] James D. Pack and Hendrik J. Monkhorst. Special points for Brillouin-zone integrations — a reply. *Physical Review B: Solid State*, 16(4):1748–1749, August 15, 1977. CODEN PLRBAQ. ISSN 0556-2805. URL `http://link.aps.org/doi/10.1103/PhysRevB.16.1748`.

Trinajstic:1977:CCP

[390] Nenad Trinajstić. Computing the characteristic polynomial of a conjugated system using the Sachs Theorem. *Croatica Chemica Acta*, 49(??):593–633, ???? 1977. CODEN CCACAA. ISSN 0011-1643 (print), 1334-417X (electronic).

Trinajstic:1977:NDH

[391] Nenad Trinajstić. New developments in Hückel theory. *International Journal of Quantum Chemistry*, 12(S11):469–477, January 16–22, 1977. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory, Collision Phenomena, and Computational Methods.

Zivkovic:1977:ERS

[392] Tomislav P. Živković. Existence and reality of solutions of the coupled-cluster equations. *International Journal of Quantum Chemistry*, 12(S11): 413–420, January 16–22, 1977. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory, Collision Phenomena, and Computational Methods.

Bonchev:1978:TCM

[393] D. Bonchev and Nenad Trinajstić. On topological characterization of molecular branching. *International Journal of Quantum Chemistry*, 14 (S12):293–303, March 12–18, 1978. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). Supplement: Proceedings of the International Symposium on Atomic, Molecular, and Solid-state Theory, Collision Phenomena, and Computational Methods.

Graovac:1978:KIV

[394] Ante Graovac, Ivan Gutman, Milan Randić, and Nenad Trinajstić. Kekulé index for valence bond structures of conjugated systems containing cyclobutane. *Collection of Czechoslovak Chemical Communications*, 43(5): 1375–1392, May 1978. CODEN CCCCAK. ISSN 0010-0765 (print), 1212-6950 (electronic). URL `http://cccc.uochb.cas.cz/43/5/1375/`.

Horvatic:1978:MKP

[395] Krešimir Horvatić and Nenad Trinajstić. Matematička kemija. Primjena teorije skupova u kemiji. (Croatian) [Mathematical chemistry. The application of set theory in chemistry]. *Kemija u Industriji*, 3(??):127–135, ???? 1978. CODEN ???? ISSN 0022-9830 (print), 1334-9090 (electronic).

Monkhorst:1979:ELM

[396] Hendrik J. Monkhorst. Exact LCAO method for two-dimensional crystals using Fourier transforms. *????*, ??(??):??, ???? 1979.

Monkhorst:1979:HFD

[397] Hendrik J. Monkhorst. Hartree–Fock density of states for extended systems. *Physical Review B: Condensed Matter and Materials Physics*, 20 (4):1504–1513, August 15, 1979. CODEN PRBMDO. ISSN 1098-0121. URL `http://link.aps.org/doi/10.1103/PhysRevB.20.1504`.

Monkhorst:1979:HTR

[398] Hendrik J. Monkhorst and James D. Pack. The high-temperature resistivity of beryllium. *Solid State Communications*, 29(9):675–676, March

1979. CODEN SSCOA4. ISSN 0038-1098 (print), 1879-2766 (electronic). URL http://www.sciencedirect.com/science/article/pii/0038109879912006.

Monkhorst:1979:NLD

[399] Hendrik J. Monkhorst and Bogumił Jeziorski. No linear dependence or many-center integral problems in momentum space quantum chemistry. *Journal of Chemical Physics*, 71(12):5268–5269, December 15, 1979. CODEN JCPSA6. ISSN 0021-9606 (print), 1089-7690 (electronic). URL http://scitation.aip.org/content/aip/journal/jcp/71/12/10.1063/1.438337.

Monkhorst:1979:XRS

[400] Hendrik J. Monkhorst, James D. Pack, and David L. Freeman. On the X-ray scattering factors of metallic and molecular hydrogen crystals. *Solid State Communications*, 29(10):735–737, March 1979. CODEN SSCOA4. ISSN 0038-1098 (print), 1879-2766 (electronic). URL http://www.sciencedirect.com/science/article/pii/0038109879910172.

Pack:1979:LCP

[401] James D. Pack, Hendrik J. Monkhorst, and David L. Freeman. Lithium crystal properties from high-quality Hartree–Fock wave functions. *Solid State Communications*, 29(10):723–725, March 1979. CODEN SSCOA4. ISSN 0038-1098 (print), 1879-2766 (electronic). URL http://www.sciencedirect.com/science/article/pii/0038109879910147.

Monkhorst:1981:EPF

[402] Hendrik J. Monkhorst and William A. Schwalm. Electrostatics for periodic films of atoms. *Physical Review B: Condensed Matter and Materials Physics*, 23(4):1729–1742, February 15, 1981. CODEN PRBMDO. ISSN 1098-0121. URL http://link.aps.org/doi/10.1103/PhysRevB.23.1729.

Koures:1995:GBE

[403] Vasilios G. Koures. Gaussian basis expansion of the QED light cone Hamiltonian. *Physics Letters B*, 348(1–2):170–177, March 30, 1995. CODEN PYLBAJ. ISSN 0370-2693 (print), 1873-2445 (electronic). URL http://www.sciencedirect.com/science/article/pii/037026939500084X.

Koures:1995:GBR

[404] Vasilios G. Koures. Gaussian basis representation of the QED light cone Hamiltonian. In ????, editor, *Proceedings DPF*, pages 1426–?? World Scientific Publishing Co. Pte. Ltd., P. O. Box 128, Farrer Road, Singapore 9128, 1995.

Koures:1996:SCS

[405] Vasilios G. Koures. Solving the Coulomb Schrödinger equation in $d = 2 + 1$ via sinc collocation. *Journal of Computational Physics*, 128(1):1–5, October 1, 1996. CODEN JCTPAH. ISSN 0021-9991 (print), 1090-2716 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0021999196901916`.

Koures:1996:SQS

[406] Vasilios G. Koures. Second quantization with sinc kets and sinc bras. Technical report UTAH-IDR-CP04, Department of Physics, University of Utah, Salt Lake City, UT, USA 84112, ???? 1996. ???? pp.

Prigogine:1967:ACP

[407] Ilya Prigogine, editor. *Advances in Chemical Physics*, volume 13. Wiley, New York, NY, USA, 1967. ISBN 0-470-14015-1. ix + 398 pp. URL `http://onlinelibrary.wiley.com/book/10.1002/9780470140154`.

Bergmann:1970:QAH

[408] Ernest David Bergmann and Bernard Pullman, editors. *Quantum aspects of heterocyclic compounds in chemistry and biochemistry: proceedings of an international symposium held in Jerusalem, 31 March–4 April 1969*, volume 2 of *The Jerusalem Symposia on Quantum Chemistry and Biochemistry*. Israel Academy of Sciences and Humanities, Jerusalem, Israel, 1970. ISSN 0075-3696. LCCN QD331 .A75.

Alder:1971:AMS

[409] Berni Alder, Sidney Fernbach, and Manuel Rotenberg, editors. *Atomic and Molecular Scattering*, volume 10 of *Methods in Computational Physics: Advances in Research and Applications*. Academic Press, New York, NY, USA, 1971. ISBN 0-12-460810-8. ISSN 0076-6860. xiii + 341 pp. LCCN QA401 .M514 v.10. URL `http://www.sciencedirect.com/science/bookseries/00766860/10/supp/C`.

Branscomb:1971:EAC

[410] Lewis M. Branscomb, H. Ehrhardt, R. Geballe, F. J. de Heer, N. V. Fedorenko, J. Kistemaker, M. Barat, E. E. Nikitin, and A. C. H. Smith, editors. *Electronic and atomic collisions: abstracts of papers of the VIIth International Conference on the Physics of Electronic and Atomic Collisions: VII ICPEAC, Amsterdam, The Netherlands, 26–30 July, 1971*. North-Holland, Amsterdam, The Netherlands, 1971. ISBN 0-7204-0234-4, 0-7204-0235-2 (vol. 1), 0-7204-0236-0 (vol. 2). LCCN QC721 I618 1971; QC794.6.C6.

Marcus:1971:CMB

[411] P. M. Marcus, J. F. Janak, and A. R. Williams, editors. *Computational Methods in Band Theory: Proceedings of a Conference held at the IBM Thomas J. Watson Research Center, Yorktown Heights, New York, May 14–15, 1970, under the joint sponsorship of IBM and the American Physical Society*, The IBM Research Symposia Series. Springer-Verlag, Berlin, Germany / Heidelberg, Germany / London, UK / etc., 1971. ISBN 1-4684-1892-0 (print), 1-4684-1890-4 (e-book). URL `http://link.springer.com/book/10.1007/978-1-4684-1890-3`.

Thewlis:1971:QMB

[412] J. Thewlis, R. C. Glass, D. J. Hughes, and A. R. Meetham, editors. *Quantum mechanics in biochemistry*, volume 4 (supplement). Pergamon Press, New York, NY, USA, 1971. ISBN 0-08-006359-4. 351–?? pp. LCCN ????

Herman:1973:CML

[413] Frank Herman, A. Douglas McLean, and Robert K. Nesbet, editors. *Computational Methods for Large Molecules and Localized States in Solids: Proceedings of a Symposium, Held May 15–17, 1972, at the IBM Research Laboratory, San Jose, California*, The IBM Research Symposia Series. Plenum Press, New York, NY, USA; London, UK, 1973. ISBN 1-4684-2015-1 (print), 1-4684-2013-5 (e-book). LCCN QD450-882. URL `http://link.springer.com/book/10.1007/978-1-4684-2013-5`.

Smith:1973:ESR

[414] Darwin W. Smith and Walter Bruce McRae, editors. *Energy, structure, and reactivity: Proceedings of the 1972 Boulder Summer Research Conference on Theoretical Chemistry*. Wiley, New York, NY, USA, 1973. ISBN 0-471-80140-2. LCCN QD462.A1 B68 1972. Proceedings of the Boulder Quantum Theory Symposium and Research Workshop, held at the University of Colorado, Boulder, CO, USA, June 1972.

Andre:1975:ESP

[415] Jean-Marie André, János Ladik, and Joseph Delhalle, editors. *Electronic Structure of Polymers and Molecular Crystals*, volume 9 of *NATO Advanced Study Institute Series. Series B, Physics*. Plenum Press, New York, NY, USA; London, UK, 1975. ISBN 1-4757-0321-X (print), 1-4757-0319-8 (e-book). LCCN QD380.N371974. URL `http://link.springer.com/book/10.1007/978-1-4757-0319-1`.

Eyring:1975:TCA

[416] Henry Eyring and Douglas Henderson, editors. *Theoretical Chemistry: Advances and Perspectives*, volume 1. Academic Press, New York, NY,

USA, 1975. CODEN THCHDM. ISBN 0-323-15958-3, 0-12-681901-7 (e-book). ISSN 0305-9995. 236 pp. LCCN ???? URL `http://www.sciencedirect.com/science/bookseries/00823961`.

Phariseau:1977:EFI

[417] P. Phariseau and L. Scheire, editors. *Electrons in Finite and Infinite Structures*, volume 24 of *NATO Advanced Study Institutes Series: Series B: Physics*. Plenum Press, New York, NY, USA; London, UK, 1977. ISBN 0-306-35724-0, 1-4684-2813-6 (print), 1-4684-2811-X (e-book). LCCN QC176.8.E4 N34 1976. URL `http://link.springer.com/book/10.1007/978-1-4684-2811-7`.

Andre:1978:QTP

[418] Jean-Marie André, Joseph Delhalle, and János Ladik, editors. *Quantum Theory of Polymers*, volume 39 of *NATO Advanced Study Institutes Series*. D. Reidel, Dordrecht, The Netherlands; Boston, MA, USA; Lancaster, UK; Tokyo, Japan, 1978. ISBN 94-009-9814-7 (print), 94-009-9812-0 (e-book). URL `http://link.springer.com/book/10.1007/978-94-009-9812-4`.

Harris:1979:PCS

[419] Frank E. Harris and Nelson H. F. Beebe, editors. *Proceedings of the conference Software Standards in Chemistry, Held at the University of Utah, July 25–27, 1979*, volume 7. Lawrence Berkeley Laboratory, University of California, Berkeley, CA, USA, July 1979. URL `http://escholarship.org/uc/item/19b1d4sw`.

Harris:1980:LNU

[420] Frank E. Harris, Josef Michl, John P. Simons, and R. P. Steiner, editors. *Lecture Notes: Utah Chemistry Workshop, September 22–27, 1980,* Modern Quantum Chemistry. Department of Chemistry, University of Utah, Salt Lake City, UT 84112, USA, 1980. Two volumes.

Lerner:1981:EP

[421] Rita G. Lerner and George L. Trigg, editors. *Encyclopedia of Physics*. Addison-Wesley, Reading, MA, USA, 1981. ISBN 0-201-04313-0. xvi + 1157 pp. LCCN QC5 .E545 1981. Foreword by Walter Sullivan.

Weatherford:1982:EMM

[422] Charles A. Weatherford and Herbert W. Jones, editors. *ETO Multicenter Molecular Integrals: Proceedings of the First International Conference held at Florida A&M University, Tallahassee, Florida, U.S.A., August 3–6, 1981*. D. Reidel, Dordrecht, The Netherlands; Boston, MA, USA;

Lancaster, UK; Tokyo, Japan, 1982. ISBN 94-009-7923-1 (print), 94-009-7921-5 (e-book). URL `http://link.springer.com/chapter/10.1007/978-94-009-7921-5_13`.

Brandas:2004:FWQ

[423] Erkki J. Brändas and Eugene S. Kryachko, editors. *Fundamental World of Quantum Chemistry: A Tribute to the Memory of Per-Olov Löwdin. Volume III*. Kluwer Academic Publishers Group, Norwell, MA, USA, and Dordrecht, The Netherlands, 2004. ISBN 90-481-6687-X (print), 94-017-0448-1 (e-book). xlvi + 677 pp. URL `http://link.springer.com/book/10.1007/978-94-017-0448-9`.

King:2006:SSS

[424] Ronald C. King, Mirosław Bylicki, and Jacek Karwowski, editors. *Symmetry, spectroscopy and SCHUR: proceedings of the Professor Brian G. Wybourne Commemorative Meeting, Toruń, 12–14 June 2005*. Nicolaus Copericus University Press, Toruń, Poland, 2006. ISBN 83-231-1901-5. LCCN QC16.W93 P76 2005.

Simos:2006:RPC

[425] Theodore E. Simos and George Maroulis, editors. *Recent progress in computational sciences and engineering: lectures presented at the International Conference of Computational Methods in Sciences and Engineering 2006 (ICCMSE 2006), Chania, Crete, Greece: recognised conference by the European Society of Computational Methods in Sciences and Engineering (ESCMSE)*, volume 7 of *Lecture series on computer and computational sciences*. VSP, International Science Publishers, Utrecht, The Netherlands, 2006. CODEN LSCCAR. ISBN 90-04-15542-2 (set). ISSN 1573-4196. LCCN Q183.9 .I524 2006.

Maroulis:2007:CMS

[426] George Maroulis and Theodore E. Simos, editors. *Computational Methods in Science and Engineering: Theory and Computation: Old Problems and New Challenges. Lectures Presented at the International Conference on Computational Methods in Science and Engineering 2007 (ICCMSE 2007): Corfu (Greece), 25–30 September 2007*, volume 963 (part 1) of *AIP Conference Proceedings (#963)*. American Institute of Physics, Woodbury, NY, USA, 2007. ISBN 0-7354-0476-3 (set), 0-7354-0477-1 (vol. 1). ISSN 0094-243X (print), 1551-7616 (electronic), 1935-0465. LCCN Q183.9.I524 2007. URL `http://scitation.aip.org/content/aip/proceeding/aipcp/963`; `http://www.springer.com/physics/atoms/book/978-0-7354-0477-9`.

Simos:2007:CMS

[427] Theodore E. Simos and George Maroulis, editors. *Computation in Modern Science and Engineering: Proceedings of the International Conference on Computational Methods in Science and Engineering 2007 (ICCMSE 2007), Corfu, Greece, 25–30 September 2007*, volume 2A. American Institute of Physics, Woodbury, NY, USA, 2007. ISBN 0-7354-0476-3 (set), 0-7354-0477-1 (vol. 1), 0-7354-0478-X (vol. 2). LCCN Q183.9 2007. Two volumes.

Paz:2009:NDQ

[428] José Luis Paz and Antonio J. Hernández, editors. *New Developments in Quantum Chemistry*. Research Signpost, Trivandrum, 695023, Kerala, India, 2009. ISBN 81-7895-446-X. LCCN QD462 .N48 2009. URL `http://www.ressign.com/UserBookDetail.aspx?bkid=1006`.

Piecuch:2009:ATA

[429] Piotr Piecuch, Jean Maruani, Gerardo Delgado-Barrio, and Stephen Wilson, editors. *Advances in the Theory of Atomic and Molecular Systems: Conceptual and Computational Advances in Quantum Chemistry*, volume 19 of *Progress in Theoretical Chemistry and Physics*. Kluwer Academic Publishers Group, Norwell, MA, USA, and Dordrecht, The Netherlands, 2009. ISBN 90-481-2595-2 (print), 90-481-2596-0 (e-book). ???? pp. URL `http://link.springer.com/book/10.1007/978-90-481-2596-8`.

Sattler:2010:HNC

[430] Klaus Sattler, editor. *Handbook of nanophysics: Clusters and Fullerenes*, volume 2. CRC Press, 2000 N.W. Corporate Blvd., Boca Raton, FL 33431-9868, USA, 2010. ISBN 1-4200-7554-3. 827 pp. LCCN QC173.4 M5. URL `http://www.crcpress.com/product/isbn/9781420075403`.

Arfken:2013:MMP

[431] George B. (George Brown) Arfken, Hans-Jürgen Weber, and Frank E. Harris. *Mathematical Methods for Physicists: a Comprehensive Guide*. Elsevier Academic Press, Amsterdam, The Netherlands, seventh edition, 2013. ISBN 0-12-384654-4 (hardcover). xiii + 1205 pp. LCCN QA37.3 .A74 2013.

Champagne:2014:ETF

[432] Benoît Champagne, Michael S. Deleuze, Frank De Proft, and Tom Leyssens, editors. *Theoretical Chemistry in Belgium: A Topical Collection from* Theoretical Chemistry Accounts, volume 6 of *Highlights in Theoretical Chemistry*. Springer-Verlag, Berlin, Germany / Heidelberg, Germany /

London, UK / etc., 2014. ISBN 3-642-41314-5 (print), 3-642-41315-3 (e-book). vi + 288 pp. URL `http://link.springer.com/book/10.1007/978-3-642-41315-5`.

Graziani:2014:FCW

[433] Frank Graziani, Michael P. Desjarlais, Ronald Redmer, and Samuel B. Trickey, editors. *Frontiers and Challenges in Warm Dense Matter*, volume 96 of *Mathematics and Statistics (Springer-11649); Lecture Notes in Computational Science and Engineering*. Springer-Verlag, Berlin, Germany / Heidelberg, Germany / London, UK / etc., 2014. ISBN 3-319-04912-7. ISSN 1439-7358. x + 282 + 89 + 64 pp. LCCN QA71-90.

Sabin:2015:CMP

[434] John R. Sabin and Remigio Cabrera-Trujillo, editors. *Concepts of mathematical physics in chemistry: a tribute to Frank E. Harris*, volume 71. Academic Press, New York, NY, USA, 2015. ISBN 0-12-802824-6, 0-12-802868-8 (e-book). xv + 382 pp. LCCN QC19.2.

Sabin:2016:CMP

[435] John R. Sabin and Remigio Cabrera-Trujillo, editors. *Concepts of mathematical physics in chemistry: a tribute to Frank E. Harris. Part B*, volume 72 of *Advances in quantum chemistry*. Academic Press, New York, NY, USA, 2016. ISBN 0-12-803984-1, 0-12-803985-X (e-book). ISSN 0065-3276. xii + 235 pp. LCCN QC19.2.

Wang:2018:CMA

[436] Yan Alexander Wang, Mark Thachuk, Roman V. Krems, and Jean Maruani, editors. *Concepts, methods and applications of quantum systems in chemistry and physics: selected proceedings of QSCP-XXI (Vancouver, BC, Canada, July 2016)*, volume 31 of *Progress in theoretical chemistry and physics*. Springer, Cham, Switzerland, 2018. ISBN 3-319-74581-6, 3-319-74582-4 (e-book). LCCN QD462.A1 F76 2015. URL `http://public.eblib.com/choice/publicfullrecord.aspx?p=5398073`.