A Complete Bibliography of Publications in *Journal of Computational Chemistry*: 1980–1989

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References

Adams:1983:CDA

[AB83] Stephen M. Adams and Shelton Bank. Calculations on the diphenylmethyl anion. *Journal of Computational Chemistry*, 4(4):470–481, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ahlrichs:1985:IES

[ABE+85] Reinhart Ahlrichs, Hans-Joachim Böhm, Claus Ehrhardt, Peter Scharf, Heinz Schiffer, Hans Lischka, and Michael Schindler. Implementation of an electronic structure program system on the CYBER 205. *Journal of Computational Chemistry*, 6(3):200–208, June 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Allinger:1980:ICR

[ABP80] Norman L. Allinger, Ulrich Burkert, and Salvatore Profeta Jr. Ab initio calculations of the rotational potential functions for propylamine and ethylmethylamine. *Journal of Computational Chemistry*, 1(3):281–284, Autumn 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Andrade:1981:BTE

[ACvRS81] Juan G. Andrade, Jayaraman Chandrasekhar, and Paul von Ragué Schleyer. Bicyclo[1.1.0]butadiene (trialene): an experimentally viable molecule? *Journal of Computational Chemistry*, 2(2):207–211, Summer 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Adamowicz:1989:CCM

[Ada89] Ludwik Adamowicz. Coupled cluster method with first-order correlation orbitals versus multireference configuration interaction method. Accurate calculations for HF, H_2O, and NH_3. *Journal of Computational Chemistry*, 10(7):928–934, October 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Alcami:1989:NIB

[ADY89] M. Alcamí, J. L. G. De Paz, and M. Yáñez. Nitrogen inversion barriers in three-membered rings. An ab initio molecular orbital study. *Journal of Computational Chemistry*, 10 (4):468–478, June 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Allinger:1983:IEM

[AF83] Norman L. Allinger and Heather L. Flanagan. Isotope effects in molecular mechanics (MM 2). Calculations deuterium compounds. *Journal of Computational Chemistry*, 4(3):399–403, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Almlof:1982:PDS

[AFK82] J. Almlöf, K. Faegri Jr., and K. Korsell. Principles for a direct SCF approach to LICAO–MO ab initio calculations. *Journal of Computational Chemistry*, 3(3):385–399, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Abraham:1988:MMS

[AG88a] Raymond J. Abraham and G. H. Grant. A molecular mechanics study of the Si O bond and alkyl-silanes. *Journal of Computational Chemistry*, 9(7):709–718, October 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Abraham:1988:CCMa

[AG88b] Raymond J. Abraham and Guy H. Grant. Charge calculations in molecular mechanics. V. Silicon compounds and π bonding. *Journal of Computational Chemistry*, 9(3):244–256, April 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Abraham:1982:ACC

[AGL82] Raymond J. Abraham, Lee Griffiths, and Philip Loftus. Approaches to charge calculations in molecular mechanics. *Journal of Computational Chemistry*, 3(3):407–416, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Abraham:1984:ACC

[AH84] Raymond J. Abraham and Brian Hudson. Approaches to charge calculations in molecular mechanics. 2 Resonance effects in conjugated systems. *Journal of Computational Chemistry*, 5(6):562–570, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Abraham:1985:CCM

[AH85] Raymond J. Abraham and Brian Hudson. Charge calculations in molecular mechanics. III: Amino acids and peptides. *Journal of Computational Chemistry*, 6(3):173–181, June 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Aida:1988:CWC

[Aid88] Misako Aida. Characteristics of the Watson-Crick type hydrogen-bonded DNA base pairs: an ab initio molecular orbital study. *Journal of Computational Chemistry*, 9(4):362–368, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Arteca:1988:SGS

[AJMM88] Gustavo A. Arteca, Victoria B. Jammal, Paul G. Mezey, and Paul G. Mezey. Shape group studies of molecular similarity and regioselectivity in chemical reactions. *Journal of Computational Chemistry*, 9(6):608–619, September 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Allinger:1988:HBM

[AKI88] Norman L. Allinger, Randall A. Kok, and Mita R. Imam. Hydrogen bonding in MM2. *Journal of Computational Chemistry*, 9(6):591–595, September 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Andzelm:1984:CCG

[AKRA84] Jan Andzelm, Mariusz Kłobukowski, and Elżbieta Radzio-Andzelm. Compact contracted Gaussian-type basis sets for halogen atoms. Basis-set superposition effects on molecular properties. *Journal of Computational Chemistry*, 5(2):146–161, April 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Allinger:1987:BAR

[AL87] Norman L. Allinger and Jenn-Huei Lii. Benzene, aromatic rings, van der Waals molecules, and crystals of aromatic molecules in molecular mechanics (MM3). *Journal of Computational Chemistry*, 8(8):1146–1153, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Arteca:1988:SCS

[AM88a] Gustavo A. Arteca and Paul G. Mezey. Shape characterization of some molecular model surfaces. *Journal of Computational Chemistry*, 9(5):554–563, July 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Arteca:1988:VHP

[AM88b] Gustavo A. Arteca and Paul G. Mezey. Validity of the Hammond postulate and constraints on general one-dimensional reaction barriers. *Journal of Computational Chemistry*, 9(7):728–744, October 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1980:Ma

[Ano80a] Anonymous. Masthead. *Journal of Computational Chemistry*, 1(1):fmi, Spring 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1980:Mb

[Ano80b] Anonymous. Masthead. *Journal of Computational Chemistry*, 1(2):fmi, Summer 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1980:Mc

[Ano80c] Anonymous. Masthead. *Journal of Computational Chemistry*, 1(3):fmi, Autumn 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1980:Md

[Ano80d] Anonymous. Masthead. *Journal of Computational Chemistry*, 1(4):fmi, Winter 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1981:Ma

[Ano81a] Anonymous. Masthead. *Journal of Computational Chemistry*, 2(1):fmi, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1981:Mb

[Ano81b] Anonymous. Masthead. *Journal of Computational Chemistry*, 2(2):fmi, Summer 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1981:Mc

[Ano81c] Anonymous. Masthead. *Journal of Computational Chemistry*, 2(3):fmi, Autumn 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1981:Md

[Ano81d] Anonymous. Masthead. *Journal of Computational Chemistry*, 2(4):fmi, Winter 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1982:A

[Ano82a] Anonymous. Announcement. *Journal of Computational Chemistry*, 3(2):274, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1982:Ma

[Ano82b] Anonymous. Masthead. *Journal of Computational Chemistry*, 3(1):fmi, Spring 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1982:Mb

[Ano82c] Anonymous. Masthead. *Journal of Computational Chemistry*, 3(2):fmi, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1982:Mc

[Ano82d] Anonymous. Masthead. *Journal of Computational Chemistry*, 3(3):fmi, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1982:Md

[Ano82e] Anonymous. Masthead. *Journal of Computational Chemistry*, 3(4):fmi, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1983:FCS

[Ano83a] Anonymous. The 1984 Florida Coast Sanibel Symposium, Sheraton Palm Coast Resort Inn, Florida, March 1–15, 1984. *Journal of Computational Chemistry*, 4(4):606, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1983:Ma

[Ano83b] Anonymous. Masthead. *Journal of Computational Chemistry*, 4(1):fmi, Spring 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1983:Mb

[Ano83c] Anonymous. Masthead. *Journal of Computational Chemistry*, 4(2):fmi, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1983:Mc

[Ano83d] Anonymous. Masthead. *Journal of Computational Chemistry*, 4(3):fmi, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1983:Md

[Ano83e] Anonymous. Masthead. *Journal of Computational Chemistry*, 4(4):fmi, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1984:A

[Ano84a] Anonymous. Announcement. *Journal of Computational Chemistry*, 5(1):113, February 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1984:Ma

[Ano84b] Anonymous. Masthead. *Journal of Computational Chemistry*, 5(1):fmi, February 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1984:Mb

[Ano84c] Anonymous. Masthead. *Journal of Computational Chemistry*, 5(2):fmi, April 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1984:Mc

[Ano84d] Anonymous. Masthead. *Journal of Computational Chemistry*, 5(3):fmi, June 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1984:Md

[Ano84e] Anonymous. Masthead. *Journal of Computational Chemistry*, 5(4):fmi, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1984:Me

[Ano84f] Anonymous. Masthead. *Journal of Computational Chemistry*, 5(5):fmi, October 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1984:Mf

[Ano84g] Anonymous. Masthead. *Journal of Computational Chemistry*, 5(6):fmi, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1984:P

[Ano84h] Anonymous. Preface. *Journal of Computational Chemistry*, 5(4):290, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1985:Aa

[Ano85a] Anonymous. Announcement. *Journal of Computational Chemistry*, 6(1):78, February 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1985:Ab

[Ano85b] Anonymous. Announcement. *Journal of Computational Chemistry*, 6(6):674, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1985:Ma

[Ano85c] Anonymous. Masthead. *Journal of Computational Chemistry*, 6(1):fmi, February 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1985:Mb

[Ano85d] Anonymous. Masthead. *Journal of Computational Chemistry*, 6(2):fmi, April 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1985:Mc

[Ano85e] Anonymous. Masthead. *Journal of Computational Chemistry*, 6(3):fmi, June 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1985:Md

[Ano85f] Anonymous. Masthead. *Journal of Computational Chemistry*, 6(4):fmi, August 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1985:Me

[Ano85g] Anonymous. Masthead. *Journal of Computational Chemistry*, 6(5):fmi, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1985:Mf

[Ano85h] Anonymous. Masthead. *Journal of Computational Chemistry*, 6(6):fmi, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1986:D

[Ano86a] Anonymous. Dedication. *Journal of Computational Chemistry*, 7(3):257–258, June 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1986:EJC

[Ano86b] Anonymous. Erratum: Journal of Computational Chemistry, Volume 6, Number 4,pp. 316–329. "Computer Program for Finding all Possible Cycles in Graphs" by A. T. Balaban, P. Filip and T.-S. Balaban. *Journal of Computational Chemistry*, 7(2):253, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [BFB85].

Anonymous:1986:Ma

[Ano86c] Anonymous. Masthead. *Journal of Computational Chemistry*, 7(1):fmi, February 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1986:Mb

[Ano86d] Anonymous. Masthead. *Journal of Computational Chemistry*, 7(2):fmi, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1986:Mc

[Ano86e] Anonymous. Masthead. *Journal of Computational Chemistry*, 7(3):fmi, June 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1986:Md

[Ano86f] Anonymous. Masthead. *Journal of Computational Chemistry*, 7(4):fmi, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1986:Me

[Ano86g] Anonymous. Masthead. *Journal of Computational Chemistry*, 7(5):fmi, October 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1986:Mf

[Ano86h] Anonymous. Masthead. *Journal of Computational Chemistry*, 7(6):fmi–fmii, December 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1986:PAI

[Ano86i] Anonymous. Preliminary announcement: 6th International Congress on Quantum Chemistry. *Journal of Computational Chemistry*, 7(2):254, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1986:SCM

[Ano86j] Anonymous. Symposium on Computational and Mathematical Chemistry. Satellite Symposium of the Canadian Institute of Chemistry Conference Saskatoon, Canada, June 1–4, 1986. *Journal of Computational Chemistry*, 7(1):89, February 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1986:WCT

[Ano86k] Anonymous. World Congress of Theoretical Organic Chemists. *Journal of Computational Chemistry*, 7(2):255, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1987:Aa

[Ano87a] Anonymous. Announcement. *Journal of Computational Chemistry*, 8(2):186, March 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1987:Ab

[Ano87b] Anonymous. Announcement. *Journal of Computational Chemistry*, 8(4):562, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1987:Ac

[Ano87c] Anonymous. Announcement. *Journal of Computational Chemistry*, 8(6):916, September 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1987:Ad

[Ano87d] Anonymous. Announcement. *Journal of Computational Chemistry*, 8(8):1232, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1987:Ma

[Ano87e] Anonymous. Masthead. *Journal of Computational Chemistry*, 8(1):fmi, January 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1987:Mb

[Ano87f] Anonymous. Masthead. *Journal of Computational Chemistry*, 8(2):fmi, March 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1987:Mc

[Ano87g] Anonymous. Masthead. *Journal of Computational Chemistry*, 8(4):fmi, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1987:Md

[Ano87h] Anonymous. Masthead. *Journal of Computational Chemistry*, 8(5):fmi, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1987:Me

[Ano87i] Anonymous. Masthead. *Journal of Computational Chemistry*, 8(6):fmi, September 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1987:Mf

[Ano87j] Anonymous. Masthead. *Journal of Computational Chemistry*, 8(7):fmi, October 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1987:Mg

[Ano87k] Anonymous. Masthead. *Journal of Computational Chemistry*, 8(8):fmi, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1988:Aa

[Ano88a] Anonymous. Announcement. *Journal of Computational Chemistry*, 9(2):188, March 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1988:Ab

[Ano88b] Anonymous. Announcement. *Journal of Computational Chemistry*, 9(4):441, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1988:CSD

[Ano88c] Anonymous. Correction: Systematic Drug Receptor Mapping: A New Approach to the Analysis of Conformational Energy Calculations of Flexible Molecules with Application to Dopaminergic and Adrenergic Agonists Lilly Sanathanan, Elizabeth Danuher, Ki-Hwan Kim, and Yvonne Martin, J. Comput. Chem., **8**, 1075 (1987). *Journal of Computational Chemistry*, 9(4):441, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [SDKM87].

Anonymous:1988:Ma

[Ano88d] Anonymous. Masthead. *Journal of Computational Chemistry*, 9(1):fmi, January 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1988:Mb

[Ano88e] Anonymous. Masthead. *Journal of Computational Chemistry*, 9(2):fmi, March 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1988:Mc

[Ano88f] Anonymous. Masthead. *Journal of Computational Chemistry*, 9(3):fmi, April 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1988:Md

[Ano88g] Anonymous. Masthead. *Journal of Computational Chemistry*, 9(4):fmi, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1988:Me

[Ano88h] Anonymous. Masthead. *Journal of Computational Chemistry*, 9(5):fmi, July 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1988:Mf

[Ano88i] Anonymous. Masthead. *Journal of Computational Chemistry*, 9(6):fmi, September 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1988:Mg

[Ano88j] Anonymous. Masthead. *Journal of Computational Chemistry*, 9(7):fmi, October 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1988:Mh

[Ano88k] Anonymous. Masthead. *Journal of Computational Chemistry*, 9(8):fmi, December 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1989:Aa

[Ano89a] Anonymous. Announcement. *Journal of Computational Chemistry*, 10(3):434, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1989:Ab

[Ano89b] Anonymous. Announcement. *Journal of Computational Chemistry*, 10(5):748, July 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1989:FYQ

[Ano89c] Anonymous. Forty years of quantum chemistry. *Journal of Computational Chemistry*, 10(1):138, January 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1989:Mb

[Ano89d] Anonymous. Masthead. *Journal of Computational Chemistry*, 10(1):fmi, January 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1989:Mc

[Ano89e] Anonymous. Masthead. *Journal of Computational Chemistry*, 10(2):fmi, March 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1989:Md

[Ano89f] Anonymous. Masthead. *Journal of Computational Chemistry*, 10(3):fmi, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1989:Me

[Ano89g] Anonymous. Masthead. *Journal of Computational Chemistry*, 10(4):fmi, June 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1989:Mf

[Ano89h] Anonymous. Masthead. *Journal of Computational Chemistry*, 10(5):fmi, July 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1989:Mg

[Ano89i] Anonymous. Masthead. *Journal of Computational Chemistry*, 10(6):fmi, September 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1989:Mh

[Ano89j] Anonymous. Masthead. *Journal of Computational Chemistry*, 10(7):fmi, October 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1989:M

[Ano89k] Anonymous. Masthead. *Journal of Computational Chemistry*, 10(8):fmi, December 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:1989:MA

[Ano89l] Anonymous. Meeting announcement. *Journal of Computational Chemistry*, 10(1):137, January 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Allinger:1980:TPF

[AP80] N. L. Allinger and S. Profeta Jr. The torsional potential function for n-butane. *Journal of Computational Chemistry*, 1(2):181–184, Summer 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Allouche:1985:IIS

[AP85] A. Allouche and G. Pouzard. Ishtar: an interactive system for quantitative investigation on dipolar and quadrupolar spin-lattice relaxation. *Journal of Computational Chemistry*, 6(6): 610–613, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Allinger:1987:FFA

[AP87] Norman L. Allinger and Ahammadunny Pathiaseril. A force field for allenes and for nonlinear acetylenes within the MM2 approximation. *Journal of Computational Chemistry*, 8(8): 1225–1231, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Andzelm:1985:CBS

[ARS85] J. Andzelm, E. Radzio, and D. R. Salahub. Compact basis sets for LCAO-LSD calculations. Part I: Method and bases for Sc to Zn. *Journal of Computational Chemistry*, 6(6):520–532, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Akins:1981:MDL

[AS81] Daniel L. Akins and Arthur David Snider. Model for diffusion-limited electrochemiluminescence. *Journal of Computational Chemistry*, 2(4):368–375, Winter 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Abraham:1988:CCMb

[AS88] Raymond J. Abraham and Paul E. Smith. Charge calculations in molecular mechanics IV: a general method for conjugated systems. *Journal of Computational Chemistry*, 9(4): 288–297, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Aped:1989:PAE

[ASFW89] Pinchas Aped, Leah Schleifer, Benzion Fuchs, and Saul Wolfe. Probing the anomeric effect. The diaminomethylene group: Calculations of N — C — N-containing molecular systems. *Journal of Computational Chemistry*, 10(2): 265–283, March 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Allinger:1985:EEA

[ASS+85] Norman L. Allinger, Lothar Schäfer, K. Siam, V. J. Klimkowski, and C. Van Alsenoy. The effect of electronegative atoms on the structures of hydrocarbons. ab initio calculations on molecules containing fluorine or (carbonyl) oxygen. *Journal of Computational Chemistry*, 6(5):331–342, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Andre:1984:ICE

[AVBF84] J. M. André, D. P. Vercauteren, V. P. Bodart, and J. G. Fripiat. Ab initio calculations of the electronic structure of helical polymers. *Journal of Computational Chemistry*, 5(6): 535–547, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Andre:1984:EDR

[AVF84] Jean-Marie André, Daniel P. Vercauteren, and Joseph G. Fripiat. Electron density and related properties in stereoregular polymers and biopolymers. *Journal of Computational Chemistry*, 5(4):349–352, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Allinger:1980:SES

[AYS80] N. L. Allinger, Y. Yuh, and J. T. Sprague. The structure and energies of some unsaturated four-membered ring carbocycles. *Journal of Computational Chemistry*, 1(1):30–35, Spring 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Burkert:1982:PUT

[BA82] Ulrich Burkert and Norman L. Allinger. Pitfalls in the use of the torsion angle driving method for the calculation of conformational interconversions. *Journal of Computational Chem-*

istry, 3(1):40–46, Spring 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bachrach:1989:TED

[Bac89] Steven M. Bachrach. Topological electron density analysis of phosphines, phosphaalkenes and phosphaalkynes. *Journal of Computational Chemistry*, 10(3):392–406, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baird:1984:MSC

[Bai84] N. Colin Baird. MNDO study of catenated sulfur: the molecules and ions S_3 to S_8. *Journal of Computational Chemistry*, 5(1):35–43, February 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bair:1986:OGV

[Bai86] Raymond A. Bair. Optimization of the Generalized Valence Bond Method for vector processors. *Journal of Computational Chemistry*, 7(4):500–512, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baker:1986:ALT

[Bak86] Jon Baker. An algorithm for the location of transition states. *Journal of Computational Chemistry*, 7(4):385–395, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baker:1987:AGO

[Bak87] Jon Baker. An algorithm for geometry optimization without analytical gradients. *Journal of Computational Chemistry*, 8 (5):563–574, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balasubramanian:1982:AGN

[Bal82a] K. Balasubramanian. An algorithm for the generation of nuclear spin species and nuclear spin statistical weights. *Journal of Computational Chemistry*, 3(1):69–74, Spring 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balasubramanian:1982:CGN

[Bal82b] K. Balasubramanian. Computer generation of nuclear spin species and nuclear spin statistical weights. *Journal of Computational Chemistry*, 3(1):75–88, Spring 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balasubramanian:1983:CGS

[Bal83] K. Balasubramanian. Computer generation of the symmetry elements of nonrigid molecules. *Journal of Computational Chemistry*, 4(3):302–307, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balasubramanian:1984:CGC

[Bal84] K. Balasubramanian. Computer generation of the characteristic polynomials of chemical graphs. *Journal of Computational Chemistry*, 5(4):387–394, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balasubramanian:1985:CPO

[Bal85] K. Balasubramanian. Characteristic polynomials of organic polymers and periodic structures. *Journal of Computational Chemistry*, 6(6):656–661, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balasubramanian:1988:CGC

[Bal88] K. Balasubramanian. Computer generation of characteristic polynomials of edge-weighted graphs, heterographs, and directed graphs. *Journal of Computational Chemistry*, 9(3): 204–211, April 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bauschlicher:1984:CTM

[Bau84] Charles W. Bauschlicher Jr. On the calculation of transition moments between states described in different orbital basis. *Journal of Computational Chemistry*, 5(5):500–505, October 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brugge:1988:TAP

[BBJ88] John A. Brugge, Bruce G. Buchanan, and Oleg Jardetzky. Toward automating the process of determining polypeptide secondary structure from ^{1}H NMR data. *Journal of Computational Chemistry*, 9(6):662–673, September 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brooks:1983:CPM

[BBO+83] Bernard R. Brooks, Robert E. Bruccoleri, Barry D. Olafson, David J. States, S. Swaminathan, and Martin Karplus. CHARMM: a program for macromolecular energy, minimization, and dynamics calculations. *Journal of Computational Chemistry*, 4(2):187–217, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bishop:1983:DPD

[BC83] David M. Bishop and Alain Cartier. Dipole polarizability derivatives calculated by the Kirkwood method. *Journal of Computational Chemistry*, 4(2):170–174, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bunge:1987:FMM

[BC87] Carlos F. Bunge and Gerardo Cisneros. Fast matrix multiplication. *Journal of Computational Chemistry*, 8(7):960–964, October 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boulu:1989:VBS

[BC89] Laurent G. Boulu and Gordon M. Crippen. Voronoi binding site models: Calculation of binding modes and influence of drug binding data accuracy. *Journal of Computational Chemistry*, 10(5):673–682, July 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bellville:1982:NPC

[BCB82] Dennis J. Bellville, Ronald Chelsky, and Nathan L. Bauld. A nonelectrocyclic path from the cyclobutene cation radical to the 1,3-butadiene cation radical. *Journal of Computational Chemistry*, 3(4):548–551, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brunvoll:1987:ECB

[BCC87] J. Brunvoll, S. J. Cyvin, and B. N. Cyvin. Enumeration and classification of benzenoid hydrocarbons. *Journal of Compu-

tational Chemistry, 8(3):189–197, April 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bonaccorsi:1983:IEA

[BCT83] R. Bonaccorsi, R. Cimiraglia, and J. Tomasi. Ab initio evaluation of absorption and emission transitions for molecular solutes, including separate consideration of orientational and inductive solvent effects. *Journal of Computational Chemistry*, 4(4):567–577, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Benzel:1982:OES

[BD82] Mark A. Benzel and Clifford E. Dykstra. An open-ended self-consistent field method. A simulation of a molecular orbital technique for small memory computers. *Journal of Computational Chemistry*, 3(2):260–264, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bair:1984:QCA

[BD84] Raymond A. Bair and Thomas H. Dunning Jr. Quantum chemistry with an attached processor. *Journal of Computational Chemistry*, 5(1):44–55, February 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boyd:1987:BCP

[BE87] Russell J. Boyd and Kenneth E. Edgecombe. Bond critical points in the electronic structures of the main group diatomic hydrides of lithium through bromine. *Journal of Computational Chemistry*, 8(4):489–498, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bersohn:1983:FAC

[Ber83] Malcom Bersohn. A fast algorithm for calculation of the distance matrix of a molecule. *Journal of Computational Chemistry*, 4(1):110–113, Spring 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bischof:1982:TPS

[BF82] P. Bischof and G. Friedrich. Thermodynamical properties and structural data of radicals calculated by MNDO–UHF. *Journal of Computational Chemistry*, 3(4):486–494, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Batana:1981:DED

[BFAG81] A. Batana, R. C. Rocha Filho, L. A. Avaca, and E. R. González. Determination of electrical double-layer parameters for the adsorption of neutral molecules at the electrode–solution interface. *Journal of Computational Chemistry*, 2(3): 221–224, Autumn 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balaban:1985:CPF

[BFB85] Alexandru T. Balaban, Petru Filip, and Teodor-Silviu Balaban. Computer program for finding all possible cycles in graphs. *Journal of Computational Chemistry*, 6(4):316–329, August 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [Ano86b].

Bersohn:1986:MMD

[BFF86] Malcolm Bersohn, Shizuo Fujiwara, and Yuzuru Fujiwara. A method for the machine detection of near equivalence of major substructures in a molecule. *Journal of Computational Chemistry*, 7(2):129–139, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bohm:1980:ITC

[BG80] Michael C. Böhm and Rolf Gleiter. INDO-type calculations on the ground state and various ionic states of transition metal tricarbonyls. *Journal of Computational Chemistry*, 1 (4):407–416, Winter 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brink:1981:SHBb

[BG81a] George Brink and Leslie Glasser. Studies in hydrogen bonding: Association in ammonia using an empirical potential. *Journal of Computational Chemistry*, 2(2):177–181, Summer 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brink:1981:SHBa

[BG81b] George Brink and Leslie Glasser. Studies in hydrogen bonding: Association in methanol using an empirical potential. *Journal of Computational Chemistry*, 2(1):14–19, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bohm:1982:KDM

[BG82a] Michael C. Böhm and Rolf Gleiter. Koopmans' defects in metal group VIII carbonyls — a many-body approach. *Journal of Computational Chemistry*, 3(2):140–153, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brink:1982:SHBa

[BG82b] George Brink and Leslie Glasser. Studies in hydrogen bonding: Association within mixed dimers of water, methanol, ammonia, and methylamine using the empirical potential EPEN. *Journal of Computational Chemistry*, 3(1):47–52, Spring 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brink:1982:SHBb

[BG82c] George Brink and Leslie Glasser. Studies in hydrogen bonding: Association within small clusters of water, methanol, and ammonia molecules using Jorgensen's intermolecular pair potentials. *Journal of Computational Chemistry*, 3(2):219–226, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boatz:1986:ISH

[BG86] Jerry A. Boatz and Mark S. Gordon. Ab initio studies of H_2PXYH molecules (X, Y = O, S). *Journal of Computational Chemistry*, 7(3):306–320, June 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bandrauk:1987:CEA

[BG87] André D. Bandrauk and Nadia Gélinas. Coupled equations approach to multiphoton molecular processes. *Journal of Computational Chemistry*, 8(4):313–323, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baker:1988:ALB

[BG88] J. Baker and P. M. W. Gill. An algorithm for the location of branching points on reaction paths. *Journal of Computational Chemistry*, 9(5):465–475, July 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bock:1984:RAC

[BGT84] Charles W. Bock, Philip George, and Mendel Trachtman. Rotation about the C N bond in 2-aza-1,3-butadiene and the N N bond in 2,3-diaza-1,3 butadiene: a molecular orbital study. *Journal of Computational Chemistry*, 5(4):395–410, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Buckingham:1986:RIC

[BHR+86] A. D. Buckingham, N. C. Handy, J. E. Rice, K. Somasundram, and C. Dijkgraaf. Reactions involving CO_2, H_2O, and NH_3: the formation of (i) carbamic acid, (ii) urea, and (iii) carbonic acid. *Journal of Computational Chemistry*, 7(3): 283–293, June 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Billeter:1987:EAM

[BHW87] M. Billeter, T. F. Havel, and K. Wüthrich. The ellipsoid algorithm as a method for the determination of polypeptide conformations from experimental distance constraints and energy minimization. *Journal of Computational Chemistry*, 8 (2):132–141, March 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bruccoleri:1986:SCM

[BK86] Robert E. Bruccoleri and Martin Karplus. Spatially constrained minimization of macromolecules. *Journal of Computational Chemistry*, 7(2):165–175, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Biegler-konig:1982:CAP

[BkBT82] Friedrich W. Biegler-könig, Richard F. W. Bader, and Ting-Hua Tang. Calculation of the average properties of atoms in molecules. II. *Journal of Computational Chemistry*, 3(3): 317–328, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bhanuprakash:1986:CIP

[BKC86] K. Bhanuprakash, G. V. Kulkarni, and Asish K. Chandra. On calculations of intermolecular potentials. *Journal of Computational Chemistry*, 7(6):731–738, December 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balasubramanian:1980:GTC

[BKKB80] K. Balasubramanian, Joyce J. Kaufman, Walter S. Koski, and Alexandru T. Balaban. Graph theoretical characterization and computer generation of certain carcinogenic benzenoid hydrocarbons and identification of bay regions. *Journal of Computational Chemistry*, 1(2):149–157, Summer 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Burke:1987:CMV

[BKL87] L. A. Burke, J. Kao, and A. C. Lilly Jr. Combination of MOMM and VEH methods to calculate electronic properties of polymers. *Journal of Computational Chemistry*, 8(2): 107–116, March 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bonchev:1982:GTC

[BKT82] D. Bonchev, D. Kamenski, and O. N. Temkin. Graph theoretical classification and coding of chemical reactions with a linear mechanism. *Journal of Computational Chemistry*, 3 (1):95–111, Spring 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boyd:1981:FFS

[BL81] Donald B. Boyd and Kenny B. Lipkowitz. Force field and self-consistent field calculations on a trans coplanar disulfide: Bis(2-pyrimidyl)disulfide. *Journal of Computational Chemistry*, 2(3):324–333, Autumn 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balasubramanian:1988:CGS

[BL88] K. Balasubramanian and Xiaoyu Liu. Computer generation of spectra of graphs: Applications to C_{60} clusters and other systems. *Journal of Computational Chemistry*, 9(4):406–415, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balaban:1985:UDCa

[BMB85a] Alexandru T. Balaban, Ovanes Mekenyan, and Danail Bonchev. Unique description of chemical structures based on hierarchically ordered extended connectivities (HOC procedures). I. Algorithms for finding graph orbits and canonical numbering of atoms. *Journal of Computational Chemistry*, 6 (6):538–551, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balaban:1985:UDCb

[BMB85b] Alexandru T. Balaban, Ovanes Mekenyan, and Danail Bonchev. Unique description of chemical structures based on hierarchically ordered extended connectivities (HOC procedures). III. Topological, chemical, and stereochemical coding of molecular structure. *Journal of Computational Chemistry*, 6(6):562–569, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baldwin:1984:MMA

[BMG84] D. Theodore Baldwin, Wayne L. Mattice, and Richard D. Gandour. Molecular mechanics assessment of the configurational statistics of polyoxyethylene. *Journal of Computational Chemistry*, 5(3):241–247, June 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Barone:1988:IPS

[BMLR88] Vincenzo Barone, Camilla Minichino, Francesco Lelj, and Nino Russo. Ab initio pseudopotential study of the fluxional behavior in tetrahydroborate complexes. Many-body contributions to the energy barriers of $NaBH_4$, AlH_2BH_4, and GaH_2BH_4. *Journal of Computational Chemistry*, 9(5):518–521, July 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bernardi:1987:TSD

[BMR87] Fernando Bernardi, Joseph J. W. McDouall, and Michael A. Robb. Transition structure in a diabatic surface formalism. *Journal of Computational Chemistry*, 8(4):296–306, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bonchev:1981:IDT

[BMT81] D. Bonchev, O. V. Mekenyan, and N. Trinajstić. Isomer discrimination by topological information approach. *Journal of Computational Chemistry*, 2(2):127–148, Summer 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boggs:1985:ICA

[BN85] James E. Boggs and Zefu Niu. Ab initio calculation of amine out-of-plane angles. *Journal of Computational Chemistry*, 6 (1):46–55, February 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baker:1986:EME

[BNR86] Jon Baker, Ross H. Nobes, and Leo Radom. The evaluation of molecular electron affinities. *Journal of Computational Chemistry*, 7(3):349–358, June 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boyd:1986:BRB

[Boy86] Richard H. Boyd. Book review: *Computer aided chemical thermodynamics of gases and liquids (theory, models and programs)*, by Paul Benedek and Ference Olti, John Wiley, New York, approx. 700 pp., $85.00 (1985). *Journal of Computational Chemistry*, 7(6):762–763, December 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Berthod:1981:MPC

[BP81] H. Berthod and A. Pullman. Molecular potential, cation binding, and hydration properties of the carboxylate anion. Ab initio studies with an extended polarized basis set. *Journal of Computational Chemistry*, 2(1):87–95, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bendl:1982:CAS

[BP82] János Bendl and Ernö Pretscn. Conformation analysis of small molecules with PCILO methods. *Journal of Computational Chemistry*, 3(4):580–587, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Back:1987:CFC

[BP87a] D. M. Back and P. L. Polavarapu. CNDO force constants for glucose. *Journal of Computational Chemistry*, 8(6):772–777, September 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bauschlicher:1987:SVS

[BP87b] Charles W. Bauschlicher Jr. and Harry Partridge. Strategies for vectorizing the sparse matrix vector product on the CRAY XMP, CRAY 2, and CYBER 205. *Journal of Computational Chemistry*, 8(5):636–644, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boggs:1982:SSF

[BPP82] James E. Boggs, Frank Pang, and Péter Pulay. Structures of some fluorinated benzenes determined by ab initio computation. *Journal of Computational Chemistry*, 3(3):344–353, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balasubramanian:1985:CGK

[BR85] K. Balasubramanian and R. Ramaraj. Computer generation of king and color polynomials of graphs and lattices and their applications to statistical mechanics. *Journal of Computational Chemistry*, 6(5):447–454, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Basilevsky:1987:TAC

[BR87] M. V. Basilevsky and V. M. Ryaboy. Two approaches to the calculation of molecular resonance states: Solution of scattering equations and matrix diagonalization. *Journal of Computational Chemistry*, 8(5):683–699, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bellido:1989:ACM

[BR89] M. N. Bellido and J. A. C. Rullmann. Atomic charge models for polypeptides derived from ab initio calculations. *Journal of Computational Chemistry*, 10(4):479–487, June 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Braga:1989:RCM

[Bra89] J. P. Braga. The rate of convergence of the S matrix for the renormalized Numerov and log-derivative methods. *Journal of Computational Chemistry*, 10(3):413–416, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Breulet:1981:ICS

[Bre81] Jacques Breulet. Ab initio calculation of spin–orbit interaction in polyatomic molecules using Gaussian-type wavefunctions. *Journal of Computational Chemistry*, 2(3):244–250, Autumn 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brown:1983:CRS

[Bro83] R. L. Brown. Counting of resonance structures for large benzenoid polynuclear hydrocarbons. *Journal of Computational Chemistry*, 4(4):556–562, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bachrach:1989:AVP

[BS89] Steven M. Bachrach and Andrew Streitwieser. Application of various population methods to some oxygenated compounds. *Journal of Computational Chemistry*, 10(4):514–519, June 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bruno:1983:TET

[BSM83] Alfredo E. Bruno, Ronald P. Steer, and Paul G. Mezey. The thioketone–enethiol tautomerism of aliphatic thiocarbonyls: an ab initio study. *Journal of Computational Chemistry*, 4(1):104–109, Spring 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boyd:1988:NST

[BSSW88] Donald B. Boyd, David W. Smith, James J. P. Stewart, and Erich Wimmer. Numerical sensitivity of trajectories across conformational energy hypersurfaces from geometry optimized molecular orbital calculations: AM1, MNDO, and MINDO/3. *Journal of Computational Chemistry*, 9(4):387–398, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ball:1980:QCIa

[BT80a] John R. Ball and Colin Thomson. Quantum chemical investigations of charge transfer interactions in relation to the electronic theory of cancer. II. *Journal of Computational Chemistry*, 1(3):275–280, Autumn 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ball:1980:QCIb

[BT80b] John R. Ball and Colin Thomson. Quantum chemical investigations of charge transfer interactions in relation to the electronic theory of cancer. IV. The interaction of formamide and the enol tautomers of several glyoxals. *Journal of Computational Chemistry*, 1(4):400–406, Winter 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baird:1981:IMC

[BT81] N. Colin Baird and Kathleen F. Taylor. Ab initio MO calculations for the oxides, oxyacids, and oxyanions of S(IV) and S(VI). *Journal of Computational Chemistry*, 2(3):225–230, Autumn 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bock:1980:ISG

[BTG80] Charles W. Bock, Mendel Trachtman, and Philip George. An ab initio study of the geometry, harmonic and anharmonic force fields, and fundamental vibrational frequencies of cis- and trans-thiolformic acid. *Journal of Computational Chemistry*, 1(2):167–177, Summer 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bock:1981:ISI

[BTG81a] Charles W. Bock, Mendel Trachtman, and Philip George. An ab initio study of the influence of substituents and intramolecular hydrogen bonding on the carbonyl bond length and stretching force constant. I. Monosubstituted carbonyl compounds. *Journal of Computational Chemistry*, 2(1):30–37, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bock:1981:CSF

[BTG81b] Charles W. Bock, Mendel Trachtman, and Philip George. A comparison of selected force constants derived from ab initio SCF calculations on β-hydroxyacrolein. Acrolein, performic acid, and formic acid. *Journal of Computational Chemistry*, 2(2):182–187, Summer 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bock:1982:ISR

[BTG82] Charles W. Bock, Mendel Trachtman, and Philip George. An ab initio study of the relationship between the O H bond length and the harmonic and anharmonic stretching force constants for planar molecules containing C OH, N OH, and O OH groups. *Journal of Computational Chemistry*, 3(4): 512–524, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bock:1985:EIP

[BTG85] Charles W. Bock, Mendel Trachtman, and Philip George. The effect of including polarization functions on the geometrical parameters calculated for benzene, fluorobenzene and cyanobenzene. *Journal of Computational Chemistry*, 6(6): 592–597, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bock:1986:EIP

[BTG86] Charles W. Bock, Mendel Trachtman, and Philip George. The effect of including polarization functions on the geometrical parameters calculated for pyridine. *Journal of Computational Chemistry*, 7(2):153–157, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bonaccorsi:1988:ICR

[BTRT88] Rosanna Bonaccorsi, Jocopo Tomasi, Christopher A. Reynolds, and C. Thomson. Ab initio calculations relevant to the mechanism of chemical carcinogenesis by *N*-nitrosamines. VIII. Effects of hydration on various reactions involved in the formation and metabolism of *N*-nitrosamines. *Journal of Computational Chemistry*, 9(7):779–783, October 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bock:1983:IIE

[BTS+83] Charles Bock, Mendel Trachtman, Ann Schmiedekamp, Philip George, and Tin S. Chin. Intramolecular interaction effects and the structure of N_2OS and N_2O_2: an ab initio study. *Journal of Computational Chemistry*, 4(3):379–389, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Burkert:1980:ICR

[Bur80a] Ulrich Burkert. Ab initio calculations of the rotational potential functions for propanol and ethyl methyl ether. *Journal of Computational Chemistry*, 1(3):285–287, Autumn 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Burkert:1980:AMM

[Bur80b] Ulrich Burkert. Applications of molecular mechanics calculations in carbohydrate chemistry. I. Conformational and constitutional equilibria of tetraoxabicyclo[4.4.0]- and -[5.3.0] decanes, bicyclic diacetals of alditols. *Journal of Computational Chemistry*, 1(2):192–198, Summer 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Burdick:1982:QMT

[Bur82] S. A. Burdick. A quantum mechanical test of Diophantine methods. *Journal of Computational Chemistry*, 3(1): 117–124, Spring 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bauld:1981:OBO

[BW81] Nathan L. Bauld and David Wirth. The origins of barriers to orbital symmetry/topology-allowed pericyclic reactions: Conjugate addition of methylene to *s*-cis-1,3-butadiene. *Journal of Computational Chemistry*, 2(1):1–6, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Berens:1983:MMA

[BW83] Peter H. Berens and Kent R. Wilson. Molecular mechanics with an array processor. *Journal of Computational Chemistry*, 4(3):313–332, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boyd:1989:EEC

[BW89] Russell J. Boyd and Liang-Chen Wang. The effect of electron correlation on the topological and atomic properties of the electron density distributions of molecules. *Journal of Computational Chemistry*, 10(3):367–375, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bystrom:1983:MMS

[Bys83] Katarina Byström. Molecular mechanics studies of enthalpies of formation and strain energies of azoxyalkanes. *Journal of Computational Chemistry*, 4(3):308–312, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cao:1989:MSI

[Cao89] Xiaoping Cao. Molecular symmetry and ab initio calculations. I. Symmetry-matrix and symmetry-supermatrix. *Journal of Computational Chemistry*, 10(7):957–962, October 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carlsen:1982:OSP

[Car82] Lars Carlsen. On the OCS_2 singlet potential energy surface. *Journal of Computational Chemistry*, 3(1):23–27, Spring 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carreira:1985:BRB

[Car85] L. A. Carreira. Book review: *Minicomputer in the laboratory*, by James W. Cooper, Wiley, New York, 1983, 381 pp. Price: $29.00. *Journal of Computational Chemistry*, 6(1): 76–77, February 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cisneros:1987:FVS

[CBR87] Gerardo Cisneros, Carlos F. Bunge, and C. C. J. Roothaan. Fast vector-scalar-multiply-and-add subroutines for VAX computers. *Journal of Computational Chemistry*, 8(5):618–624, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Clark:1983:EDF

[CCSvRS83] Timothy Clark, Jayaraman Chandrasekhar, Günther W. Spitznagel, and Paul von Ragué Schleyer. Efficient diffuse function-augmented basis sets for anion calculations. III. The 3-21+G basis set for first-row elements, Li–F. *Journal of Computational Chemistry*, 4(3):294–301, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Clark:1989:VGP

[CCV89] Matthew Clark, Richard D. Cramer III, and Nicole Van Opdenbosch. Validation of the general purpose Tripos 5.2 force field. *Journal of Computational Chemistry*, 10(8):982–1012, December 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Clavero:1987:TSA

[CDL+87] Carmen Clavero, Miquel Duran, Agustí Lledós, Oscar N. Ventura, and Juan Bertrán. Theoretical study of the addition of hydrogen halides to olefins: a comparison between $(HCl)_2$ and $(HF)_2$ additions to ethylene. *Journal of Computational Chemistry*, 8(4):481–488, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Choi:1989:ASP

[CDL89] Jae Young Choi, Ernest R. Davidson, and Ikchoon Lee. AM1 studies on the potential energy surface for the proton transfer in protonated water clusters, $H^+ (H_2O)_n$. *Journal of Computational Chemistry*, 10(2):163–175, March 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cruickshank:1987:RFI

[CE87] D. W. J. Cruickshank and M. Eisenstein. The role of d functions in ab initio calculations. II. The deformation densities of SO_2, NO_2, and their ions. *Journal of Computational Chemistry*, 8(1):6–27, January 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:1983:RPC

[CF83] Chia-Chung Chen and Marye Anne Fox. Reaction path calculations for the interaction of the ethylene radical cation with triplet oxygen. *Journal of Computational Chemistry*, 4(4): 488–493, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chirlian:1987:ACD

[CF87] Lisa Emily Chirlian and Michelle Miller Francl. Atomic charges derived from electrostatic potentials: a detailed study. *Journal of Computational Chemistry*, 8(6):894–905, September 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carsky:1985:EUP

[ČFHS85] P. Čársky, J. Fabian, B. A. Hess Jr., and L. J. Schaad. An efficient UMP2 program. *Journal of Computational Chemistry*, 6(5):429–431, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cremer:1986:USM

[CG86a] Dieter Cremer and JüRgen Gauss. An unconventional SCF method for calculations on large molecules. *Journal of Computational Chemistry*, 7(3):274–282, June 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cvetkovic:1986:CSG

[CG86b] Dragoš Cvetković and Ivan Gutman. The computer system GRAPH: a useful tool in chemical graph theory. *Journal of Computational Chemistry*, 7(5):640–644, October 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cummins:1989:CSO

[CG89] Peter L. Cummins and Jill E. Gready. Computational strategies for the optimization of equilibrium geometries and transition-state structures at the semiempirical level. *Journal of Computational Chemistry*, 10(7):939–950, October 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Contreras:1987:TST

[CGN87] R. H. Contreras, H. O. Gavarini, and M. A. Natiello. The through-space transmission of ^{77}Se–^{77}Se coupling constants. *Journal of Computational Chemistry*, 8(3):265–271, April 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chang:1983:ORR

[Cha83] Tse-Chiang Chang. Orbital relaxation in the Rydberg series of the lithium atom. An excited state SCF calculation. *Journal of Computational Chemistry*, 4(4):563–566, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:1989:MCS

[Che89] R. S. Chen. Monte Carlo simulations for the study of hemoglobin-fragment conformations. *Journal of Computational Chemistry*, 10(4):488–494, June 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carsky:1984:UMS

[ČHS84] P. Čársky, B. A. Hess Jr., and L. J. Schaad. Use of molecular symmetry in two-electron integral transformation: an MP 2 program compatible with HONDO 5. *Journal of Computational Chemistry*, 5(3):280–287, June 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cioslowski:1987:CEP

[Cio87] J. Cioslowski. Computer enumeration of polyhexes using the compact naming approach. *Journal of Computational Chemistry*, 8(6):906–915, September 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Crowder:1985:CAS

[CL85] G. A. Crowder and Lorelei Lynch. Conformational analysis of some dimethylheptanes with the aid of normal coordinate calculations. *Journal of Computational Chemistry*, 6(6):625–633, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Clark:1981:TEB

[Cla81] Timothy Clark. Three electron bonds. I. The H_2SSH radical cation. *Journal of Computational Chemistry*, 2(3):261–265, Autumn 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Clark:1982:TEB

[Cla82] Timothy Clark. Three-electron bonds. II. SS and SCL three-electron bonds. *Journal of Computational Chemistry*, 3(1): 112–116, Spring 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Clark:1983:TEB

[Cla83] Timothy Clark. Three-electron bonds. III. Phosphorus and chlorine σ^* radical cations. *Journal of Computational Chem-*

istry, 4(3):404–409, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chesnut:1989:LDB

[CM89] D. B. Chesnut and K. D. Moore. Locally dense basis sets for chemical shift calculations. *Journal of Computational Chemistry*, 10(5):648–659, July 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carballeira:1988:MMP

[CMR88] Luis Carballeira, Ricardo A. Mosquera, and Miguel A. Ríos. Molecular mechanics of peroxides. I. Parametrization and conformational analysis of linear compounds. *Journal of Computational Chemistry*, 9(8):851–860, December 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carballeira:1989:MMP

[CMR89] L. Carballeira, R. A. Mosquera, and M. A. Rios. Molecular mechanics of peroxides. II. Cyclic compounds. *Journal of Computational Chemistry*, 10(7):911–920, October 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Curtiss:1986:TSH

[CMRW86] Larry A. Curtiss, Carlos A. Melendres, Alan E. Reed, and Frank Weinhold. Theoretical studies of O_2^-:$(H_2O)_n$ clusters. *Journal of Computational Chemistry*, 7(3):294–305, June 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cooper:1977:MLE

[Coo77] James William Cooper. *The minicomputer in the laboratory: with examples using the PDP-11*. John Wiley, New York, NY, USA, 1977. ISBN 0-471-01883-X. xvii + 365 pp. LCCN QA76.6 .C653 1977. URL `http://catalog.hathitrust.org/api/volumes/oclc/2524627.html`.

Cooper:1980:IPS

[Coo80] James William Cooper. *Introduction to PASCAL for scientists*. John Wiley, New York, NY, USA, 1980. ISBN 0-471-08785-8. xv + 260 pp. LCCN QA76.73.P2 C68.

Cooper:1980:SCP

[CP80] Ian L. Cooper and Christopher N. M. Pounder. A systematic CI procedure with modified virtual orbitals. *Journal of Computational Chemistry*, 1(1):69–75, Spring 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cotrait:1981:CEC

[CP81] Michel Cotrait and Marius Ptak. Conformational energy calculation on the neurotensin *c*-terminal pentapeptide Arg–Pro–Tyr–Ile–Leu OH. *Journal of Computational Chemistry*, 2(4):460–469, Winter 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cimiraglia:1987:RAM

[CP87a] Renzo Cimiraglia and Maurizio Persico. Recent advances in multireference second order perturbation CI: the CIPSI method revisited. *Journal of Computational Chemistry*, 8(1):39–47, January 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Crippen:1987:DEE

[CP87b] Gordon M. Crippen and P. K. Ponnuswamy. Determination of an empirical energy function for protein conformational analysis by energy embedding. *Journal of Computational Chemistry*, 8(7):972–981, October 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chung-Phillips:1989:DAO

[CP89a] Alice Chung-Phillips. Deorthogonalization of atomic originals in the CNDO approach. *Journal of Computational Chemistry*, 10(1):17–34, January 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chung-Phillips:1989:MFS

[CP89b] Alice Chung-Phillips. Methods for the Fourier-series expansion of torsional energies. *Journal of Computational Chemistry*, 10(5):733–747, July 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chang:1985:ORR

[CPH85] T. C. Chang, Chien Hua Pao, and Chen-Shiung Hsue. Orbital relaxation in the Rydberg series of the He atom. *Jour-*

nal of Computational Chemistry, 6(4):282–286, August 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cimiraglia:1984:ECR

[CPTC84] R. Cimiraglia, M. Persico, J. Tomasi, and O. P. Charkin. Electron correlation and relative energetic characteristics of complex hydrides of light elements. I. Beryllohydrides. *Journal of Computational Chemistry*, 5(3):263–271, June 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cortes:1984:CAH

[CPV84] Joaquin Cortés, Heinrich Puschmann, and Eliana Valencia. On computationally adjusting the Hill equation of adsorption. *Journal of Computational Chemistry*, 5(1):104–112, February 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cramer:1985:BRB

[Cra85] Richard Cramer. Book review: *Logic and combinational algorithms for drug design*, by V. E. Golender and A. B. Rosenblit, John Wiley, New York, 289 pp. $63.95 (1984). *Journal of Computational Chemistry*, 6(1):77, February 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cremer:1982:TDIa

[Cre82a] Dieter Cremer. Thermochemical data from ab initio calculations. I. Estimation of SCF energies for augmented basis sets and Hartree–Fock limit energies. *Journal of Computational Chemistry*, 3(2):154–164, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cremer:1982:TDIb

[Cre82b] Dieter Cremer. Thermochemical data from ab initio calculations. II. Total correlation energies, Schrödinger energies, and theoretical heats of formation. *Journal of Computational Chemistry*, 3(2):165–177, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Crippen:1982:CAE

[Cri82] Gordon M. Crippen. Conformational analysis by energy embedding. *Journal of Computational Chemistry*, 3(4):471–476, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Crippen:1984:CAS

[Cri84] Gordon M. Crippen. Conformational analysis by scaled energy embedding. *Journal of Computational Chemistry*, 5(6): 548–554, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Crippen:1987:VBS

[Cri87] Gordon M. Crippen. Voronoi binding site models. *Journal of Computational Chemistry*, 8(7):943–955, October 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Crippen:1989:LEN

[Cri89] Gordon M. Crippen. Linearized embedding: a new metric matrix algorithm for calculating molecular conformations subject to geometric constraints. *Journal of Computational Chemistry*, 10(7):896–902, October 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Canfield:1985:DWM

[CRR85] E. R. Canfield, R. W. Robinson, and D. H. Rouvray. Determination of the Wiener molecular branching index for the general tree. *Journal of Computational Chemistry*, 6(6):598–609, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Collins:1980:ISE

[CS80] John B. Collins and Andrew Streitwieser Jr. Integrated spatial electron populations in molecules: Application to simple molecules. *Journal of Computational Chemistry*, 1(1):81–87, Spring 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Collis:1982:SEH

[CS82] F. P. Collis and J. A. Schwarz. Selectivity effects and hydrocarbon-chain growth during Fischer–Tropsch synthesis. *Journal of Computational Chemistry*, 3(2):135–139, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Catalan:1989:TTM

[CSCD+89] Javier Catalán, Marta Sánchez-Cabezudo, José Luis G. De Paz, José Elguero, Robert W. Taft, and Frederick Anvia. The tautomerism of 1,2,3-triazole, 3(5)-methylpyrazole and their cations. *Journal of Computational Chemistry*, 10(3): 426–433, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cremer:1987:ISC

[CT87] Dieter Cremer and Walter Thiel. On the importance of size-consistency corrections in semiempirical MNDOC calculations. *Journal of Computational Chemistry*, 8(1):48–50, January 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chang:1989:PED

[CU89] D. K. Chang and D. W. Urry. Polypentapeptide of elastin: Damping of internal chain dynamics on extension. *Journal of Computational Chemistry*, 10(6):850–855, September 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cho:1989:CDA

[CUCP89] Soo Gyeong Cho, Rayomand J. Unwalla, Frank K. Cartledge, and Salvatore Profeta Jr. Chlorosilanes: Development and application of MM2 force field parameters. *Journal of Computational Chemistry*, 10(6):832–849, September 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Clark:1981:CPV

[CvRS81] Timothy Clark and Paul von Ragué Schleyer. Conformational preferences of 34 valence electron A_2X_4 molecules: an ab initio Study of B_2F_4, B_2Cl_4, N_2O_4, and C_2O. *Journal of Computational Chemistry*, 2(1):20–29, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chandrasekhar:1981:CSE

[CvRSKJ81] Jayaraman Chandrasekhar, Paul von Ragué Schleyer, and Karsten Krogh-Jespersen. Carbodications. I. The structures and energies of C_4H isomers. *Journal of Computational*

Chemistry, 2(3):356–360, Autumn 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chesnut:1980:SOI

[CW80] D. B. Chesnut and F. W. Whitehurst. A simplex optimized INDO calculation of ^{13}C chemical shifts in hydrocarbons. *Journal of Computational Chemistry*, 1(1):36–45, Spring 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cox:1981:RME

[CW81] S. R. Cox and D. E. Williams. Representation of the molecular electrostatic potential by a net atomic charge model. *Journal of Computational Chemistry*, 2(3):304–323, Autumn 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chesnut:1988:MMC

[CZ88] D. B. Chesnut and C. Zhang. Modified MINDO/3 ^{13}C chemical shift calculations for simple hydrocarbons. *Journal of Computational Chemistry*, 9(4):416–423, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DeLeeuw:1983:CAP

[DA83] Frank A. A. M. De Leeuw and Cornelis Altona. Computer-assisted pseudorotation analysis of five-membered rings by means of proton spin–spin coupling constants: Program PSEUROT. *Journal of Computational Chemistry*, 4(3):428–437, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Darden:1989:MFS

[Dar89] Tom Darden. A method for fitting a smooth ribbon to curved DNA. *Journal of Computational Chemistry*, 10(4):529–551, June 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Damewood:1988:MMS

[DAU88] James R. Damewood Jr., Wayne P. Anderson, and Joseph J. Urban. A molecular mechanics study of neutral molecule complexation with crown ethers. *Journal of Computational Chemistry*, 9(2):111–124, March 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Delgado-barrio:1986:MEA

[DbCV+86] G. Delgado-barrio, A. M. Cortina, A. Varadé, P. Mareca, P. Villarreal, and S. Miret-artés. Matrix elements for anharmonic potentials: Application to I_2 Morse oscillator. *Journal of Computational Chemistry*, 7(2):208–212, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Delgado-Barrio:1984:VPV

[DBVMB84] G. Delgado-Barrio, P. Villarreal, P. Mareca, and J. A. Beswick. Vibrational predissociation of the van der Waals complex $Ne\cdots I_2(B3\Pi)$. A quasiclassical approach. *Journal of Computational Chemistry*, 5(4):322–325, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dykstra:1981:RCD

[DCG81] Clifford E. Dykstra, Richard A. Chiles, and Michael D. Garrett. Recent computational developments with the self-consistent electron pairs method and application to the stability of glycine conformers. *Journal of Computational Chemistry*, 2(3):266–272, Autumn 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Diz:1985:TST

[DCNG85] A. C. Diz, R. H. Contreras, M. A. Natiello, and H. O. Gavarini. The through-space transmission of ^{31}P–^{31}P coupling constants. *Journal of Computational Chemistry*, 6(6): 647–651, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

David:1981:LAS

[DD81] Carl W. David and Elaine Eisler David. Li^+F^- in aqueous solution. *Journal of Computational Chemistry*, 2(4):414–415, Winter 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DeOliveiraNeto:1986:RLPa

[De 86a] Marçal De Oliveira Neto. Rapid location of the preferred interaction sites between small polar molecules and macromolecules. I. Binding of water to the component units of nucleic acids. *Journal of Computational Chemistry*, 7(5):

617–628, October 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DeOliveiraNeto:1986:RLPb

[De 86b] Marçal De Oliveira Neto. Rapid location of the preferred interaction sites between small polar molecules and macromolecules. II. Binding of water to a model segment of B-DNA. *Journal of Computational Chemistry*, 7(5):629–639, October 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Davis:1983:TDS

[DE83] Michael I. Davis and M. Lawrence Ellzey Jr. A technique for determining the symmetry properties of molecular graphs. *Journal of Computational Chemistry*, 4(2):267–275, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DelBene:1981:ISM

[Del81a] Janet E. Del Bene. Ab initio study of 4-monosubstituted pyrimidines in ground and excited $n \rightarrow \pi^*$ states. *Journal of Computational Chemistry*, 2(3):251–260, Autumn 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DelBene:1981:MOTa

[Del81b] Janet E. Del Bene. Molecular orbital theory of the hydrogen bond. 24. Ground-state water–uracil complexes. *Journal of Computational Chemistry*, 2(2):188–199, Summer 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DelBene:1981:MOTb

[Del81c] Janet E. Del Bene. Molecular orbital theory of the hydrogen bond. 25. Water–uracil complexes in excited $n \rightarrow \pi$ states. *Journal of Computational Chemistry*, 2(2):200–206, Summer 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DelBene:1981:MOTc

[Del81d] Janet E. Del Bene. Molecular orbital theory of the hydrogen bond. 26. The hydration of uracil. *Journal of Computational*

Chemistry, 2(4):416–421, Winter 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DelBene:1981:MOTd

[Del81e] Janet E. Del Bene. Molecular orbital theory of the hydrogen bond. 27. Substituent effects in water: 4-R-pyrimidine complexes. *Journal of Computational Chemistry*, 2(4):422–432, Winter 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DelBene:1983:MOT

[Del83] Janet E. Del Bene. Molecular orbital theory of the hydrogen bond. XXX. Water-cytosine complexes. *Journal of Computational Chemistry*, 4(2):226–233, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DelBene:1984:GBS

[Del84] Janet E. Del Bene. Geometry, basis set, and correlation energy dependence of computed protonation energies of imino bases. *Journal of Computational Chemistry*, 5(4):381–386, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DelBene:1985:BSC

[Del85] Janet E. Del Bene. Basis set and correlation effects on computed proton affinities of some oxygen and nitrogen bases. *Journal of Computational Chemistry*, 6(4):296–301, August 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DelBene:1986:BSC

[Del86] Janet E. Del Bene. Basis set and correlation effects on computed lithium ion affinities of some oxygen and nitrogen bases. *Journal of Computational Chemistry*, 7(3):259–264, June 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DelBene:1987:BSC

[Del87] Janet E. Del Bene. Basis set and correlation effects on computed positive ion hydrogen bond energies of the complexes $AH_n \cdot AH_{n+1}^{+1}$: $AH_n = NH_3$, OH_2, and FH. *Journal of Computational Chemistry*, 8(6):810–815, September 1987. CO-

DEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DelBene:1989:IMO

[Del89] Janet E. Del Bene. An ab initio molecular orbital study of the structures and energies of neutral and charged bimolecular complexes of NH_3 with the hydrides AH_n (A = N, O, F, P, S, and Cl). *Journal of Computational Chemistry*, 10(5):603–615, July 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dewar:1984:CEE

[DFC+84] Michael J. S. Dewar, Marye Anne Fox, Kay A. Campbell, Chia-Chung Chen, James E. Friedheim, Mary K. Holloway, Shi Choon Kim, Phillip B. Liescheski, Ali M. Pakiari, Tze-Pei Tien, and Eve G. Zoebisch. Calculation of energies of excited states using MNDO. *Journal of Computational Chemistry*, 5 (5):480–485, October 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Davis:1981:MCC

[DGW+81] L. P. Davis, R. M. Guidry, J. R. Williams, M. J. S. Dewar, and H. S. Rzepa. MNDO calculations for compounds containing aluminum and boron. *Journal of Computational Chemistry*, 2(4):433–445, Winter 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dewar:1983:GSMc

[DH83] Michael J. S. Dewar and Eamonn Healy. Ground states of molecules. 64. MNDO calculations for compounds containing bromine. *Journal of Computational Chemistry*, 4(4):542–551, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dobbs:1986:MOT

[DH86] K. D. Dobbs and W. J. Hehre. Molecular orbital theory of the properties of inorganic and organometallic compounds 4. Extended basis sets for third- and fourth-row, main-group elements. *Journal of Computational Chemistry*, 7(3):359–378, June 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dobbs:1987:MOTa

[DH87a] K. D. Dobbs and W. J. Hehre. Molecular orbital theory of the properties of inorganic and organometallic compounds 5. Extended basis sets for first-row transition metals. *Journal of Computational Chemistry*, 8(6):861–879, September 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [DH88].

Dobbs:1987:MOTb

[DH87b] K. D. Dobbs and W. J. Hehre. Molecular orbital theory of the properties of inorganic and organometallic compounds. 6. Extended basis sets for second-row transition metals. *Journal of Computational Chemistry*, 8(6):880–893, September 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dobbs:1988:EMO

[DH88] K. D. Dobbs and W. J. Hehre. Erratum: Molecular orbital theory of the properties of inorganic and organometallic compounds 5. Extended basis sets for first-row transition metals. *Journal of Computational Chemistry*, 9(7):801, October 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [DH87a].

Dingle:1989:CWT

[DHK89] T. W. Dingle, S. Huzinaga, and M. Klobukowski. Contraction of the well-tempered Gaussian basis sets: the first-row diatomic molecules. *Journal of Computational Chemistry*, 10(6):753–769, September 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DeLaMare:1983:SMM

[DHP83] Peter B. D. De La Mare, David Hall, and Nicola Pavitt. A study by molecular mechanics of the geometric isomers of benzene hexachloride, benzene tetrachloride, and naphthalene tetrachloride. *Journal of Computational Chemistry*, 4 (1):114–122, Spring 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dewar:1984:GSM

[DHS84] Michael J. S. Dewar, Eamonn F. Healy, and James J. P. Stewart. Ground states of molecules. 67. MNDO Calculations for compounds containing iodine. *Journal of Computational Chemistry*, 5(4):358–362, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dillen:1986:UCM

[Dil86] Jan L. M. Dillen. On the use of constraints in molecular mechanics. Rigid group refinement. *Journal of Computational Chemistry*, 7(4):476–481, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dillen:1987:UCM

[Dil87] Jan L. M. Dillen. On the use of constraints in molecular mechanics. II. The Lagrange multiplier method and non-full-matrix Newton–Raphson minimization. *Journal of Computational Chemistry*, 8(8):1099–1103, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dagher:1984:DVR

[DK84] Mounzer Dagher and Hafez Kobeissi. On the diatomic vibration–rotation eigenvalue equation: Highly accurate results for high levels. *Journal of Computational Chemistry*, 5 (6):576–580, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dagher:1985:HAV

[DK85] Mounzer Dagher and Hafez Kobeissi. Highly accurate vibration–rotation Franck–Condon factors for high levels. *Journal of Computational Chemistry*, 6(5):360–367, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dagher:1988:VEA

[DK88] Mounzer Dagher and Hafez Kobeissi. Vibrational eigenvalues for all levels for the Lennard-Jones potential. *Journal of Computational Chemistry*, 9(6):647–649, September 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dreux:1985:SPM

[DLMR85] J. Dreux, P. Lhoste, M. Moreau, and J. Royer. Studies of a proposed mechanism for the reaction between 2H-pyran-2-ones and organomagnesium compounds. *Journal of Com-*

putational Chemistry, 6(1):9–12, February 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dewar:1983:GSMa

[DM83] Michael J. S. Dewar and Michael L. McKee. Ground states of molecules. 56. MNDO calculations for molecules containing sulfur. *Journal of Computational Chemistry*, 4(1):84–103, Spring 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Defrees:1986:IDP

[DM86a] D. J. Defrees and A. D. McLean. Ab initio determination of the proton affinities of small neutral and anionic molecules. *Journal of Computational Chemistry*, 7(3):321–333, June 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dosen-Micovic:1986:ACQ

[DM86b] Ljiljana Došen-Mićović. Atomic charges in the quadrupole solvation energy calculations. *Journal of Computational Chemistry*, 7(4):523–527, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Davis:1989:SFD

[DM89] M. E. Davis and J. A. McCammon. Solving the finite difference linearized Poisson–Boltzmann equation: a comparison of relaxation and conjugate gradient methods. *Journal of Computational Chemistry*, 10(3):386–391, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dosen-Micovic:1988:LE

[DMB88] Lj. Došen-Mićović and B. Blaive. Letter to the editor. *Journal of Computational Chemistry*, 9(1):91, January 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dodziuk:1984:CCA

[Dod84] Helena Dodziuk. Classical conformational analysis of strained organic molecules. I. $[l, m, n]$ Propellanes with l, m, n equal to 2, 3, and 4. *Journal of Computational Chemistry*, 5(6):571–575, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Demare:1980:CES

[DPCS80] G. R. Demaré, M. R. Peterson, I. G. Csizmadia, and O. P. Strausz. Conformational energy surfaces of triplet-state isomeric methyloxiranes. *Journal of Computational Chemistry*, 1(2):141–148, Summer 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Diez:1988:ESC

[DPSF+88] Ernesto Diez, Jesús Palma, Jesús San-Fabián, Joaquin Guilleme, Angel L. Esteban, and Maria P. Galache. Effect of the substituents on the conformational behavior of five-membered rings: Application to the cis- and trans-2,5-dimethoxytetrahydrofuran. *Journal of Computational Chemistry*, 9(3):189–199, April 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dewar:1983:GSMb

[DR83] Michael J. S. Dewar and Henry S. Rzepa. Ground states of molecules. 53. MNDO calculations for molecules containing chlorine. *Journal of Computational Chemistry*, 4(2):158–169, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dewar:1986:ISM

[DR86] Michael J. S. Dewar and Charles H. Reynolds. An improved set of MNDO parameters for sulfur. *Journal of Computational Chemistry*, 7(2):140–143, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

De:1980:CSS

[DS80] B. R. De and A. B. Sannigrahi. A comparative study of the structure and bonding of HOO, HOS, HSO, and HSS radicals by CNDO /2 and INDO methods. *Journal of Computational Chemistry*, 1(4):334–340, Winter 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Datta:1987:RFC

[DS87] N. C. Datta and B. Sen. Recursion formulae for calculation of overlap integrals. *Journal of Computational Chemistry*, 8 (1):1–5, January 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DelValle:1985:ICI

[DTPR85] F. J. Olivares Del Valle, S. Tolosa, A. Lopez Piñeiro, and A. Requena. Ab initio calculations of intermolecular potentials. The ground state of the Ar H_2 van der Waals molecule. *Journal of Computational Chemistry*, 6(1):39–45, February 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DeLeeuw:1983:TSE

[DVA83] Frank A. A. M. De Leeuw, Aart A. Van Beuzekom, and Cornelis Altona. Through-space effects on vicinal proton spin–spin coupling constants mediated via hetero atoms: Nonequivalence of cis couplings in five-membered rings. *Journal of Computational Chemistry*, 4(3):438–448, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dykstra:1988:ECE

[Dyk88] Clifford E. Dykstra. Efficient calculation of electrically based intermolecular potentials of weakly bonded clusters. *Journal of Computational Chemistry*, 9(5):476–487, July 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

El-Basil:1987:CPF

[EB87] Sherif El-Basil. On color polynomials of Fibonacci graphs. *Journal of Computational Chemistry*, 8(7):956–959, October 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Esteban:1989:LRP

[EGM+89] Angel L. Esteban, Maria P. Galache, Francisco Mora, Ernesto Diez, and Jesus San Fabian. Long-range proton-proton coupling constants. I. Propanic coupling involving a methyl group $^4J_{MeH}$. *Journal of Computational Chemistry*, 10(7): 887–895, October 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Eisenstein:1983:SEC

[EH83] M. Eisenstein and F. L. Hirshfeld. Substituent effects on the charge density in the formyl group. *Journal of Compu-*

tational Chemistry, 4(1):15–22, Spring 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ehrenson:1981:CBE

[Ehr81] S. Ehrenson. Cavity boundary effects within the Onsager theory for dielectrics. *Journal of Computational Chemistry*, 2(1):41–52, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ehrenson:1984:SDA

[Ehr84] S. Ehrenson. Solvent dielectric attenuation of substituent effects. Dependence on boundary representation in prolate spheroidal cavity models. *Journal of Computational Chemistry*, 5(1):56–63, February 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ehrenson:1986:OMC

[Ehr86] S. Ehrenson. Offcenter molecular charge distribution corrections to Born equation electrostatic solvation energies. *Journal of Computational Chemistry*, 7(5):648–656, October 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ehrenson:1989:CRD

[Ehr89] S. Ehrenson. Continuum radial dielectric functions for ion and dipole solution systems. *Journal of Computational Chemistry*, 10(1):77–93, January 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ermer:1985:CPP

[EIO85] Otto Ermer, Petko M. Ivanov, and Eiji Osawa. Conformational properties of permethylcyclohexane as compared to cyclohexane: a force field study. *Journal of Computational Chemistry*, 6(5):401–428, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Egan:1984:CEP

[EM84] John T. Egan and Robert D. MacElroy. Calculating the electrostatic potential of molecular models with separate evaluations by conventional, vector, and array processors. *Journal of Computational Chemistry*, 5(1):72–83, February 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Essen:1983:GTM

[Ess83] Hanno Essén. On the general transformation from molecular geometric parameters to Cartesian coordinates. *Journal of Computational Chemistry*, 4(2):136–141, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Edwards:1987:QMM

[EW87] W. Daniel Edwards and Gary R. Weisman. Quantum mechanical modeling of a transannular interaction in a bicyclic amidinium ion. *Journal of Computational Chemistry*, 8(2): 149–157, March 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Eatock:1985:ISM

[EWM85] Beverley G. Eatock, William L. Waltz, and Paul G. Mezey. Ab initio SCF MO calculations on the reactions of hydroxyl radical with imidazole and monoprotonated imidazole. *Journal of Computational Chemistry*, 6(1):68–75, February 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Faegri:1986:EOG

[FA86] Knut Faegri Jr. and Jan Almlof. Energy-optimized GTO basis sets for LCAO Calculations. A Gradient Approach. *Journal of Computational Chemistry*, 7(4):396–405, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fabian:1988:ACR

[Fab88] Walter M. F. Fabian. AM1 calculations of rotation around essential single bonds and preferred conformations in conjugated molecules. *Journal of Computational Chemistry*, 9(4): 369–377, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Faegri:1989:BSQ

[FB89] Knut Faegri Jr. and Gil Biran. Basis set quality versus size II. Approximate GTO wave functions for second row transition metal atoms. *Journal of Computational Chemistry*, 10(4): 495–502, June 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fripiat:1986:CFS

[FBBA86] J. G. Fripiat, C. Barbier, V. P. Bodart, and J. M. André. Calculations of first- and second-order nonlinear molecular hyperpolarizabilities by perturbation methods: I. An efficient method for evaluating time-independent hyperpolarizabilities. *Journal of Computational Chemistry*, 7(6):756–760, December 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Feller:1980:TSP

[FBD80] David Feller, Weston Thatcher Borden, and Ernest R. Davidson. A theoretical study of paths for decomposition and rearrangement of dihydroxycarbene. *Journal of Computational Chemistry*, 1(2):158–166, Summer 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fantucci:1985:UMV

[FBKK85] P. Fantucci, V. BonačiCć-Koutecký, and J. Koutecký. Usefulness of modified virtual orbitals in multireference CI procedure illustrated by calculations on lithium clusters. *Journal of Computational Chemistry*, 6(5):462–468, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Froelich:1988:SOT

[FC88] P. Froelich and F. T. Chan. On the second-order terms of perturbation theory. *Journal of Computational Chemistry*, 9 (5):578–580, July 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fried:1987:PSP

[FE87] Laurence E. Fried and Gregory S. Ezra. PERTURB: a special-purpose algebraic manipulation program for classical perturbation theory. *Journal of Computational Chemistry*, 8 (4):397–411, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ferguson:1989:MMC

[FGR89] David M. Ferguson, William A. Glauser, and Douglas J. Raber. Molecular mechanics conformational analysis of cyclononane using the RIPS method and comparison with quantum-mechanical calculations. *Journal of Computational*

Chemistry, 10(7):903–910, October 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Froimowitz:1984:SBA

[FK84] Mark Froimowitz and Peter Kollman. A study of the biologically active conformers for prodine opiates and their derivatives. *Journal of Computational Chemistry*, 5(6):507–516, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Frenking:1985:IIP

[FKS85] Gernot Frenking, Wolfram Koch, and Michael Schaale. Ab initio investigation of the potential energy surfaces of $C_2H_2F_2$ and $C_2H_2F_2^+$. *Journal of Computational Chemistry*, 6(3): 189–199, June 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Frenking:1986:TIF

[FKS86] Gernot Frenking, Wolfram Koch, and Helmut Schwarz. Theoretical investigations on fluorine-substituted ethylene dications $C_2H_nF_{4-n}^{2+}$ ($n = 0$–4). *Journal of Computational Chemistry*, 7(4):406–416, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fujita:1987:MDS

[FM87] T. Fujita and E. F. Meyer Jr. Molecular dynamics simulation of the 1:1 enzyme-ligand complex between porcine pancreatic elastase and acetyl-alanine-proline-alanine. *Journal of Computational Chemistry*, 8(6):801–809, September 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Favini:1984:CSO

[FMTS84] Giorgio Favini, Giorgio Moro, Roberto Todeschini, and Massimo Simonetta. Conformational studies of octalene and its benzo-derivatives. *Journal of Computational Chemistry*, 5 (4):343–348, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Farras:1986:SEL

[FOSV86] Jaume Farrás, Santiago Olivella, Albert Solé, and Jaume Vilarrasa. Substituent effects on the low-lying singlet and triplet states of methylene. *Journal of Computational Chemistry*, 7 (4):428–442, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fraga:1982:SFS

[Fra82] Serafin Fraga. A semiempirical formulation for the study of molecular interactions. *Journal of Computational Chemistry*, 3(3):329–334, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fraser:1987:DMG

[Fra87] Simon J. Fraser. Discrete models of growth and dynamical percolation in chemistry. *Journal of Computational Chemistry*, 8(4):428–435, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Froimowitz:1986:CPP

[Fro86] Mark Froimowitz. Conformational Properties of 3-Phenylpiperidine and 3-Phenylpyrrolidine Opioid Analgesics. *Journal of Computational Chemistry*, 7(4):513–522, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Frenking:1982:CSC

[FS82] Gernot Frenking and Helmut Schwarz. The calculated structures of the $C_4H_8NO^+$ cations resulting from the unimolecular gas-phase dissociation $(CH_3)_2NCOCH_2X^{\cdot +} \rightarrow C_4H_8NO^+ + X\cdot(X = CL, NO_2)$. *Journal of Computational Chemistry*, 3(2):251–259, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ford:1983:MCP

[FS83] George P. Ford and John D. Scribner. MNDO calculations of proton and methyl-and ethyl-cation affinities of neutral carbon, nitrogen, and oxygen bases. *Journal of Computational Chemistry*, 4(4):594–604, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ford:1989:MMO

[FS89] George P. Ford and Christopher T. Smith. An MNDO molecular orbital study of the reactions of protonated oxirane derivatives ($XCHCH_2OH^+$, X = CN, Cl, CH_3, Ph) with simple nucleophiles. Implications for regioselectivity in the reactions of electrophiles with nucleic acid bases. *Journal of*

Computational Chemistry, 10(4):568–592, June 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Froimowitz:1984:CPA

[FSH+84] Mark Froimowitz, P. Salva, G. J. Hite, G. Gianutsos, P. Suzdak, and R. Heyman. Conformational properties of α- and β-azabicyclane opiates. The effect of conformation on pharmacological activity. *Journal of Computational Chemistry*, 5 (4):291–298, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Felder:1984:ICM

[FSL84] Clifford E. Felder, Abraham Shanzer, and Shneior Lifson. Initial conformations of macrocyclic compounds with rotational symmetry generated from a molecular fragment. *Journal of Computational Chemistry*, 5(2):170–174, April 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Favini:1982:GEO

[FSST82] G. Favini, M. Simonetta, M. Sottocornola, and R. Todeschini. Geometry and energy of overcrowded ethylenes. II. Bornanylidene, fenchylidene, and bifluorenylidene derivatives. *Journal of Computational Chemistry*, 3(2):178–184, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Favini:1981:GET

[FST81] G. Favini, M. Simonetta, and R. Todeschini. Geometry and energy of tetra-tert-butylethylene. *Journal of Computational Chemistry*, 2(2):149–156, Summer 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Floris:1989:EDC

[FT89] F. Floris and J. Tomasi. Evaluation of the dispersion contribution to the solvation energy. A simple computational model in the continuum approximation. *Journal of Computational Chemistry*, 10(5):616–627, July 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fujita:1987:SID

[Fuj87] T. Fujita. A specific inhibitor design approach by means of molecular dynamics calculation for porcine pancreatic elastase. *Journal of Computational Chemistry*, 8(5):645–650, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Francois:1985:GEM

[FVV85] J. P. François, R. Voets, and L. C. Van Poucke. General expressions for monocenter repulsion integrals in a basis of real atomic orbitals. *Journal of Computational Chemistry*, 6 (5):343–349, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fleischman:1985:STM

[FWB85] Stephen H. Fleischman, Eugen E. Weltin, and C. Hackett Bushweller. Stereodynamics of triethylamine: Molecular mechanics calculations on the direct rotational racemization of the C_3-symmetric conformers. *Journal of Computational Chemistry*, 6(3):249–255, June 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Farcasiu:1989:CNF

[FWS89] Dan Fărcaşiu, Patrick Walter, and Kelly Sheils. Calculation of number and free energy of the conformers of linear alkanes with medium and long chains. Implications for catalysis. *Journal of Computational Chemistry*, 10(4):520–528, June 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gallup:1982:ICE

[Gal82] G. A. Gallup. Iterative calculation of eigenvalues and eigenvectors of large, real matrix systems with overlap. *Journal of Computational Chemistry*, 3(2):127–129, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garst:1982:BRBb

[Gar82a] John F. Garst. Book review: *Computational chemistry, An introduction to numerical analysis*, A. C. Norris, Wiley, New York, 1981, 454 pp. Price: \$46.95. *Journal of Computational*

Chemistry, 3(4):604, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garst:1982:BRBa

[Gar82b] John F. Garst. Book review: *Personal computers in chemistry*, Peter Lykos, ed., Wiley, New York, 1981, 262 pp. *Journal of Computational Chemistry*, 3(2):273, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garmer:1989:ETS

[Gar89] David R. Garmer. Extrapolation of the time-step bias in diffusion quantum Monte Carlo by a differential sampling technique. *Journal of Computational Chemistry*, 10(2):176–185, March 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gowda:1983:ESH

[GB83] B. Thimme Gowda and Sidney W. Benson. Energetics and structure of the hydrated gaseous halide anions. *Journal of Computational Chemistry*, 4(3):283–293, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gilliom:1985:MTS

[GBP85] Richard D. Gilliom, Jean-Paul Beck, and William P. Purcell. An MNDO treatment of sigma values. *Journal of Computational Chemistry*, 6(5):437–440, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

George:1980:ISG

[GBT80] Phillip George, Charles W. Bock, and Mendel Trachtman. An ab initio study of the geometry and energy of six planar conformers of β-hydroxyacrolein. *Journal of Computational Chemistry*, 1(4):373–385, Winter 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

George:1982:ISG

[GBT82] Philip George, Charles W. Bock, and Mendel Trachtman. An ab initio study of the geometry, energy, and selected force constants for the three planar conformers of carbonic acid, and the bicarbonate ion; and of the energy for the reaction

$H_2O + CO_2 \rightarrow H_2CO_3$. *Journal of Computational Chemistry*, 3(3):283–296, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ghose:1985:GFB

[GC85] Arup K. Ghose and Gordon M. Crippen. Geometrically feasible binding modes of a flexible ligand molecule at the receptor site. *Journal of Computational Chemistry*, 6(5):350–359, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ghose:1986:APP

[GC86] Arup K. Ghose and Gordon M. Crippen. Atomic physicochemical parameters for three-dimensional structure-directed quantitative structure-activity relationships I. Partition coefficients as a measure of hydrophobicity. *Journal of Computational Chemistry*, 7(4):565–577, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grunewald:1988:CPA

[GCW88] Gary L. Grunewald, Mary W. Creese, and H. J. R. Weintraub. Conformational preferences in alkylbenzenes and arylalkylamines: a comparative study using CAMSEQ, MM2 and molecular dynamics methods. *Journal of Computational Chemistry*, 9(4):315–326, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gimarc:1989:ISM

[GDO89] Benjamin M. Gimarc, Baiching Dai, and Jane J. Ott. Ab initio SCF MO results for the carborane isomers 3,5-$C_2B_6H_8$, 1, 7-$C_2B_7H_9$, and 1,2-$C_2B_7H_9$. *Journal of Computational Chemistry*, 10(1):14–16, January 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gilbert:1985:PRT

[GDP+85] Mary M. Gilbert, Jack J. Donn, Martha Peirce, Kenneth R. Sundberg, and Klaus Ruedenberg. Pictorial representation of three-dimensional electron distributions through a perspective view of contour diagrams in a set of parallel planes. *Journal of Computational Chemistry*, 6(3):209–215, June 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Genest:1987:TSW

[Gen87] Monique Genest. Theoretical study of water-pyridine complexes using intermolecular potentials. *Journal of Computational Chemistry*, 8(1):67–80, January 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gidiotis:1987:CAM

[GF87] Grigorios Gidiotis and Wendell Forst. Computational aspects of master equation transformation in terms of moments. *Journal of Computational Chemistry*, 8(4):420–427, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gregory:1989:FFP

[GG89] D. H. Gregory and J. T. Gerig. Force field parameterization for the 4-fluorophenyl group. *Journal of Computational Chemistry*, 10(5):711–717, July 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Georgian:1987:HDC

[GHF87] T. Georgian, J. M. Halpin, and G. L. Findley. Hamiltonian dynamics of chemical reactions. Consecutive first-order reactions and reactions possessing one autocatalytic intermediate. *Journal of Computational Chemistry*, 8(5):744–751, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Graimann:1985:MMC

[GHHS85] Christof Graimann, Helmut Hönig, Klaus Hummel, and Franz Stelzer. Molecular mechanics calculations on cyclopentenyl compounds, products obtained by olefin metathesis of norbornadiene derivatives. *Journal of Computational Chemistry*, 6(4):302–311, August 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Glidewell:1987:IRS

[GHT87] Christopher Glidewell, Derek Higgins, and Colin Thomson. An investigation of the relative stabilities of the isomers of CF_2N_2: Comparison of ab initio and MNDO calculations. *Journal of Computational Chemistry*, 8(8):1170–1178, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gilliom:1984:CSR

[Gil84] Richard D. Gilliom. A computational study of the reaction of methane with methyl radical. *Journal of Computational Chemistry*, 5(3):237–240, June 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gilbert:1987:BRB

[Gil87] Kevin E. Gilbert. Book review: *Scientific and engineering applications with personal computer*, R. Annino and R. D. Driver. Wiley, New York, 1986, $45.00, 577 pp. *Journal of Computational Chemistry*, 8(7):1066–1067, October 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grigoras:1987:ICE

[GL87] Stelian Grigoras and Thomas H. Lane. Ab initio calculations on the effect of polarization functions on disiloxane. *Journal of Computational Chemistry*, 8(1):84–93, January 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grigoras:1988:MMP

[GL88] Stelian Grigoras and Thomas H. Lane. Molecular mechanics parameters for organosilicon compounds calculated from ab initio computations. *Journal of Computational Chemistry*, 9(1):25–39, January 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See correction [GL89].

Grigoras:1989:CMM

[GL89] Stelian Grigoras and Thomas H. Lane. Correction. Molecular mechanics parameters for organosilicon compounds calculated from ab initio computations. *Journal of Computational Chemistry*, 10(1):136, January 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [GL88].

Glaser:1989:DIA

[Gla89] Rainer Glaser. The density integration approach to populations. A critical comparison of projection populations to populations defined by the theory of atoms in molecules. *Journal of Computational Chemistry*, 10(1):118–135, January 1989.

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gonzalez-Lafont:1988:HFM

[GLLOB88] A. González-Lafont, J. M. Lluch, A. Oliva, and J. Bertrán. Hydration of Fe^{+}: a Monte Carlo simulation of water clusters and of a dilute aqueous solution. *Journal of Computational Chemistry*, 9(8):819–826, December 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ganti:1986:TPM

[GM86] Girija Ganti and J. Andrew McCammon. Transport properties of macromolecules by Brownian dynamics simulation: Vectorization of Brownian dynamics on the Cyber-205. *Journal of Computational Chemistry*, 7(4):457–463, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Goddard:1987:CSD

[God87] John D. Goddard. Computational studies of 1,2-dithiete and dithioglyoxal. *Journal of Computational Chemistry*, 8(4): 389–396, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Goldblum:1987:IHB

[Gol87] Amiram Goldblum. Improvement of the hydrogen bonding correction to MNDO for calculations of biochemical interest. *Journal of Computational Chemistry*, 8(6):835–849, September 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gordon:1988:NRV

[Gor88] R. L. Gordon. Note on the role of vibrational modes in molecular electronic transitions. *Journal of Computational Chemistry*, 9(8):924–929, December 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ghose:1988:APP

[GPC88] Arup K. Ghose, Avis Pritchett, and Gordon M. Crippen. Atomic physicochemical parameters for three dimensional structure directed quantitative structure-activity relationships III: Modeling hydrophobic interactions. *Journal of*

Computational Chemistry, 9(1):80–90, January 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gresh:1983:TSI

[Gre83] Nohad Gresh. A theoretical study of the interaction of monomethylammonium with double-stranded oligonucleotides. *Journal of Computational Chemistry*, 4(3):390–398, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gready:1984:VBO

[Gre84] Jill E. Gready. The value of the π-bond order–bond length relationship in geometry prediction and chemical bonding interpretation. *Journal of Computational Chemistry*, 5(5): 411–426, October 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gready:1985:TSP

[Gre85] Jill E. Gready. Theoretical studies on pteridines. 2. Geometries, tautomer, ionization and reduction energies of substrates and inhibitors of dihydrofolate reductase. *Journal of Computational Chemistry*, 6(5):377–400, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gropen:1987:GBS

[Gro87] Odd Gropen. Gaussian basis sets for the fifth row elements, Mo-Cd, and the sixth row elements W-RN. *Journal of Computational Chemistry*, 8(7):982–1003, October 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Glauser:1988:EDA

[GRS88] William A. Glauser, Douglas J. Raber, and Brian Stevens. Electron donor-acceptor complexes: Evaluation of MNDO as a computational tool to probe intermolecular interactions. *Journal of Computational Chemistry*, 9(5):539–553, July 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gersten:1985:SEI

[GS85] Joel I. Gersten and Anne Marie Sapse. Solvent-effect investigations through the use of an extended Born equation.

Journal of Computational Chemistry, 6(5):481–485, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gibson:1987:RAB

[GS87a] K. D. Gibson and H. A. Scheraga. Revised algorithms for the build-up procedure for predicting protein conformations by energy minimization. *Journal of Computational Chemistry*, 8(6):826–834, September 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gilliom:1987:MMS

[GS87b] Richard D. Gilliom and Gerald L. Stoner. Molecular mechanics study of myelin basic protein. *Journal of Computational Chemistry*, 8(8):1104–1108, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gowda:1985:PFA

[GSB85] B. Thimme Gowda, B. S. Sherigara, and Sidney W. Benson. Potential functions for alkali halide molecules. *Journal of Computational Chemistry*, 6(2):93–107, April 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gilson:1988:CEP

[GSH88] Michael K. Gilson, Kim A. Sharp, and Barry H. Honig. Calculating the electrostatic potential of molecules in solution: Method and error assessment. *Journal of Computational Chemistry*, 9(4):327–335, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Glidewell:1982:SAB

[GT82] Chistopher Glidewell and Colin Thomson. The structure and acid–base properties of methyl and silyl amines and phosphines: an ab-initio SCF study. *Journal of Computational Chemistry*, 3(4):495–506, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Glidewell:1983:KTI

[GT83] Christopher Glidewell and Colin Thomson. Koopmans' theorem ionization potentials of methyl and silyl halides, chalcogenides, amines, and phosphines: an ab initio SCF study. *Journal of Computational Chemistry*, 4(1):9–14, Spring 1983.

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Glidewell:1984:ICE

[GT84] Christopher Glidewell and Colin Thomson. Ab initio calculations on the effect of different basis sets and electron correlation on the transition state for the reactions HNC $\rightleftharpoons$ HCN and BCN $\rightleftharpoons$ BNC. *Journal of Computational Chemistry*, 5 (1):1–10, February 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

George:1981:RSR

[GTB81] Philip George, Mendel Trachtman, and Charles W. Bock. A reassessment of some restricted Hartree–Fock limit molecular energies and an investigation of the applicability of Ermler and Kern's procedure for their estimation. *Journal of Computational Chemistry*, 2(3):334–346, Autumn 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Haser:1989:IDS

[HA89] Marco Häser and Reinhart Ahlrichs. Improvements on the direct SCF method. *Journal of Computational Chemistry*, 10 (1):104–111, January 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hosoya:1987:AES

[HAKW87] Haruo Hosoya, Misako Aida, Reiko Kumagai, and Kazu Watanabe. Analysis of the π-electronic structure of infinitely large networks. I. Some remarks on the characteristic polynomial and density of states of large polycyclic aromatic hydrocarbons. *Journal of Computational Chemistry*, 8(4):358–366, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hambley:1987:SEM

[Ham87] Trevor W. Hambley. Strain energy minimization study of the mechanism of, and the barrier to, conformational interconversion in five-membered diamine chelate rings. *Journal of Computational Chemistry*, 8(5):651–657, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hasanein:1984:GSP

[Has84] Ahmed A. Hasanein. The ground state potential energy surface of methyl fluoride dimer. *Journal of Computational Chemistry*, 5(6):528–534, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hasselbarth:1987:IPI

[Häs87] Werner Hässelbarth. The inverse problem of isomer enumeration. *Journal of Computational Chemistry*, 8(5):700–717, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hase:1982:DER

[HB82] William L. Hase and Daniel G. Buckowski. Dynamics of ethyl radical decomposition. II. Applicability of classical mechanics to large-molecule unimolecular reaction dynamics. *Journal of Computational Chemistry*, 3(3):335–343, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Herndon:1987:LNM

[HB87] William C. Herndon and Steven H. Bertz. Linear notations and molecular graph similarity. *Journal of Computational Chemistry*, 8(4):367–374, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hosoya:1989:CAM

[HB89] Haruo Hosoya and K. Balasubramanian. Computational algorithms for matching polynomials of graphs from the characteristic polynomials of edge-weighted graphs. *Journal of Computational Chemistry*, 10(5):698–710, July 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hendrickson:1980:SSD

[HBK80] James B. Hendrickson and Elaine Braun-Keller. Systematic synthesis design. 8. Generation of reaction sequences. *Journal of Computational Chemistry*, 1(4):323–333, Winter 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hurst:1988:IDC

[HD88] G. J. B. Hurst and M. Dupuis. Integral data compression for FPS 64-bit processors: Improved I/O and reduced storage. *Journal of Computational Chemistry*, 9(2):148–157, March 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Harding:1985:PAV

[HE85] Lawrence B. Harding and Walter C. Ermler. Polyatomic, anharmonic, vibrational–rotational analysis. Application to accurate ab initio results for formaldehyde. *Journal of Computational Chemistry*, 6(1):13–27, February 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hsieh:1988:IVT

[HE88] Hsiuchin C. Hsieh and Walter C. Ermler. Ab initio vibrational transition dipole moments and intensities of formaldehyde. *Journal of Computational Chemistry*, 9(2):95–106, March 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Higo:1989:ARC

[HG89] Jun'Ichi Higo and Nobuhiro Gō. Algorithm for rapid calculation of excluded volume of large molecules. *Journal of Computational Chemistry*, 10(3):376–379, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hall:1980:AMP

[HH80] David Hall and Christine E. L. Headford. An analysis of the molecular packing of maleic hydrazide. *Journal of Computational Chemistry*, 1(3):261–265, Autumn 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Halim:1986:MMC

[HHK+86] Herman Halim, Nikolaus Heinrich, Wolfram Koch, Jochen Schmidt, and Gernot Frenking. MINDO/3 and MNDO calculations of closed- and open-shell cations containing C, H, N, and O. *Journal of Computational Chemistry*, 7(2):93–104, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huige:1987:SIO

[HHR87] C. J. M. Huige, A. M. F. Hezemans, and Kjeld Rasmussen. Small imines and oximes as model compounds in the optimization of a consistent force field potential energy function. *Journal of Computational Chemistry*, 8(3):204–225, April 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hilal:1980:LMO

[Hil80a] Rifaat Hilal. Localized molecular orbitals and chemical binding in five-membered heterocycles. II. *Journal of Computational Chemistry*, 1(4):358–367, Winter 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hilal:1980:MCD

[Hil80b] Rifaat Hilal. Molecular charge distribution and chemical binding in five-membered heterocycles. I. *Journal of Computational Chemistry*, 1(4):348–357, Winter 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hinchliffe:1980:BIR

[Hin80] Alan Hinchliffe. The barrier to internal rotation in Ge_2H_6. *Journal of Computational Chemistry*, 1(2):185–188, Summer 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Houser:1988:NTR

[HK88] John J. Houser and Gilles Klopman. A new tool for the rapid estimation of charge distribution. *Journal of Computational Chemistry*, 9(8):893–904, December 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huber:1983:PLC

[HL83] Hanspeter Huber and Zdzisław Latajka. Proton and lithium cation affinities calculated with floating orbital geometry optimization (FOGO). *Journal of Computational Chemistry*, 4 (2):252–259, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hermansson:1988:VSM

[HLC88] Kersti Hermansson, George C. Lie, and Enrico Clementi. On velocity scaling in molecular dynamics simulations. *Journal* of *Computational Chemistry*, 9(3):200–203, April 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hammarstrom:1988:EIM

[HLG88] Lars-Gunnar Hammarström, Tommy Liljefors, and Johann Gasteiger. Electrostatic interactions in molecular mechanics (MM2) calculations via PEOE partial charges I. Haloalkanes. *Journal of Computational Chemistry*, 9(4):424–440, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hout:1982:EEC

[HLH82] Robert F. Hout Jr., Beverly A. Levi, and Warren J. Hehre. Effect of electron correlation on theoretical vibrational frequencies. *Journal of Computational Chemistry*, 3(2):234–250, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hout:1983:MCN

[HLH83] Robert F. Hout Jr., Beverly A. Levi, and Warren J. Hehre. A method for the calculation of normal-mode vibrational frequencies using symmetry coordinates. Application to the calculation of secondary deuterium isotope effects on carbocations. *Journal of Computational Chemistry*, 4(4):499–505, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hall:1982:CM

[HLPT82] David Hall, Paul John Lyons, Nicola Pavitt, and John A. Trezise. The conformation of malformin A. *Journal of Computational Chemistry*, 3(1):89–94, Spring 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hass:1982:TSA

[HMA82] Ernst C. Hass, Paul G. Mezey, and Suzanne R. Abrams. Theoretical studies on "acetylenic zipper" reaction intermediates. *Journal of Computational Chemistry*, 3(2):185–190, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hopkinson:1983:TSS

[HML83] A. C. Hopkinson, M. A. McKinney, and M. H. Lien. A theoretical study of α-substituted isopropyl and cyclopropyl anions. *Journal of Computational Chemistry*, 4(4):513–523, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hosoya:1983:OTO

[HO83] Haruo Hosoya and Noriko Ohkami. Operator technique for obtaining the recursion formulas of characteristic and matching polynomials as applied to polyhex graphs. *Journal of Computational Chemistry*, 4(4):585–593, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hall:1984:AMF

[HP84a] David Hall and Nicola Pavitt. An appraisal of molecular force fields for the representation of polypeptides. *Journal of Computational Chemistry*, 5(5):441–450, October 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hopfinger:1984:MMF

[HP84b] A. J. Hopfinger and R. A. Pearlstein. Molecular mechanics force-field parameterization procedures. *Journal of Computational Chemistry*, 5(5):486–499, October 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hout:1983:OP

[HPH83] Robert F. Hout Jr., William J. Pietro, and Warren J. Hehre. Orbital photography. *Journal of Computational Chemistry*, 4(2):276–282, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hinde:1980:TAS

[HPR80] Alan L. Hinde, Addy Pross, and Leo Radom. A theoretical approach to substituent effects. Interactions between directly bonded groups in the neutrals X NH_2, X OH, and X F and the anions X NH^- and X O^-. *Journal of Computational Chemistry*, 1(2):118–128, Summer 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hall:1982:CP

[HPW82] David Hall, Nicola Pavitt, and Murray K. Wood. The conformation of pithomycolide. *Journal of Computational Chemistry*, 3(3):381–384, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hafelinger:1985:ISO

[HR85] Günter Häfelinger and Claus Regelmann. Ab initio STO-3G optimization of planar, perpendicular, and twisted molecular structures of biphenyl. *Journal of Computational Chemistry*, 6(5):368–376, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hafelinger:1987:RIS

[HR87] Günter Häfelinger and Claus Regelmann. Refined ab initio 6-31G split-valence basis set optimization of the molecular structures of biphenyl in twisted, planar, and perpendicular conformations. *Journal of Computational Chemistry*, 8(7): 1057–1065, October 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hafelinger:1989:BSD

[HRKW89] Günter Häfelinger, Claus Ulrich Regelmann, Tadeusz Marek Krygowski, and Krzysztof Wozniak. Basis set dependence, precision, and accuracy of full ab initio gradient optimizations of molecular structures of nonstrained hydrocarbons. I. CC bond lengths. *Journal of Computational Chemistry*, 10 (3):329–343, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hall:1982:MPA

[HS82] David Hall and K. Barry Sexton. A molecular packing analysis of some ferrous porphyrin complexes. *Journal of Computational Chemistry*, 3(4):588–592, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hess:1983:ISC

[HSEČ83] B. A. Hess Jr., L. J. Schaad, C. S. Ewig, and P. Čársky. Ab initio studies on calicene. *Journal of Computational Chemistry*, 4(1):53–57, Spring 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Herzig:1983:ISP

[HSS83] L. Herzig, A. M. Sapse, and G. Snyder. Ab initio studies of a proposed mechanism for N-nitrosamine formation. *Journal of Computational Chemistry*, 4(1):68–72, Spring 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Harris:1982:MSC

[HSW82] J. Milton Harris, Steven G. Shafer, and S. D. Worley. MINDO /3 Calculation of carbocation heats of formation. *Journal of Computational Chemistry*, 3(2):208–213, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Handler:1982:ILC

[HT82] George S. Handler and Carl Trindle. The imposition of linear constraints upon eigenvalue problems. *Journal of Computational Chemistry*, 3(1):37–39, Spring 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Higgins:1988:TSR

[HT88] Derek Higgins and Colin Thomson. A theoretical study of the rotational isomers of nitrosomethanol by semiempirical (AM1) and ab initio methods. *Journal of Computational Chemistry*, 9(3):212–221, April 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Higgins:1988:CSM

[HTT88] Derek Higgins, Colin Thomson, and Walter Thiel. Comparison of semiempirical MO methods for open-shell systems. *Journal of Computational Chemistry*, 9(6):702–707, September 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hurley:1988:CFF

[Hur88] A. C. Hurley. The computation of floating functions and their use in force constant calculations. *Journal of Computational Chemistry*, 9(1):75–79, January 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hall:1980:PCS

[HW80] David Hall and Murray K. Wood. Prediction of the crystal structure of a cyclic tetrapeptide. *Journal of Computational Chemistry*, 1(4):368–372, Winter 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ha:1982:ICC

[HW82] Tae-Kyu Ha and Urs P. Wild. An ab initio CI calculation of the triplet–triplet absorption spectrum of naphthalene. *Journal of Computational Chemistry*, 3(1):1–5, Spring 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Holder:1988:CED

[HW88] Andrew J. Holder and David L. Wertz. Conformational energetics of 1,3-dichloropropane as predicted by several calculations methods. *Journal of Computational Chemistry*, 9(6): 684–688, September 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ibrahim:1987:CEH

[IFvRSS87] Mustafa R. Ibrahim, Zacharia A. Fataftah, Paul von Ragué Schleyer, and Peter D. Stout. Calculation of enthalpies of hydrogenation of hydrocarbons. *Journal of Computational Chemistry*, 8(8):1131–1138, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ikuta:1984:IMC

[Iku84] Shigeru Ikuta. Ab initio MO calculations on the acidities of water and methanol, and hydrogen bond energies of the conjugate ions with a water molecule. *Journal of Computational Chemistry*, 5(4):374–380, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ikuta:1985:TSR

[Iku85] Shigeru Ikuta. Theoretical study of the relative stabilities of $H^+ (X)_2$ and $H^+ (X)_3$ conformers and their clustering energies: X CO and N_2. *Journal of Computational Chemistry*, 6 (2):116–121, April 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Iratcabal:1986:CDD

[IL86] P. Iratçabal and D. Liotard. Conformational dynamics of 9,9-dimethyl-1,5-dihetero-spiro [5.5] undecanes by molecular mechanics calculations: a three-dimensional topological approach. *Journal of Computational Chemistry*, 7(4):482–493, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ivanov:1984:RAT

[IŌ84] Petko M. Ivanov and Eiji Ōsawa. Remarks on the analysis of torsional energy surfaces of cycloheptane and cyclooctane by molecular mechanics. *Journal of Computational Chemistry*, 5(4):307–313, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Iroff:1980:GMG

[Iro80] Linda D. Iroff. On the gearing of methyl groups in hexamethylbenzene. *Journal of Computational Chemistry*, 1(1):76–80, Spring 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ibrahim:1985:AER

[IvRS85] Mustafa R. Ibrahim and Paul von Ragué Schleyer. Atom equivalents for relating ab initio energies to enthalpies of formation. *Journal of Computational Chemistry*, 6(3):157–167, June 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jaffe:1988:TSM

[Jaf88] H. H. Jaffé. Treatment of symmetry in MO calculations. II. Numerical projection operators for molecular orbitals. *Journal of Computational Chemistry*, 9(6):604–607, September 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jug:1985:CSR

[JB85] Karl Jug and Sabine Buss. Comparative studies on the reactivity of molecules by atomic valences. *Journal of Computational Chemistry*, 6(6):507–513, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jerman-Blazic:1986:CSM

[JBFR86] B. Jerman-Blažič, I. Fabič, and M. Randić. Comparison of sequences as a method for evaluation of the molecular similarity. *Journal of Computational Chemistry*, 7(2):176–188, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jenneskens:1987:MCM

[JdKdWB87] Leonardus W. Jenneskens, Franciscus J. J. de Kanter, Willem H. de Wolf, and Friedrich Bickelhaupt. MNDO calculations on [n]metacyclophanes. *Journal of Computational Chemistry*, 8(8):1154–1169, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jain:1989:TSS

[JDS89] Duli C. Jain, Denyse De Gale, and Anne-Marie Sapse. A theoretical study of solvation energies of FCH_2COO^-, FCH_2COOH, and F_2CHCOO^-. *Journal of Computational Chemistry*, 10(8):1031–1037, December 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jug:1989:CCV

[JFG89] Karl Jug, Eckhard Fasold, and M. S. Gopinathan. A concept of charge and valence for ab initio wave functions. *Journal of Computational Chemistry*, 10(8):965–974, December 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jordan:1989:GTR

[JG89] Meredith J. Jordan and Jill E. Gready. Guanidinium-type resonance stabilization and its biological implications. 2. The doubly-extended-guanidine series. *Journal of Computational Chemistry*, 10(2):186–202, March 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jug:1983:PES

[JH83] Karl Jug and Gerhard Hahn. Properties of excited states of aromatic rings containing nitrogen. *Journal of Computational Chemistry*, 4(3):410–418, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jorgensen:1981:ISR

[JI81] William L. Jorgensen and Mustafa Ibrahim. Ab initio studies of RO^- ... HOR' complexes. Solvent effects on the relative acidities of water and methanol. *Journal of Computational Chemistry*, 2(1):7–11, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jug:1987:ASS

[JI87] Karl Jug and Rüdiger Iffert. Application of SINDO1 to sulphur compounds. *Journal of Computational Chemistry*, 8(7): 1004–1015, October 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jug:1988:ASS

[JI88] Karl Jug and Rüdiger Iffert. Application of SINDO1 to silicon, aluminum, and magnesium compounds. *Journal of Computational Chemistry*, 9(1):51–62, January 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jayaram:1987:MCS

[JMB87] B. Jayaram, M. Mezei, and D. L. Beveridge. Monte Carlo study of the aqueous hydration of dimethylphosphate conformations. *Journal of Computational Chemistry*, 8(7):917–942, October 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jorgensen:1981:BRB

[Jor81] William L. Jorgensen. Book review: *Computational methods in Chemistry*, J. Bargon, Ed., Plenum, New York, 1980, 335 pp. *Journal of Computational Chemistry*, 2(2):218, Summer 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jug:1987:ASC

[JS87] Karl Jug and Joachim Schulz. Application of SINDO1 to chlorine and sodium compounds. *Journal of Computational Chemistry*, 8(7):1040–1050, October 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jug:1988:ASP

[JS88] Karl Jug and Joachim Schulz. Application of SINDO1 to phosphorus compounds. *Journal of Computational Chemistry*, 9(1):40–50, January 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jug:1988:SPS

[JSKI88] Karl Jug, Hans-Peter Schluff, Hans Kupka, and Rüdiger Iffert. Structure and properties of small silicon and aluminum clusters. *Journal of Computational Chemistry*, 9(8):803–809, December 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jeffrey:1980:AMM

[JT80] G. A. Jeffrey and R. Taylor. The application of molecular mechanics to the structures of carbohydrates. *Journal of Computational Chemistry*, 1(1):99–109, Spring 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jug:1984:UTV

[Jug84] Karl Jug. A unified treatment of valence and bond order from density operators. *Journal of Computational Chemistry*, 5(6): 555–561, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jurs:1988:BRB

[Jur88] Peter C. Jurs. Book review: *Similarity and clustering in chemical information systems*, by Peter Willett, Research Studies Press, Letchworth, Hertfordshire, England, 230 + xii pp, $54.95, (1987). *Journal of Computational Chemistry*, 9 (7):798, October 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kaldor:1987:OSC

[Kal87] Uzi Kaldor. Open-shell coupled-cluster method: Electron affinities of Li and Na. *Journal of Computational Chemistry*, 8(4):448–453, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kao:1988:TSC

[Kao88] J. Kao. Theoretical studies of conjugated systems containing C C and C N fragments and their alkyl and amino derivatives. *Journal of Computational Chemistry*, 9(8):905–923, December 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karlstrom:1981:PII

[Kar81] Gunnar Karlström. On the possibility of improving the integral evaluation section in ab initio Hartree–Fock calculations on large molecules. *Journal of Computational Chemistry*, 2 (1):83–86, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karfunkel:1986:FAI

[Kar86] H. R. Karfunkel. A fast algorithm for the interactive docking maneuver with flexible macromolecules and probes. *Journal of Computational Chemistry*, 7(2):113–128, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karfunkel:1987:MMD

[Kar87] H. R. Karfunkel. Molecular mechanics and the deformation of macromolecules: the use of a very short cutoff combined with a quadratic approximation. *Journal of Computational Chemistry*, 8(2):174–184, March 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karpfen:1984:ISPa

[KB84a] Alfred Karpfen and Anton Beyer. Ab initio studies on polymers. VI. Torsional potential in regular polyethylene chains. *Journal of Computational Chemistry*, 5(1):11–18, February 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karpfen:1984:ISPb

[KB84b] Alfred Karpfen and Anton Beyer. Ab initio studies on polymers. VII. Polyoxymethylene. *Journal of Computational Chemistry*, 5(1):19–23, February 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kreye:1988:ASS

[KBS88] W. C. Kreye, Prem Batra, and Gordon Skinner. Analytic solutions to sets of first-order rate equations with up to six rate constants using a symbolic computer language SMP and application to biochemical kinetics. *Journal of Computational Chemistry*, 9(6):674–683, September 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kim:1987:HSE

[KC87] Kwang S. Kim and E. Clementi. Hydration structures and energetics of phospholipid. *Journal of Computational Chemistry*, 8(1):57–66, January 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kuhl:1984:CAC

[KCF84] F. S. Kuhl, G. M. Crippen, and D. K. Friesen. A combinatorial algorithm for calculating ligand binding. *Journal of Computational Chemistry*, 5(1):24–34, February 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kobeissi:1989:CME

[KDEHK89] H. Kobeissi, M. Dagher, A. El-Hajj, and M. Kobeissi. On the computation of matrix elements between numerical wave functions: the canonical functions method. *Journal of Computational Chemistry*, 10(3):358–366, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kobeissi:1983:NTV

[KDKC83] Hafez Kobeissi, Mounzer Dagher, Mahmoud Korek, and Ahmad Chaalan. A new treatment of the vibration–Rotation eigenvalue problem for a diatomic molecule. *Journal of Computational Chemistry*, 4(2):218–225, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karfunkel:1989:ARC

[KE89] Heinrich R. Karfunkel and Veronique Eyraud. An algorithm for the representation and computation of supermolecular surfaces and volumes. *Journal of Computational Chemistry*, 10(5):628–634, July 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kelsey:1980:OTB

[Kel80a] Donald R. Kelsey. Orbital topology. I. A basic topological model for chemical systems, an orbital mapping technique, and analyses of model, thermal electrocyclic reactions. *Journal of Computational Chemistry*, 1(1):3–20, Spring 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kelsey:1980:OTI

[Kel80b] Donald R. Kelsey. Orbital topology. II. Orbital mapping of unsymmetrical molecules. A survey of the thermal isomerizations of Dewar isomers of isoelectronically substituted benzenes, cyclopentadienes, and cyclopentadienyl ions. *Journal of Computational Chemistry*, 1(1):21–29, Spring 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kelsey:1982:OTI

[Kel82] Donald R. Kelsey. Orbital topology. III. Orbital mapping of unsymmetrical molecules. A survey of the thermal ring opening of isoelectronically substituted cyclobutenes and benzocyclobutenes. *Journal of Computational Chemistry*, 3(3):436–444, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

King:1988:COT

[KF88] Harry F. King and Thomas R. Furlani. Computation of one and two electron spin-orbit integrals. *Journal of Computational Chemistry*, 9(7):771–778, October 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kaufman:1987:IMC

[KHRvH87] Joyce J. Kaufman, P. C. Hariharan, Szczepan Roszak, and Marc van Hemert. Ab-initio MRD–CI calculations on a CNO_2 decomposition pathway of nitrobenzene. *Journal of Computational Chemistry*, 8(5):736–743, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klein:1986:TMM

[KHS86] D. J. Klein, G. E. Hite, and T. G. Schmalz. Transfer-matrix method for subgraph enumeration: Applications to polypyrene fusenes. *Journal of Computational Chemistry*, 7

(4):443–456, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klopman:1981:CPC

[KI81] Gilles Klopman and Linda D. Iroff. Calculation of partition coefficients by the charge density method. *Journal of Computational Chemistry*, 2(2):157–160, Summer 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kim:1985:MEA

[Kim85] Kwang S. Kim. Microscopic effect of an applied voltage on the solvated gramicidin a transmembrane channel in the presence of Na^+ and K^+ cations. *Journal of Computational Chemistry*, 6(3):256–263, June 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

King:1983:A

[Kin83] R. Bruce King. Announcement. *Journal of Computational Chemistry*, 4(1):124, Spring 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

King:1987:CAT

[Kin87] R. B. King. Chemical applications of topology and group theory. 23. A comparison of graph-theoretical and extended Hückel methods for study of bonding in octahedral and icosahedral boranes. *Journal of Computational Chemistry*, 8(4):341–349, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Krogh-Jespersen:1982:ESB

[KJ82] Karsten Krogh-Jespersen. Electronic states and barriers to internal rotation in silaallenes. *Journal of Computational Chemistry*, 3(4):571–579, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Krogh-Jespersen:1985:TDA

[KJ85] Mary-Beth Krogh-Jespersen. Theoretically derived absorption and MCD spectral data for the cellular species produced in the hydrolysis of cis-diamminedichloroplatinum(II). *Journal of Computational Chemistry*, 6(6):614–624, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kruger:1987:GPS

[KJ87] Thomas Krüger and Karl Jug. Generalized potential surfaces under inclusion of nuclear motion. *Journal of Computational Chemistry*, 8(4):350–357, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kondo:1984:GOU

[KJLW84] H. Kondo, H. H. Jaffé, H. Y. Lee, and William J. Welsh. Geometry optimization using symmetry coordinates. *Journal of Computational Chemistry*, 5(1):84–88, February 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klopman:1985:CSA

[KK85] Gilles Klopman and Alexander N. Kalos. Causality in structure–activity studies. *Journal of Computational Chemistry*, 6(5):492–506, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kobeissi:1988:TDE

[KKE88] Hafez Kobeissi, Majida Kobeissi, and Ali El Hajj. On testing difference equations for the diatomic eigenvalue problem. *Journal of Computational Chemistry*, 9(8):844–850, December 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kozmutza:1982:TLP

[KKR+82] C. Kozmutza, E. Kapuy, M. A. Robb, R. Daudel, and I. G. Csizmadia. Theory of lone pairs. IV. Molecular ion hole states of ten-electron hydrides. Molecular ionization potentials and proton affinities by direct SCF calculations. *Journal of Computational Chemistry*, 3(1):14–22, Spring 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klobukowski:1983:NQM

[Klo83] M. Klobukowski. Nonrelativistic and quasirelativistic model potential calculations on AgH and Ag_2. *Journal of Computational Chemistry*, 4(3):350–361, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kirkpatrick:1985:LMO

[KM85] Carol M. Kirkpatrick and Dennis S. Marynick. Localized molecular orbital studies of transition metal complexes. II: Simple π-accepting ligands. *Journal of Computational Chemistry*, 6(2):142–147, April 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klimkowski:1985:MSI

[KMS85] V. J. Klimkowski, J. P. Manning, and Lothar Schäfer. Molecular structures and intramolecular interactions in dimethyl cyclohexane isomers. *Journal of Computational Chemistry*, 6 (6):570–580, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Knop:1987:CEG

[KMS+87] J. V. Knop, W. R. Müller, K. Szymanski, H. W. Kroto, and N. Trinajstić. Computer enumeration and generation of physical trees. *Journal of Computational Chemistry*, 8(4):549–554, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Knop:1986:EFP

[KMST86] J. V. Knop, W. R. Müller, K. Szymanski, and N. Trinajstić. On the enumeration of 2-factors of polyhexes. *Journal of Computational Chemistry*, 7(4):547–564, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klopman:1985:SMC

[KNS85] Gilles Klopman, Krishnan Namboodiri, and Melvin Schochet. Simple method of computing the partition coefficient. *Journal of Computational Chemistry*, 6(1):28–38, February 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kikuchi:1986:SGA

[KNS86] Takeshi Kikuchi, George Némethy, and Harold A. Scheraga. Spatial geometric arrangements of disulfide-crosslinked loops in proteins. *Journal of Computational Chemistry*, 7(1):67–88, February 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kikuchi:1989:SGA

[KNS89] Takeshi Kikuchi, George Némethy, and Harold A. Scheraga. Spatial geometric arrangements of disulfide-crosslinked loops in nonplanar proteins. *Journal of Computational Chemistry*, 10(3):287–294, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kozmutza:1986:EMU

[KO86] C. Kozmutza and Zs. Ozoróczy. An efficient method for using molecular symmetry. In advance selection of zero integrals. *Journal of Computational Chemistry*, 7(4):494–499, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kozmutza:1987:IPT

[Koz87] C. Kozmutza. Ab initio program for treatment of related molecules. II. Integral transformation in extended systems. *Journal of Computational Chemistry*, 8(8):1179–1190, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klimkowski:1984:CCI

[KPE+84] V. J. Klimkowski, P. Pulay, J. D. Ewbank, D. C. McKean, and Lothar Schäfer. Critical comparison of the ab initio and spectroscopic methyl-C — H bond length difference in acetyl compounds, $CH_3C(=O)X$. *Journal of Computational Chemistry*, 5(6):517–522, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kemister:1981:TAS

[KPRT81] Gary Kemister, Addy Pross, Leo Radom, and Robert W. Taft. A theoretical approach to substituent effects. A comparison of the isoelectronic BH, CH_3, and NH groups and their interaction with substituents in disubstituted benzenes. *Journal of Computational Chemistry*, 2(4):470–477, Winter 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klein:1987:IDF

[KR87] D. J. Klein and M. Randić. Innate degree of freedom of a graph. *Journal of Computational Chemistry*, 8(4):516–521, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klopman:1988:NAU

[KR88] Gilles Klopman and Chandan Raychaudhury. A novel approach to the use of graph theory in structure–activity relationship studies. Application to the qualitative evaluation of mutagenicity in a series of nonfused ring aromatic compounds. *Journal of Computational Chemistry*, 9(3):232–243, April 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kroutil:1988:BRB

[Kro88] Robert T. Kroutil. Book review: *Chemometrics*, by M. A. Sharaf, D. L. Illman, and B. R. Kowalski, Wiley, New York, 1986, 332 pp. $49.95. *Journal of Computational Chemistry*, 9(7):799–800, October 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kincaid:1982:ACM

[KS82] Robert H. Kincaid and Harold A. Scheraga. Acceleration of convergence in Monte Carlo simulations of aqueous solutions using the Metropolis algorithm. Hydrophobic hydration of methane. *Journal of Computational Chemistry*, 3(4):525–547, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Krauss:1983:ESU

[KS83] M. Krauss and W. J. Stevens. Electronic structure of UH, UF, and their ions. *Journal of Computational Chemistry*, 4(2):127–135, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kao:1984:CAA

[KS84] James Kao and Jeffrey I. Seeman. Conformational analysis of allylamine. An ab initio molecular orbital study. *Journal of Computational Chemistry*, 5(2):200–206, April 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klimkowski:1984:ISSb

[KSB84] V. J. Klimkowski, Lothar Schäfer, and Robert K. Bohn. Ab initio studies of structural features not easily amenable to experiment. 32. Conformational analysis and molecular structures of isopropyl and ethyl formate and comparison with spectroscopic data. *Journal of Computational Chemistry*, 5 (2):175–181, April 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Krauss:1985:REP

[KSB85] M. Krauss, W. J. Stevens, and Harold Basch. Relativistic effective potential SCF calculations of AgH and AuH. *Journal of Computational Chemistry*, 6(4):287–295, August 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kliesch:1988:CSP

[KSHD88] Wolfgang Kliesch, Klaus Schenk, Dietmar Heidrich, and Holger Dachsel. On the computation of stationary points on potential energy hypersurfaces. *Journal of Computational Chemistry*, 9(8):810–818, December 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kimura:1988:AHO

[KSI88] Toshiyasu Kimura, Nobuyuki Sato, and Suehiro Iwata. Application of the higher order finite-element method to one-dimensional Schrödinger equation. *Journal of Computational Chemistry*, 9(8):827–835, December 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Krauss:1982:SOD

[KSJ82] M. Krauss, W. J. Stevens, and P. S. Julienne. Spin–orbit and dispersion energy effects in XeF. *Journal of Computational Chemistry*, 3(3):372–380, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Knop:1983:CEG

[KSJT83] J. V. Knop, K. Szymanski, Ž. Jeričević, and N. Trinajstić. Computer enumeration and generation of benzenoid hydrocarbons and identification of bay regions. *Journal of Computational Chemistry*, 4(1):23–32, Spring 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koehler:1987:CEE

[KSL87] J. E. H. Koehler, W. Saenger, and B. Lesyng. Cooperative effects in extended hydrogen bonded systems involving O — H groups. Ab initio studies of the cyclic S_4 water tetramer. *Journal of Computational Chemistry*, 8(8):1090–1098, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klimkowski:1983:ISS

[KSS83] V. J. Klimkowski, J. N. Scarsdale, and Lothar Schäfer. Ab initio studies of structural features not easily amenable to experiment. 25. Conformational analysis of methyl propanoate and comparison with the methyl ester of glycine. *Journal of Computational Chemistry*, 4(4):494–498, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kao:1988:MMR

[KT88] S. C. Kao and T. J. Tseng. The MT-MSXα(R) method: Applications to Li_2, F_2, and N_2 molecules. *Journal of Computational Chemistry*, 9(8):890–892, December 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kaufmann:1986:RII

[KTvRS86] Elmar Kaufmann, Bruce Tidor, and Paul von Ragué Schleyer. The remarkably invariant interaction energies of lithium first-row compounds with water and with ammonia. *Journal of Computational Chemistry*, 7(3):334–344, June 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kausch:1980:ISP

[KvRS80] Michael Kausch and Paul von Ragué Schleyer. Isomeric structures of protonated ozone: a theoretical study. *Journal of Computational Chemistry*, 1(1):94–98, Spring 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kaufmann:1989:DLH

[KvRS89] Elmar Kaufmann and Paul von Ragué Schleyer. Degenerate lithium-hydrogen exchange reactions: Ab initio models for metallation mechanisms involving H_2, CH_4, NH_3, H_2O, and HF. *Journal of Computational Chemistry*, 10(4):437–448, June 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klimkowski:1984:ISSa

[KVV+84] V. J. Klimkowski, P. Van Nuffel, L. Van Den Enden, C. Van Alsenoy, H. J. Geise, J. N. Scarsdale, and Lothar Schäfer. Ab initio studies of structural features not easily amenable to experiment. 30. Conformational analysis and molecular structures of propanal and butanal. *Journal of Computational Chemistry*, 5(2):122–128, April 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kraus:1986:VCT

[KW86] Wayne A. Kraus and Albert F. Wagner. Vectorization of a classical trajectory code on a Floating Point Systems, Inc. Model 164 attached processor. *Journal of Computational Chemistry*, 7(2):219–229, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kim:1988:IWS

[KYJ88] Seungmoak Kim, Chang No Yoon, and Mu Shik Jhon. Intermediate water structures in solution of N^{α}-acetyl-N-methylphenylalaninamide. *Journal of Computational Chemistry*, 9(2):125–132, March 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liljefors:1985:NTF

[LA85] Tommy Liljefors and Norman L. Allinger. A note on torsional force constants in molecular mechanics for a methyl group attached to a conjugated system. *Journal of Computational Chemistry*, 6(5):478–480, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Laube:1988:CBS

[Lau88] Thomas Laube. Construction of the best set of four orthonormal $2s$–$2p$ hybrid orbitals by least-squares methods. *Journal of Computational Chemistry*, 9(4):356–361, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lipkowitz:1986:SFO

[LB86] Kenny Lipkowitz and Anthony Burkett. Structural features of organic anions: 7-Norbornadienyllithium. *Journal of Computational Chemistry*, 7(6):745–755, December 1986. CO-

DEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Laidlaw:1987:HFI

[LB87] W. G. Laidlaw and M. Bénard. Hartree–Fock instabilities of sulfur-nitrogen ring systems: S_2N_2. *Journal of Computational Chemistry*, 8(5):727–735, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:1989:CGE

[LB89a] Xiaoyu Liu and K. Balasubramanian. Computer generation of edge groups and edge colorings of graphs. *Journal of Computational Chemistry*, 10(1):1–13, January 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:1989:CGC

[LB89b] Xiaoyu Liu and K. Balasubramanian. Computer generation of the character tables of the symmetric groups (S_n). *Journal of Computational Chemistry*, 10(3):417–425, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:1989:BSS

[LBM89] Yoon Sup Lee, Kyoung Koo Baeck, and A. D. McLean. Basis set selections for relativistic self-consistent field calculations. *Journal of Computational Chemistry*, 10(1):112–117, January 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lipkowitz:1989:TSMb

[LBZ89] Kenny B. Lipkowitz, Brian Baker, and Richard Zegarra. Theoretical studies in molecular recognition: Enantioselectivity in chiral chromatography. *Journal of Computational Chemistry*, 10(5):718–732, July 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Largo-Cabrerizo:1987:HCM

[LCC87] A. Largo-Cabrerizo and E. Clementi. The Hylleraas–CI method in molecular calculations: Two-electron integrals. *Journal of Computational Chemistry*, 8(8):1191–1198, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:1984:DRM

[LCL84] Ikchoon Lee, Jeoung Ki Cho, and Bon-Su Lee. Determination of reactivity by MO theory. 27. Molecular orbital study of the gas-phase decarboxylation of but-3-enoic acid. *Journal of Computational Chemistry*, 5(3):217–224, June 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:1982:ISN

[LCY82] Ikchoon Lee, Young Gu Cheun, and Kiyull Yang. Ab-initio studies on π-nonbonded and through-bonds interactions in n-alkanes, n-alkyl radicals, and polymethylene diradicals. *Journal of Computational Chemistry*, 3(4):565–570, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Loushin:1987:PCC

[LD87] Sharilyn K. Loushin and Clifford E. Dykstra. Polarization counterpoise corrections to correlated hydrogen bond interaction energies. *Journal of Computational Chemistry*, 8(1): 81–83, January 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lipkowitz:1988:EMP

[LDL+88] Kenny B. Lipkowitz, David A. Demeter, Jo. M. Landwer, Carol A. Parish, and Thomas Darden. Explorations on the multidimensional potential energy surface of a chiral stationary phase. *Journal of Computational Chemistry*, 9(1):63–66, January 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Labanowski:1989:OEA

[LDM89] Jan K. Labanowski, Richard A. Dammkoehler, and Ioan Motoc. Orbital electronegativity and analytical representation of atom valence state energy. *Journal of Computational Chemistry*, 10(8):1016–1030, December 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lavery:1980:EPY

[LDP80] Richard Lavery, Marcal De Oliveira, and Bernard Pullman. The electrostatic potential of yeast tRNA^{Phe}. II. The potentials of the phosphate groups in their various conformational states. *Journal of Computational Chemistry*, 1(3):301–306, Autumn 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lipkowitz:1987:CDT

[LDP+87] Kenny B. Lipkowitz, David A. Demeter, Carol A. Parish, Jo M. Landwer, and Thomas Darden. Column design. 3. Theoretical studies of a chiral stationary phase used in column chromatography. *Journal of Computational Chemistry*, 8(6):753–760, September 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lewis:1987:MOC

[Lew87] David F. V. Lewis. Molecular orbital calculations on solvents and other small molecules: Correlation between electronic and molecular properties ν, α MOL, π^*, and β. *Journal of Computational Chemistry*, 8(8):1084–1089, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lewis:1989:CMP

[Lew89] David F. V. Lewis. The calculation of molar polarizabilities by the CNDO/2 method: Correlation with the hydrophobic parameter, $\log P$. *Journal of Computational Chemistry*, 10 (2):145–151, March 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lii:1989:MMM

[LGB+89] Jenn-Huei Lii, Steven Gallion, Charles Bender, Håkan Wikström, Norman L. Allinger, Kenneth M. Flurchick, and M. M. Teeter. Molecular mechanics (MM2) calculations on peptides and on the protein Crambin using the CYBER 205. *Journal of Computational Chemistry*, 10(4):503–513, June 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lien:1985:TSS

[LH85] M. H. Lien and A. C. Hopkinson. A theoretical study of α-substituted cyclopropyl and isopropyl radicals. *Journal of Computational Chemistry*, 6(4):274–281, August 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lohr:1987:CDM

[LH87] Lawrence L. Lohr and A. J. Helman. Centrifugal distortions in molecules: an ab initio approach with application to ozone. *Journal of Computational Chemistry*, 8(4):307–312, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:1984:MSS

[LHC84] Ikchoon Lee, Eun Sook Han, and Jae Young Choi. A MINDO /3 study of the hetero-Diels–Alder reaction. *Journal of Computational Chemistry*, 5(6):606–611, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:1984:TSP

[LHOM84] Choi Chuck Lee, Ernst C. Hass, Craig A. Obafemi, and Paul G. Mezey. A theoretical study on the protonation of cycloalkanes C_nH_{2n} ($n = 3$ to 6). *Journal of Computational Chemistry*, 5(2):190–196, April 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liljefors:1987:BRB

[Lil87] Tommy Liljefors. Book review: *Macromolecular structure and specificity: Computer-assisted modeling and applications*, Edited by Babu Venkataraghavan and Richard J. Feldmann, Annals of the New York Academy of Sciences, New York, 209 pp. Price: $48.00 (1985). *Journal of Computational Chemistry*, 8(2):185, March 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Linse:1988:GAC

[Lin88] Per Linse. General algorithm for calculating vibrational–librational states of a rigid molecule in an external potential. Application to benzene–water complexes. *Journal of Computational Chemistry*, 9(5):505–517, July 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lipkowitz:1983:BRBb

[Lip83a] Kenny Lipkowitz. Book review: *Molecular mechanics*, by Ulrich Burkert and Norman L. Allinger, published by the American Chemical Society, 1982. 339 pages, $64.95. *Journal* *of Computational Chemistry*, 4(4):605, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lipkowitz:1983:BRBa

[Lip83b] Kenny Lipkowitz. Book review: *Progress in theoretical organic chemistry*, volume 3, L. Radom et al. Elsevier, New York, 1982. Price: $103. *Journal of Computational Chemistry*, 4(1):123, Spring 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lipkowitz:1986:BRB

[Lip86] Kenny Lipkowitz. Book review: *A handbook of computational chemistry: A practical guide to chemical structure and energy calculations*, by Tim Clark, John Wiley, New York, 332 pp. Price: $35.00 (1985). *Journal of Computational Chemistry*, 7 (3):379–380, June 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lipson:1987:SSB

[Lip87] J. E. G. Lipson. Simulation studies of branched polymer molecules. *Journal of Computational Chemistry*, 8(4):333–340, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:1987:TSA

[LKL87] Ikchoon Lee, Chang Kon Kim, and Byung Choon Lee. Theoretical studies on the acid hydrolysis of methyl carbamate. *Journal of Computational Chemistry*, 8(6):794–800, September 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:1985:TSG

[LLC85] Ikchoon Lee, Bon-Su Lee, and Jae Young Choi. Theoretical study of the gas-phase reaction of hydrogen isocyanate with water. *Journal of Computational Chemistry*, 6(2):79–87, April 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:1985:TSH

[LLSC85] Bon-Su Lee, Ikchoon Lee, Chang Hyun Song, and Jae Young Choi. Theoretical studies on the hydrogen atom transfer reaction. *Journal of Computational Chemistry*, 6(5):486–491, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lindh:1989:SAM

[LM89] Roland Lindh and Per-Årke Malmquist. A submatrix algorithm for the matrix-vector multiplication of very large matrices. *Journal of Computational Chemistry*, 10(3):344–345, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lejeune:1986:IFM

[LMV86] J. Lejeune, A. Michel, and D. P. Vercauteren. Improving the flexible molecular fitting technique using distance matrices. *Journal of Computational Chemistry*, 7(6):739–744, December 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lees:1985:PSP

[LMW85] W. Lees, S. Manoli, and M. A. Whitehead. The α and α parameters for spin polarized Hartree–Fock–Slater calculations. *Journal of Computational Chemistry*, 6(1):56–60, February 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lopez:1989:SPP

[Lop89] Jesus P. Lopez. Stationary points on the potential energy surface of O_2^-HF and $O_2^-H_2O$. *Journal of Computational Chemistry*, 10(1):55–62, January 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lindblad:1988:SMZ

[LP88] Marina Lindblad and Tapani A. Pakkanen. Surface model for ZnS thin films: ZnS clusters and chemisorption of $ZnCl_2$ on ZnS surface. *Journal of Computational Chemistry*, 9(5):581–590, July 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lieb:1984:TDG

[LPB84] S. G. Lieb, W. L. Perry, and J. W. Bevan. Theoretical development of a Gaussian potential function in the description of the radial portion of isotropic bending vibrations. *Journal* of *Computational Chemistry*, 5(2):115–121, April 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liotard:1987:TCI

[LR87] D. Liotard and M. Roche. Topology of conical intersections and Jahn–Teller crossing: Application to the standard model for XY_4 molecules in T_2 ground states. *Journal of Computational Chemistry*, 8(6):850–860, September 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Laitinen:1987:MVC

[LRP87] Risto S. Laitinen, Bruce Randolph, and Tapani A. Pakkanen. Molecular valence calculations on cyclohexasulfur, cycloheptasulfur, and cyclooctasulfur. *Journal of Computational Chemistry*, 8(5):658–662, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Leugers:1984:RTV

[LS84] M. A. Leugers and C. J. Seliskar. A rotation–torsion vibronic band contour program. *Journal of Computational Chemistry*, 5(5):457–465, October 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Latajka:1987:BSMa

[LS87a] Zdzislaw Latajka and Steve Scheiner. Basis sets for molecular interactions. 1. Construction and tests on $(HF)_2$ and $(H_2O)_2$. *Journal of Computational Chemistry*, 8(5):663–673, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Latajka:1987:BSMb

[LS87b] Zdzislaw Latajka and Steve Scheiner. Basis sets for molecular interactions. 2. Application to H_3NHF, H_3NHOH, H_2OHF, $(NH_3)_2$, and H_3CHOH_2. *Journal of Computational Chemistry*, 8(5):674–682, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lipton:1988:MMP

[LS88] Mark Lipton and W. Clark Still. The multiple minimum problem in molecular modeling. Tree searching internal coordinate conformational space. *Journal of Computational*

Chemistry, 9(4):343–355, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lambert:1989:PRPa

[LS89a] Millard H. Lambert and Harold A. Scheraga. Pattern recognition in the prediction of protein structure. I. Tripeptide conformational probabilities calculated from the amino acid sequence. *Journal of Computational Chemistry*, 10(6):770–797, September 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lambert:1989:PRPb

[LS89b] Millard H. Lambert and Harold A. Scheraga. Pattern recognition in the prediction of protein structure. II. Chain conformation from a probability-directed search procedure. *Journal of Computational Chemistry*, 10(6):798–816, September 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lambert:1989:PRPc

[LS89c] Millard H. Lambert and Harold A. Scheraga. Pattern recognition in the prediction of protein structure. III. An importance-sampling minimization procedure. *Journal of Computational Chemistry*, 10(6):817–831, September 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Latajka:1980:PSH

[LSROT80] Z. Latajka, M. M. Szczęśniak, H. Ratajczak, and W. J. Orville-Thomas. Properties of strong hydrogen-bonded systems. II. Ab initio SCF–MO study of the hydrogen bond between nitric acid and ammonia. *Journal of Computational Chemistry*, 1(4):417–419, Winter 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liljefors:1987:PDA

[LTLA87] Tommy Liljefors, Julia C. Tai, Shusen Li, and Norman L. Allinger. On the out-of-plane deformation of aromatic rings, and its representation by molecular mechanics. *Journal of Computational Chemistry*, 8(7):1051–1056, October 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lipkowitz:1985:SFB

[LUNV85] Kenny B. Lipkowitz, Christopher Uhegbu, Adel M. Naylor, and Robert Vance. Structural features of benzylic carbanions. A theoretical study. *Journal of Computational Chemistry*, 6 (6):662–673, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

LaManna:1982:CSI

[LV82] Gianfranco La Manna and Eduardo Venuti. Computational study on the interaction of water with 2- and 3-hydroxypyridine and the corresponding pyridones. *Journal of Computational Chemistry*, 3(4):593–602, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:1988:FDA

[LV88] Zong Jie Liu and Roland Van Rapenbusch. A fast, direct algorithm for the least-squares fitting of two sets of atomic coordinates of macromolecular structures. *Journal of Computational Chemistry*, 9(6):596–599, September 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lugosi:1988:SWP

[LW88] Erzsebet Lugosi and Arthur T. Winfree. Simulation of wave-propagation in three dimensions using Fortran on the CYBER 205. *Journal of Computational Chemistry*, 9(6):689–701, September 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lochmann:1982:IDL

[LWD82] R. Lochmann, Th. Weller, and D. Deininger. An improved description of lone pairs by a modified PCILO method. *Journal of Computational Chemistry*, 3(4):507–511, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lopez:1987:ESC

[LYH87] Jesus P. Lopez, Cary Y. Yang, and C. R. Helms. Electronic structure of clusters modeling silica. *Journal of Computational Chemistry*, 8(3):198–203, April 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lipkowitz:1989:TSMa

[LZ89] Kenny B. Lipkowitz and Richard Zegarra. Theoretical studies in molecular recognition: Rebek's cleft. *Journal of Computational Chemistry*, 10(5):595–602, July 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lavery:1984:OME

[LZP84] Richard Lavery, Krystyna Zakrzewska, and Alberte Pullman. Optimized monopole expansions for the representation of the electrostatic properties of the nucleic acids. *Journal of Computational Chemistry*, 5(4):363–373, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Magnusson:1984:SES

[Mag84] Eric Magnusson. Substituent effects in second-row molecules: Basis set performance in calculations of normal valency phosphorus and sulfur compounds. *Journal of Computational Chemistry*, 5(6):612–628, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mercau:1984:MVC

[MAR+84] N. Mercau, R. Aroca, E. A. Robinson, J. Aron, J. Bunnell, and T. A. Ford. Molecular vibrational constants of some simple polyatomic molecules. Methyl, silyl, and germyl halides. *Journal of Computational Chemistry*, 5(5):427–440, October 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

March:1987:DAP

[Mar87] N. H. March. The density amplitude $\rho^{1/2}$ and the potential which generates it. *Journal of Computational Chemistry*, 8 (4):375–379, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Masamura:1988:EAS

[Mas88] M. Masamura. An efficient algorithm for solving eigenvalue problems of the type $HC = SCe$ or $FC = SCe$. *Journal of Computational Chemistry*, 9(3):257–268, April 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Matyska:1988:FAR

[Mat88] Luděk Matyska. Fast algorithm for ring perception. *Journal of Computational Chemistry*, 9(5):455–459, July 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mezei:1984:GSS

[MB84] Mihaly Mezei and David L. Beveridge. Generic solvent sites in a crystal. *Journal of Computational Chemistry*, 5(6):523–527, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mekenyan:1984:UDC

[MBB84] Ovanes Mekenyan, Danail Bonchev, and Alexandru T. Balaban. Unique description of chemical structures based on hierarchically ordered extended connectivities (HOC procedures). V. New topological indices, ordering of graphs, and recognition of graph similarity. *Journal of Computational Chemistry*, 5(6):629–639, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mekenyan:1985:UDC

[MBB85] Ovanes Mekenyan, Danail Bonchev, and Alexandru T. Balaban. Unique description of chemical structures on hierarchically ordered extended connectivities (HOC procedures). II. Mathematical proofs for the HOC algorithm. *Journal of Computational Chemistry*, 6(6):552–561, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Margheritis:1988:AWI

[MC88] C. Margheritis and G. Corongiu. Acetylcholine in water: Abinitio potential and Monte Carlo simulation. *Journal of Computational Chemistry*, 9(1):1–10, January 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Meyer:1980:MMO

[Mey80a] A. Y. Meyer. Molecular mechanics of organic halides. III. Fluorinated olefins. *Journal of Computational Chemistry*, 1 (2):111–117, Summer 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Meyer:1980:CAC

[Mey80b] Edgar F. Meyer Jr. The computational application of the Cahn–Ingold–Prelog rules 1 and 2. *Journal of Computational Chemistry*, 1(3):229–232, Autumn 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Meyer:1981:MMO

[Mey81] A. Y. Meyer. Molecular mechanics of organic halides. V. Conformational equilibria in solution. *Journal of Computational Chemistry*, 2(4):384–391, Winter 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Meyer:1984:RMM

[Mey84] A. Y. Meyer. Remarks on the molecular mechanical calculations of functionalized hydrocarbons. *Journal of Computational Chemistry*, 5(4):299–306, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Meyer:1986:MMM

[Mey86] A. Y. Meyer. Molecular mechanics and molecular shape. III. Surface area and cross-sectional areas of organic molecules. *Journal of Computational Chemistry*, 7(2):144–152, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Meyer:1988:MMM

[Mey88] A. Y. Meyer. Molecular mechanics and molecular shape. V. on the computation of the bare surface area of molecules. *Journal of Computational Chemistry*, 9(1):18–24, January 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mezey:1987:I

[Mez87a] Paul G. Mezey. Introduction. *Journal of Computational Chemistry*, 8(4):281, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mezey:1987:SMC

[Mez87b] Paul G. Mezey. The shape of molecular charge distributions: Group theory without symmetry. *Journal of Computational Chemistry*, 8(4):462–469, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Meyer:1985:TCM

[MF85] A. Y. Meyer and F. R. F. Forrest. Towards the convergence of molecular-mechanical force fields. *Journal of Computational Chemistry*, 6(1):1–4, February 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Martin:1989:ISP

[MFG89a] J. M. L. Martin, J. P. François, and R. Gijbels. Ab initio study of the proton affinity of a number of ortho-substituted pyridines. *Journal of Computational Chemistry*, 10(3):346–357, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Martin:1989:CBPb

[MFG89b] J. M. L. Martin, J. P. François, and R. Gijbels. Combined bond-polarization basis sets for accurate determination of dissociation energies. II. Basis set superposition error as a function of the parent basis set. *Journal of Computational Chemistry*, 10(7):875–886, October 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Martin:1989:CBPa

[MFG89c] J. M. L. Martin, J. P. François, and R. Gijbels. Combined bond polarization function basis sets for accurate ab initio calculation of the dissociation energies of AH_n molecules (A = Li to F). *Journal of Computational Chemistry*, 10(2): 152–162, March 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mezey:1983:PBS

[MH83] Paul G. Mezey and Ernst-C. Hass. The propagation of basis-set error and geometry optimization in ab initio calculations. II. Correlation between the balance of Gaussian basis sets and calculated molecular properties. *Journal of Computational Chemistry*, 4(4):482–487, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Miller:1989:FSD

[MHA89] Kenneth J. Miller, Robert J. Hinde, and Janet Anderson. First and second derivative matrix elements for the stretching, bending, and torsional energy. *Journal of Computational*

Chemistry, 10(1):63–76, January 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Millett:1987:SIF

[Mil87] Kenneth C. Millett. Stereotopological indices for a family of chemical graphs. *Journal of Computational Chemistry*, 8(4): 536–548, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mitin:1988:DLS

[Mit88] A. V. Mitin. The dynamic “level shift” method for improving the convergence of the SCF procedure. *Journal of Computational Chemistry*, 9(2):107–110, March 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Masut:1984:MMV

[MK84a] Remo A. Masut and Joseph N. Kushick. The molecular mechanics of valinomycin. I. Energy minimization calculations on the uncomplexed ionophore. *Journal of Computational Chemistry*, 5(4):336–342, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Miller:1984:IMN

[MK84b] Kenneth J. Miller and Paul J. Kowalczyk. Interactions of molecules with nucleic acids. IX. Evaluation and presentation of electrostatic contours on a steric surface with the removal of hidden lines. *Journal of Computational Chemistry*, 5(1): 89–103, February 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mach:1985:CBB

[MK85a] P. Mach and O. Kysel. Comparison between 6-31 + bond functions and 6-31 G* basis sets in UMP calculations of dissociation energies of the first row element compounds. I. *Journal of Computational Chemistry*, 6(4):312–315, August 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Masut:1985:MMV

[MK85b] Remo A. Masut and Joseph N. Kushick. The molecular mechanics of valinomycin. II: Comparative studies of alkali ion binding. *Journal of Computational Chemistry*, 6(2):148–155, April 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Miller:1983:IMN

[MKSW83] Kenneth J. Miller, Paul Kowalczyk, Wolfgang Segmuller, and George Walker. Interactions of molecules with nucleic acids. VII. Evaluation and presentation of steric contours and molecules in bonding sites. *Journal of Computational Chemistry*, 4(3):366–378, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mullally:1983:FFD

[MM83] D. J. Mullally and J. W. McIver Jr. Faster finite-difference calculations of molecular properties. *Journal of Computational Chemistry*, 4(4):552–555, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

McCourt:1987:SCE

[MM87] Mary McCourt and James W. McIver Jr. On the SCF calculation of excited states: Singlet states in the two-electron problem. *Journal of Computational Chemistry*, 8(4):454–458, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Muller:1989:SER

[MM89] Paul Müller and Jiri Mareda. Steric effects on reaction rates. XI. Solvolysis of tertiary carbon substrates rationalized by molecular mechanics calculations. *Journal of Computational Chemistry*, 10(7):863–868, October 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mom:1981:CSA

[Mom81] V. Mom. On the construction of self-avoiding chains. *Journal of Computational Chemistry*, 2(4):446–459, Winter 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Morin:1985:CRD

[Mor85] François Morin. Computation of reequilibration data in solids. *Journal of Computational Chemistry*, 6(6):514–519, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mezey:1980:RIC

[MR80] Paul G. Mezey and Ch. V. S. Ramachandra Rao. On the relative importance of core and valence shell representations in the calculation of conformational energies using small Gaussian basis sets. *Journal of Computational Chemistry*, 1(2): 134–140, Summer 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Murthy:1983:UCF

[MR83] A. S. N. Murthy and Shoba Ranganathan. The use of CNDO/force and compliance constant methods in evaluating quadratic potential functions of carbonyl and formyl fluorides. *Journal of Computational Chemistry*, 4(2):175–180, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Miyoshi:1988:AMP

[MS88] Eisaku Miyoshi and Yoshiko Sakai. Applications of the model potential method to transition metal compounds. *Journal of Computational Chemistry*, 9(7):719–727, October 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Michalska:1988:BSE

[MSČ+88] D. Michalska, L. J. Schaad, P. Čarsky, B. Andes Hess Jr., and C. S. Ewig. Basis set effects and the choice of reference geometry in ab initio calculations of vibrational spectra. *Journal of Computational Chemistry*, 9(5):495–504, July 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mezey:1980:NDM

[MSG80] P. G. Mezey, O. P. Strausz, and R. K. Gosavi. A note on density matrix extrapolation and multiple solutions of the unrestricted Hartree–Fock equations. *Journal of Computational Chemistry*, 1(2):178–180, Summer 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Muller:1987:ACM

[MSKT87] W. R. Müller, K. Szymanski, J. V. Knop, and N. Trinajstić. An algorithm for construction of the molecular distance matrix. *Journal of Computational Chemistry*, 8(2):170–173, March 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

McManus:1982:EMS

[MSS82] Samuel P. McManus, Maurice R. Smith, and Steven G. Shafer. Evaluation of MINDO /3 calculated structures. III. Saturated acyclic compounds with chlorine, nitrogen, oxygen, or sulfur. *Journal of Computational Chemistry*, 3(2): 229–233, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

McManus:1980:EMS

[MSSS80] Samuel P. McManus, Maurice R. Smith, Margaret B. Smith, and Steven G. Shafer. Evaluation of MINDO /3 calculated structures. II. Branching errors in alkanes and cycloalkanes. *Journal of Computational Chemistry*, 1(3):233–239, Autumn 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mohar:1982:CTR

[MT82] B. Mohar and N. Trinajstić. On computation of the topological resonance energy. *Journal of Computational Chemistry*, 3 (1):28–36, Spring 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Matias:1987:ISV

[MTN87] Manuel Matías, Luis M. Tel, and Juan J. Novoa. Ab initio studies on van der Waals molecules. A comparative study with several basis sets of the C_{2v} $HeLi_2$ system. *Journal of Computational Chemistry*, 8(1):51–56, January 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mullay:1988:MCA

[Mul88a] John Mullay. A method for calculating atomic charges in large molecules. *Journal of Computational Chemistry*, 9(4): 399–405, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mullay:1988:SMC

[Mul88b] John Mullay. A simple method for calculating reliable atomic charges in large molecules. *Journal of Computational Chem-*

istry, 9(7):764–770, October 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Matias:1987:ISL

[MV87] M. A. Matías and A. J. C. Varandas. Ab initio study of the He(^{1}S)-Li$_2$(X$^-$, $^1\Sigma$) interaction by the SCF and MP2 methods. *Journal of Computational Chemistry*, 8(6):761–771, September 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nilar:1984:MAV

[NF84] S. H. M. Nilar and Serafin Fraga. Molecular associations: Values of the expansion parameters for new classes of atoms. *Journal of Computational Chemistry*, 5(3):261–262, June 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nilsson:1986:EEF

[NK86] Lennart Nilsson and Martin Karplus. Empirical energy functions for energy minimization and dynamics of nucleic acids. *Journal of Computational Chemistry*, 7(5):591–616, October 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nguyen:1985:PMD

[NKC85] H. L. Nguyen, H. Khanmohammadbaigi, and E. Clementi. A parallel molecular dynamics strategy. *Journal of Computational Chemistry*, 6(6):634–646, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Norskov-Lauritsen:1984:MMT

[NLA84] Leif Nørskov-Lauritsen and Norman L. Allinger. A molecular mechanics treatment of the anomeric effect. *Journal of Computational Chemistry*, 5(4):326–335, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Norskov-Lauritsen:1985:CAP

[NLB85] L. Nørskov-Lauritsen and H. B. Bürgi. Cluster analysis of periodic distributions; application to conformational analysis. *Journal of Computational Chemistry*, 6(3):216–228, June 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Neuberger:1987:NCE

[NN87] J. W. Neuberger and D. W. Noid. Numerical calculation of eigenvalues for the Schrödinger equation. III. *Journal of Computational Chemistry*, 8(4):459–461, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Norman:1980:MMB

[NR80] Joe G. Norman Jr. and P. Barry Ryan. Metal–metal bond energies in Mo_2, Mo_2Cl, and $Mo_2(O_2CH)_4$. *Journal of Computational Chemistry*, 1(1):59–63, Spring 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Natiello:1985:GFQ

[NRM85] Mario A. Natiello, Héctor F. Reale, and Jorge A. Medrano. A generalized formalism of the quantum theory of valence and bonding. *Journal of Computational Chemistry*, 6(2):108–115, April 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nobes:1982:GBS

[NRR82] Ross H. Nobes, William R. Rodwell, and Leo Radom. The 6-31 G^{++} basis set: an economical basis set for correlated wavefunctions. *Journal of Computational Chemistry*, 3(4):561–564, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nguyen:1984:AIF

[NRS84] T. T. Nguyen, P. N. Raychowdhury, and D. D. Shillady. Application of an ion-fitted pseudopotential to HF, H_2O, NH_3, BeO, and HCl in a Gaussian lobe basis. *Journal of Computational Chemistry*, 5(6):640–649, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Naaray-Szabo:1981:SCE

[NSGK+81] G. Náaray-Szabó, A. Grofcsik, K. Kósa, M. Kubinyi, and A. Martin. Simple calculation of electrostatic isopotential maps from bond fragments. *Journal of Computational Chemistry*, 2(1):58–62, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Naray-Szabo:1987:TQC

[NSKNK87] Gábor Náray-Szabó, György Kramer, Péter Nagy, and Sándor Kugler. Towards a quantum chemical software package utilizing transferable fragments as molecular building blocks. *Journal of Computational Chemistry*, 8(4):555–561, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Namboodiri:1981:ESS

[NVGB81] K. P. Krishnan Namboodiri, S. Viswanathan, R. Ganesan, and V. C. Jyothi Bhasu. The electronic structure, spectra, and reactivity of nitrophenols. *Journal of Computational Chemistry*, 2(4):392–401, Winter 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Onuchic:1988:DWG

[OC88] J. N. Onuchic and G. Corongiu. Determination of the water geometry in violuric acid monohydrate with a Monte Carlo simulation. *Journal of Computational Chemistry*, 9(1):11–17, January 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Olefirowicz:1989:CAM

[OE89] Edward M. Olefirowicz and Ernest L. Eliel. Conformational analysis. 48. A molecular mechanics (MMP2) approach to the conformational analysis of methyl-, dimethyl- and trimethylisochromanes. *Journal of Computational Chemistry*, 10(3):407–412, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ott:1986:OSR

[OG86] Jane J. Ott and Benjamin M. Gimarc. Optimized structures and relative stabilities of the carboranes from ab initio calculations. *Journal of Computational Chemistry*, 7(5):673–692, October 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Oie:1983:ISC

[OLBM83] Tetsuro Oie, Gilda H. Loew, Stanley K. Burt, and Robert D. Macelroy. Ab initio study of catalyzed and uncatalyzed amide bond formation as a model for peptide bond formation: Ammonia-Glycine reactions. *Journal of Computational*

Chemistry, 4(4):449–460, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Okuyama:1988:CAS

[OMK+88] Tohru Okuyama, Yoshikatsu Miyashita, Shigehiko Kanaya, Hiroyuki Katsumi, Shin-Ichi Sasaki, and Milan Randić. Computer assisted structure–taste studies on sulfamates by pattern recognition method using graph theoretical invariants. *Journal of Computational Chemistry*, 9(6):636–646, September 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Osawa:1982:MCC

[Ōsa82] Eiji Ōsawa. Mechanisms of conformational chirality inversion in bicyclo[4.2.1]nonan-9-one and bicyclo[4.2.2]decane as studied in two-parametric torsional energy surfaces. *Journal of Computational Chemistry*, 3(3):400–406, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Orchard:1987:MMP

[OTPH87] B. J. Orchard, S. K. Tripathy, R. A. Pearlstein, and A. J. Hopfinger. Molecular modeling of polymers: I. Correct and efficient enumeration of intrachain conformational energetics. *Journal of Computational Chemistry*, 8(1):28–38, January 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Osman:1981:EDR

[OTW81] Roman Osman, Sid Topiol, and Harel Weinstein. Electron density redistribution in the stabilization of a molecular stacking complex: the nature and correction of basis set superposition errors. *Journal of Computational Chemistry*, 2(1):73–82, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Olivella:1984:EMC

[OUV84] Santiago Olivella, Felix Urpi, and Jaume Vilarrasa. Evaluation of MNDO calculated proton affinities. *Journal of Computational Chemistry*, 5(3):230–236, June 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pascual-Ahuir:1987:EIS

[PASTB87] J. L. Pascual-Ahuir, E. Silla, J. Tomasi, and R. Bonaccorsi. Electrostatic interaction of a solute with a continuum. Improved description of the cavity and of the surface cavity bound charge distribution. *Journal of Computational Chemistry*, 8(6):778–787, September 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Phillips:1983:TRL

[PD83] Philip Phillips and Ernest R. Davidson. Theory of the radiative lifetime of the $^3B_1$ state of SO_2. *Journal of Computational Chemistry*, 4(3):337–344, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Perry:1984:MIT

[Per84] W. L. Perry. A monotone iterative technique for solution of pth order ($p < 0$) reaction–diffusion problems in permeable catalysis. *Journal of Computational Chemistry*, 5(4): 353–357, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pople:1982:SSA

[PFRS82] John A. Pople, Michael J. Frisch, Krishnan Raghavachari, and Paul V. R. Schleyer. The structure and stability of the acetylene dication. *Journal of Computational Chemistry*, 3 (4):468–470, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pietro:1983:MOT

[PH83] William J. Pietro and Warren J. Hehre. Molecular orbital theory of the properties of inorganic and organometallic compounds. 3. STO-3G basis sets for first- and second-row transition metals. *Journal of Computational Chemistry*, 4(2): 241–251, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Price:1989:IDM

[PHG89] S. L. Price, R. J. Harrison, and M. F. Guest. An ab initio distributed multipole study of the electrostatic potential around an undecapeptide cyclosporin derivative and a comparison with point charge electrostatic models. *Journal of*

Computational Chemistry, 10(4):552–567, June 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Panchenko:1988:IVA

[PKB88] Yurii N. Panchenko, Sergei V. Krasnoshchiokov, and Charles W. Bock. Ab initio vibrational analysis of three rotamers of 2-propen-1-imine, $H_2C{=}CH{-}HC{=}N{-}H$, and methanimine, $H_2C{=}N{-}H$. *Journal of Computational Chemistry*, 9(5):443–454, July 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pelissier:1988:OCE

[PKD88] M. Pelissier, N. Komiha, and J. P. Daudey. One-center expansion for pseudopotential matrix elements. *Journal of Computational Chemistry*, 9(4):298–302, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pettersson:1987:BBP

[PL87] Ingrid Pettersson and Tommy Liljefors. Benzene-benzene (phenyl-phenyl) interactions in MM2/MMP2 molecular mechanics calculations. *Journal of Computational Chemistry*, 8(8):1139–1145, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pattabiraman:1985:CGR

[PLFL85] N. Pattabiraman, M. Levitt, T. E. Ferrin, and R. Langridge. Computer graphics in real-time docking with energy calculation and minimization. *Journal of Computational Chemistry*, 6(5):432–436, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Poirier:1986:SCS

[PMZ86] Raymond A. Poirier, Dariush Majlessi, and Theresa J. Zielinski. An SCF and CI study of the 1,3 shift in the $HX{-}CH{=}Y \rightleftharpoons X{=}CH{-}YH$ isoelectronic series: X, Y = CH_2, NH, and O. *Journal of Computational Chemistry*, 7(4):464–475, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pottle:1980:CAP

[PPT+80] C. Pottle, M. S. Pottle, R. W. Tuttle, R. J. Kinch, and H. A. Scheraga. Conformational analysis of proteins: Algorithms and data structures for array processing. *Journal of Computational Chemistry*, 1(1):46–58, Spring 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Palmieri:1983:EOA

[PPV83] P. Palmieri, G. Poggi, and J. Vrbancich. Electronic optical activity of (-)-α-phellandrene. *Journal of Computational Chemistry*, 4(2):260–266, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pross:1980:TAS

[PR80] Addy Pross and Leo Radom. A theoretical approach to substituent effects. Structural consequences of electrostatic and orbital interactions in model mono- and disubstituted methanes. *Journal of Computational Chemistry*, 1(3):295–300, Autumn 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pietila:1984:PCC

[PR84] Lars-Olof Pietilä and Kjeld Rasmussen. A program for calculation of crystal conformations of flexible molecules using convergence acceleration. *Journal of Computational Chemistry*, 5(3):252–260, June 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ponder:1987:ENL

[PR87] Jay W. Ponder and Frederic M. Richards. An efficient Newton-like method for molecular mechanics energy minimization of large molecules. *Journal of Computational Chemistry*, 8(7):1016–1024, October 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Poirier:1987:ASL

[PS87] Raymond A. Poirier and Péter R. Surján. The application of strictly localized geminals to the description of chemical bonds. *Journal of Computational Chemistry*, 8(4):436–441, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pople:1980:SCT

[PSSS80] John A. Pople, Ute Seeger, Rolf Seeger, and Paul V. R. Schleyer. The structure of carbon trioxide. *Journal of Com-*

putational Chemistry, 1(2):199–203, Summer 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Profeta:1989:SAM

[PUC89] Salvatore Profeta Jr., Rayomand J. Unwalla, and Frank K. Cartledge. Simple alkyldisilanes: MM2 and ab initio studies of their structures and barriers to rotation. *Journal of Computational Chemistry*, 10(1):99–103, January 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pulay:1982:ISC

[Pul82] P. Pulay. Improved SCF convergence acceleration. *Journal of Computational Chemistry*, 3(4):556–560, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Profeta:1986:CRP

[PUNC86] Salvatore Profeta Jr., Rayomand J. Unwalla, Binh T. Nguyen, and Frank K. Cartledge. A comparison of the rotational potential functions in butane, propylsilane, ethylmethylsilane, and 1,2-disilylethane: Ab initio and MM2 results. *Journal of Computational Chemistry*, 7(4):528–538, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Putnam:1982:CMF

[PV82a] B. F. Putnam and L. L. Van Zandt. Calculation of macromolecular force constants. *Journal of Computational Chemistry*, 3(3):297–304, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Putnam:1982:PNV

[PV82b] B. F. Putnam and L. L. Van Zandt. Planar and nonplanar vibrations of cytosine. *Journal of Computational Chemistry*, 3(3):305–316, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pasternak:1981:SSO

[PW81] R. Pasternak and G. Wagnière. Semiempirical spin–orbit coupling calculations. I. Theory and method. Benzophenone as a test case. *Journal of Computational Chemistry*, 2(3):347–355, Autumn 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Parry:1982:EPF

[PW82] D. E. Parry and M. A. Whitehead. Empirical penetration functions and two-center electron repulsion integrals for semiempirical calculations of electronic structure. *Journal of Computational Chemistry*, 3(2):265–268, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Radzio:1987:RGB

[RA87] Elżbieta Radzio and Jan Andzelm. Reliable Gaussian basis sets for closed-shell atoms. *Journal of Computational Chemistry*, 8(2):117–131, March 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Randic:1980:RWT

[Ran80] Milan Randić. Random walks and their diagnostic value for characterization of atomic environment. *Journal of Computational Chemistry*, 1(4):386–399, Winter 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Randic:1982:ECP

[Ran82] Milan Randić. On evaluation of the characteristic polynomial for large molecules. *Journal of Computational Chemistry*, 3 (3):421–435, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Randic:1983:SPC

[Ran83] Milan Randić. Symmetry properties of chemical graphs. V. Internal rotation in $XY{\cdot}_3XY{\cdot}_2XY_3$. *Journal of Computational Chemistry*, 4(1):73–83, Spring 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Randic:1986:BRB

[Ran86] Milan Randic. Book review: *Computer generation of certain classes of molecules*, by J. V. Knop, W. R. Muller, K. Szymnsky, and N. Trinajstic, association of chemists and technologists of croatia berislaviceva 6/1, YU-41000 Zagreb and INA Research & development, Proleterskih Brigada 78, YU 41000 Zagreb, Yugoslavia, 250 pp. price: $9.00 (19XX). *Journal of Computational Chemistry*, 7(6):761–762, December 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rappe:1984:VQC

[Rap84] A. K. Rappé. Vectorization of quantum chemical algorithms: MC–SCF procedures. *Journal of Computational Chemistry*, 5(5):471–479, October 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Radzio:1985:CBS

[RAS85] E. Radzio, J. Andzelm, and D. R. Salahub. Compact basis sets for LCAO-LSD calculations. Part II: Tests for Cr_2 and Ni_4. *Journal of Computational Chemistry*, 6(6):533–537, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ramaraj:1985:CGM

[RB85] Ramamani Ramaraj and K. Balasubramanian. Computer generation of matching polynimials of chemical graphs and lattices. *Journal of Computational Chemistry*, 6(2):122–141, April 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ritchie:1987:SMA

[RB87] James P. Ritchie and Steven M. Bachrach. Some methods and applications of electron density distribution analysis. *Journal of Computational Chemistry*, 8(4):499–509, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rothman:1980:PSM

[RBEV80] Michael J. Rothman, Lawrence S. Bartell, Carl S. Ewig, and John R. Van Wazer. A pseudopotential SCF-MO study of Te. *Journal of Computational Chemistry*, 1(1):64–68, Spring 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rauk:1987:IAG

[RD87] Arvi Rauk and Remo Dutler. Implementation and applications of Gaussian 82 on a CDC Cyber 205. *Journal of Computational Chemistry*, 8(4):324–332, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rico:1983:RHFa

[RDAF83] J. Fernández Rico, J. M. Garcia De La Vega, J. I. Fernández Alonso, and P. Fantucci. Restricted Hartree–Fock approximation. I. Techniques for the energy minimization. *Journal of Computational Chemistry*, 4(1):33–40, Spring 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rys:1983:CER

[RDK83] J. Rys, M. Dupuis, and H. F. King. Computation of electron repulsion integrals using the Rys quadrature method. *Journal of Computational Chemistry*, 4(2):154–157, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rasmussen:1988:ACC

[RDW88] Edie M. Rasmussen, Geoffrey M. Downs, and Peter Willett. Automatic classification of chemical structure databases using a highly parallel array processor. *Journal of Computational Chemistry*, 9(4):378–386, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Redondo:1989:MSU

[RFLC89] P. Redondo, J. R. Flores, and J. Largo-Cabrerizo. Multiple solutions of unrestricted Hartree–Fock equations: the SNH^+ radical as an example. *Journal of Computational Chemistry*, 10(3):295–301, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ragazzi:1986:FFS

[RFP86] Massimo Ragazzi, Dino R. Ferro, and Augusto Provasoli. A force-field study of the conformational characteristics of the iduronate ring. *Journal of Computational Chemistry*, 7(2): 105–112, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rossler:1987:QCH

[RH87] O. E. Rössler and M. Hoffmann. Quasiperiodization in classical hyperchaos. *Journal of Computational Chemistry*, 8(4): 510–515, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Randic:1989:CMP

[RHP89] Milan Randić, Haruo Hosoya, and Oskar E. Polansky. On the construction of the matching polynomial for unbranched catacondensed benzenoids. *Journal of Computational Chemistry*, 10(5):683–697, July 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ritchie:1986:EVA

[Rit86] James P. Ritchie. The effects of vinylic and allylic fluorine substitution in iso-butylene. *Journal of Computational Chemistry*, 7(1):1–12, February 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Randhawa:1981:CSF

[RK81] H. S. Randhawa and J. L. Kapoor. CN stretching frequencies in amide systems. *Journal of Computational Chemistry*, 2 (1):12–13, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ralev:1985:UDC

[RKM+85] Nikolai Ralev, Stoyan Karabunarliev, Ovanes Mekenyan, Danail Bonchev, and Alexandru T. Balaban. Unique description of chemical structures based on hierarchically ordered extended connectivities (HOC procedures). VIII. General principles for computer implementation. *Journal of Computational Chemistry*, 6(6):587–591, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rico:1988:COE

[RLR88] J. Fernández Rico, R. López, and G. Ramírez. Calculation of the one-electron two-center integrals with STOS using recurrence-based algorithms. *Journal of Computational Chemistry*, 9(7):790–797, October 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rico:1989:IAC

[RLR89] J. Fernández Rico, R. López, and G. Ramírez. Improved algorithm for the calculation of one-electron two-center integrals with STOs. *Journal of Computational Chemistry*, 10 (7):869–874, October 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ravishanker:1986:CSF

[RMB86] G. Ravishanker, M. Mezei, and D. L. Beveridge. Conformational stability and flexibility of the ala dipeptide in free space and water: Monte Carlo computer simulation studies. *Journal of Computational Chemistry*, 7(3):345–348, June 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Randic:1986:SPC

[ROK86] Milan Randić, David O. Oakland, and Douglas J. Klein. Symmetry properties of chemical graphs. IX. The valence tautomerism in the P_7^{3-} skeleton. *Journal of Computational Chemistry*, 7(1):35–54, February 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rouvray:1987:MCP

[Rou87] Dennis H. Rouvray. The modeling of chemical phenomena using topological indices. *Journal of Computational Chemistry*, 8(4):470–480, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rauk:1980:ESO

[RP80] Arvi Rauk and H. Allan Peoples. The electronic structure and optical activity of conjugated dienes: 1,3-Butadiene and α- and β-phellandrene. *Journal of Computational Chemistry*, 1(3):240–256, Autumn 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rico:1983:RHFb

[RPAF83] J. Fernández Rico, M. Paniagua, J. I. Fernández Alonso, and P. Fantucci. Restricted Hartree–Fock approximation. II. Computational aspects of the direct minimization procedure. *Journal of Computational Chemistry*, 4(1):41–47, Spring 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). Check garbled author names??

Rico:1986:MMT

[RPD+86] J. Fernández Rico, M. Paniagua, J. M. García De La Vega, J. I. Fernández-alonso, and P. Fantucci. A minimal multiconfigurational technique. *Journal of Computational Chemistry*, 7(2):201–207, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rothstein:1987:TSE

[RPV87] Stuart M. Rothstein, Narayan Patil, and Jan Vrbik. Time step error in diffusion Monte Carlo simulations: an empirical study. *Journal of Computational Chemistry*, 8(4):412–419, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Raychaudhury:1984:DIS

[RRG+84] C. Raychaudhury, S. K. Ray, J. J. Ghosh, A. B. Roy, and S. C. Basak. Discrimination of isomeric structures using information theoretic topological indices. *Journal of Computational Chemistry*, 5(6):581–588, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Raghavachari:1986:GPN

[RRH86] Krishnan Raghavachari, W. D. Reents Jr., and R. C. Haddon. Gas-phase nitrosation of benzene: Theoretical investigations. *Journal of Computational Chemistry*, 7(3):265–273, June 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rubio:1988:DIM

[RRI88] J. Rubio, J. M. Ricart, and F. Illas. Doublet instability and the molecular structure of AlO_2. *Journal of Computational Chemistry*, 9(8):836–843, December 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Redfern:1985:EAU

[RS85] Paul Redfern and Steve Scheiner. Effects of alkylation upon the proton affinities of nitrogen and oxygen bases. *Journal of Computational Chemistry*, 6(3):168–172, June 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ruelle:1987:TSM

[Rue87] P. Ruelle. Theoretical study on the mechanism of the thermal decarboxylation of acrylic and benzoic acids. Models for aqueous solution. *Journal of Computational Chemistry*, 8(2):158–169, March 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ruttink:1985:UPT

[RV85] P. J. A. Ruttink and M. M. M. Van Schaik. On the use of perturbation theory corrections to numerically selected MRDCI calculations. *Journal of Computational Chemistry*, 6(2):88–92, April 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Randic:1987:GG

[RWKH87] Milan Randić, Wayne L. Woodworth, Alexander F. Kleiner, and Haruo Hosoya. Graph generators. *Journal of Computational Chemistry*, 8(4):522–535, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sprague:1980:GMM

[SA80] Joseph T. Sprague and Norman L. Allinger. Graphite: a molecular mechanics treatment. *Journal of Computational Chemistry*, 1(3):257–260, Autumn 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schmitz:1988:SHH

[SAF88] Lawrence R. Schmitz, Norman L. Allinger, and Kenneth M. Flurchick. The stepwise heats of hydrogenation of barrelene, an ab initio study. *Journal of Computational Chemistry*, 9(4):281–287, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Symposia:1982:A

[San82] Sanibel Symposia. Announcements. *Journal of Computational Chemistry*, 3(4):605, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schmitz:1988:RAC

[SAP88] Lawrence R. Schmitz, Norman L. Allinger, and Salvatore Profeta Jr. Rotation around the C1 C2 bond of propylamine, an ab initio study. *Journal of Computational Chemistry*, 9(5):460–464, July 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sidrak:1987:OCO

[SAS87] Yousry L. Sidrak and A. Aboul-Seoud. An objective computer-oriented method for the calculation of formation constants from the formation function. A weighted least-squares curve fitting. *Journal of Computational Chemistry*, 8 (5):575–580, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Saunders:1989:SSC

[Sau89] Martin Saunders. Stochastic search for the conformations of bicyclic hydrocarbons. *Journal of Computational Chemistry*, 10(2):203–208, March 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sanz:1988:TCP

[SAV88] Javier Fernández Sanz, Julio Anguiano, and Jaume Vilarrasa. Theoretical calculations of proton affinities of azines. Prediction of the relative basicities and preferred protonation sites. *Journal of Computational Chemistry*, 9(7):784–789, October 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sax:1985:PCS

[Sax85] Alexander F. Sax. Pseudopotential calculations on Si_2H_6 and Si_2H_4. *Journal of Computational Chemistry*, 6(5):469–477, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Spiekermann:1982:CCV

[SBS82] M. Spiekermann, D. Bougeard, and B. Schrader. Coupled calculations of vibrational frequencies and intensities. III. IR and Raman spectra of ethylene oxide and ethylene sulfide. *Journal of Computational Chemistry*, 3(3):354–362, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Spitznagel:1982:SMA

[SCCvRS82] Günther W. Spitznagel, Timothy Clark, Jayaraman Chandrasekhar, and Paul von Ragué Schleyer. Stabilization of methyl anions by first-row substituents. The superiority of diffuse function-augmented basis sets for anion calculations. *Journal of Computational Chemistry*, 3(3):363–371, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Scharfenberg:1982:IME

[Sch82a] Peter Scharfenberg. An improved method for the evaluation of transition states. *Journal of Computational Chemistry*, 3 (3):277–282, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schlegel:1982:OEG

[Sch82b] H. Bernhard Schlegel. Optimization of equilibrium geometries and transition structures. *Journal of Computational Chemistry*, 3(2):214–218, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schelly:1986:BRB

[Sch86] Z. A. Schelly. Book review: *Physical chemistry on a microcomputer*, by J. H. Noggle, Little, Brown and Co., Boston, 239 pp. price: $12.95 (1985). *Journal of Computational Chemistry*, 7(6):761, December 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schlick:1988:MSG

[Sch88] Tamar Schlick. A modular strategy for generating starting conformations and data structures of polynucleotide helices for potential energy calculations. *Journal of Computational Chemistry*, 9(8):861–889, December 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schlick:1989:RED

[Sch89] Tamar Schlick. A recipe for evaluating and differentiating $\cos\varphi$ expressions. *Journal of Computational Chemistry*, 10 (7):951–956, October 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stewart:1982:FSC

[SCP82] J. J. P. Stewart, P. Császár, and P. Pulay. Fast semiempirical calculations. *Journal of Computational Chemistry*, 3(2):227–228, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Spitznagel:1987:EPD

[SCvRSH87] Günther W. Spitznagel, Timothy Clark, Paul von Ragué Schleyer, and Warren J. Hehre. An evaluation of the performance of diffuse function-augmented basis sets for second row elements, Na-Cl. *Journal of Computational Chemistry*, 8(8): 1109–1116, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stewart:1987:SEC

[SDB87] James J. P. Stewart, Larry P. Davis, and Larry W. Burggraf. Semi-empirical calculations of molecular trajectories: Method and applications to some simple molecular systems. *Journal of Computational Chemistry*, 8(8):1117–1123, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sanathanan:1987:SDR

[SDKM87] Lilly Sanathanan, Elizabeth Danaher, Ki-Hwan Kim, and Yvonne Martin. Systematic drug receptor mapping: a new approach to the analysis of conformational energy calculations of flexible molecules with application to dopaminergic and adrenergic agonists. *Journal of Computational Chemistry*, 8(8):1075–1083, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See correction [Ano88c].

Seel:1982:QOD

[SDL82] M. Seel, G. Del Re, and J. Ladik. Quasi-one-dimensional systems and localized defects: Some results of the Green's matrix formalism. *Journal of Computational Chemistry*, 3 (4):451–467, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Seeger:1981:PPM

[See81] Rolf Seeger. Parallel processing on minicomputers: a powerful tool for quantum chemistry. *Journal of Computational Chemistry*, 2(2):168–176, Summer 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Senn:1987:NEA

[Sen87] Peter Senn. A note on the efficient and accurate computation of the phase functions φ and χ in semiclassical approximations. *Journal of Computational Chemistry*, 8(7):965–971, October 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schoenenberger:1985:CAL

[SF85] Christian Schoenenberger and Wendell Forst. Computational aspects of Laplace transform inversion of thermal unimolecular rate constant. *Journal of Computational Chemistry*, 6(5): 455–461, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sordo:1986:MAV

[SF86] J. A. Sordo and S. Fraga. Molecular associations: Values of the expansion parameters for new classes of atoms. *Journal of Computational Chemistry*, 7(1):55–57, February 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stromberg:1983:GBS

[SGW83] Ann Strömberg, Odd Gropen, and Ulf Wahlgren. Gaussian basis sets for the fourth-row main group elements, In–Xe. *Journal of Computational Chemistry*, 4(2):181–186, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Saldanha:1989:DGP

[SHDP89] José W. Saldanha, Brendan Howlin, Louis Du Toit, and Rex A. Palmer. The dynamics of gallamine: a potent neuromuscular blocker. A determination by quantum mechanics and molecular dynamics (i) in vacuo studies. *Journal of Computational Chemistry*, 10(8):975–981, December 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sokalski:1983:GDB

[SHK83] W. A. Sokalski, P. C. Hariharan, and Joyce J. Kaufman. Guidelines for development of basis sets for the first-order intermolecular interaction energy calculations. *Journal of Computational Chemistry*, 4(4):506–512, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sato:1988:AFE

[SI88] Nobuyuki Sato and Suehiro Iwata. Application of finite-element method to the two-dimensional Schrödinger equation. *Journal of Computational Chemistry*, 9(3):222–231, April 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Siegbahn:1985:INP

[Sie85] Per E. M. Siegbahn. An investigation of NO_3 as a possible intermediate in the oxidation of nitric oxide. *Journal of Computational Chemistry*, 6(3):182–188, June 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Silver:1981:SMA

[Sil81] G. L. Silver. Space modification: an alternative approach to chemistry problems involving geometry. *Journal of Computational Chemistry*, 2(4):478–482, Winter 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Silver:1985:OMD

[Sil85] G. L. Silver. Operational method of data treatment. *Journal of Computational Chemistry*, 6(3):229–236, June 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Silver:1989:BIE

[Sil89] G. L. Silver. Bivariate interpolation for experimental designs. *Journal of Computational Chemistry*, 10(8):1013–1015, December 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Simon:1987:MGT

[Sim87] Jonathan Simon. Molecular graphs as topological objects in space. *Journal of Computational Chemistry*, 8(5):718–726, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Saunders:1986:NMM

[SJ86] Martin Saunders and Ronald M. Jarret. A new method for molecular mechanics. *Journal of Computational Chemistry*, 7(4):578–588, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Singh:1984:ACE

[SK84a] U. Chandra Singh and Peter A. Kollman. An approach to computing electrostatic charges for molecules. *Journal of*

Computational Chemistry, 5(2):129–145, April 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Szamosi:1984:EMC

[SK84b] Janos Szamosi and Sandor Kristyan. Experimental mathematics. I. Computational study on the limit cycle behavior of a two-dimensional chemical oscillator. *Journal of Computational Chemistry*, 5(2):186–189, April 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Singh:1985:ECA

[SK85] U. Chandra Singh and Peter Kollman. Energy component analysis calculations on neutral atom ... base interactions. *Journal of Computational Chemistry*, 6(1):5–8, February 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Singh:1986:CIQ

[SK86] U. Chandra Singh and Peter A. Kollman. A combined ab initio quantum mechanical and molecular mechanical method for carrying out simulations on complex molecular systems: Applications to the CH_3Cl + Cl^- exchange reaction and gas phase protonation of polyethers. *Journal of Computational Chemistry*, 7(6):718–730, December 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sax:1989:MSC

[SK89] Alexander F. Sax and Josef Kalcher. MC–SCF and CI calculations on the Si_4H_4 system. *Journal of Computational Chemistry*, 10(3):309–328, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Skancke:1983:DCP

[Ska83] Per N. Skancke. Divinylketone: Conformational preferences. Molecular geometry and vibrational force field in the ground state. *Journal of Computational Chemistry*, 4(2):142–149, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Siam:1984:ISS

[SKE+84] K. Siam, V. J. Klimkowski, J. D. Ewbank, Lothar Schäfer, and C. Van Alsenoy. Ab initio studies of structural features not easily amenable to experiment. 38. Structural and conformational investigations of propanoic, 2-methylpropanoic, and butanoic acid. *Journal of Computational Chemistry*, 5 (5):451–456, October 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sax:1988:MSC

[SKJ88] Alexander F. Sax, Josef Kalcher, and Rudolf Janoschek. MC–SCF and CI calculations on four isomers of Si_6H_6. *Journal of Computational Chemistry*, 9(5):564–577, July 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schafer:1985:ISS

[SKV+85] Lothar Schäfer, V. J. Klimkowski, C. Van Alsenoy, J. D. Ewbank, and J. N. Scarsdale. Ab initio studies of structural features not easily amenable to experiment. 42. Molecular geometries and conformational analysis of methylbutanoate. *Journal of Computational Chemistry*, 6(1):61–67, February 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schneider:1981:EIT

[SL81] W. J. Schneider and J. J. Ladik. On efficient integration techniques for oscillatory integrals in periodic system calculations. *Journal of Computational Chemistry*, 2(4):376–383, Winter 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sawaryn:1983:ENE

[SLB83] Andrezej Sawaryn, Bernd Leps, and Hans Bradaczek. Energetics of the neighbor exclusion model of intercalation. *Journal of Computational Chemistry*, 4(3):333–336, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sonnenschein:1986:TRM

[SLC86] Roland Sonnenschein, Aatto Laaksonen, and Enrico Clementi. The treatment of rotational motion in molecular dynamics. *Journal of Computational Chemistry*, 7(5):645–647, October 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sokalski:1986:NAA

[SLR+86] W. A. Sokalski, A. H. Lowrey, S. Roszak, V. Lewchenko, J. Blaisdell, P. C. Hariharan, and Joyce J. Kaufman. Nonempirical atom-atom potentials for main components of intermolecular interaction energy. *Journal of Computational Chemistry*, 7(5):693–700, October 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Srivastava:1980:ESB

[SM80] S. K. Srivastava and P. C. Mishra. Electronic structure of benzaldehyde: a comparative study of the lowest excited singlet $\pi^* \leftarrow \pi$ and $\pi^* \leftarrow n$ states. *Journal of Computational Chemistry*, 1(3):288–294, Autumn 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sotomatsu:1989:CAS

[SMF89] Tomoko Sotomatsu, Yoshiyuki Murata, and Toshio Fujita. Correlation analysis of substituent effects on the acidity of benzoic acids by the AM1 method. *Journal of Computational Chemistry*, 10(1):94–98, January 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Streitwieser:1987:SBS

[SMG87] Andrew Streitwieser Jr., Robert S. McDowell, and Rainer Glaser. A study of basis set effects on structures and electronic structures of phosphine oxide and fluorophosphine oxide. *Journal of Computational Chemistry*, 8(6):788–793, September 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sakai:1987:MPMa

[SMKH87a] Yoshiko Sakai, Eisaku Miyoshi, Mariusz Klobukowski, and Sigeru Huzinaga. Model potentials for molecular calculations. I. The *sd*-MP set for transition metal atoms Sc through Hg. *Journal of Computational Chemistry*, 8(3):226–255, April 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sakai:1987:MPMb

[SMKH87b] Yoshiko Sakai, Eisaku Miyoshi, Mariusz Klobukowski, and Sigeru Huzinaga. Model potentials for molecular calculations. II. The *spd*-MP set for transition metal atoms Sc through Hg. *Journal of Computational Chemistry*, 8(3):256–264, April 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sanchez-Marin:1985:SMS

[SMOT85] J. Sánchez-Marín, E. Ortí, and F. Tomás. Study of a medium-size biological molecular association by means of a pair potential semiempirical approach: β-carboline–lumiflavin. *Journal of Computational Chemistry*, 6(5):441–446, October 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Smeyers:1987:CTS

[SN87] Yves G. Smeyers and A. Niño. Character tables and symmetry eigenvectors for two C_{3v} rotor molecular systems. *Journal of Computational Chemistry*, 8(4):380–388, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sanjeevi:1983:MSA

[SNR83] R. Sanjeevi, R. Nagarajan, and V. Sri Ram. Multicollinearity and some applications in biological chemistry. *Journal of Computational Chemistry*, 4(3):362–365, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schlick:1987:PTN

[SO87] Tamar Schlick and Michael Overton. A powerful truncated Newton method for potential energy minimization. *Journal of Computational Chemistry*, 8(7):1025–1039, October 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sanyal:1986:IESa

[SOR86a] Nitish K. Sanyal, Rajendra Prasad Ojha, and M. Roychoudhury. Interaction energy studies of pyrrolopyrimidine nucleoside antibiotics-toyocamycin. *Journal of Computational Chemistry*, 7(1):13–19, February 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sanyal:1986:IESb

[SOR86b] Nitish K. Sanyal, Rajendra Prasad Ojha, and M. Roychoudhury. Interaction energy studies of pyrrolopyrimidine nucleoside antibiotics: Tubercidin. *Journal of Computational Chemistry*, 7(1):20–29, February 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sanyal:1987:IES

[SOR87] Nitish K. Sanyal, Rajendra Prasad Ojha, and M. Roychoudhury. Interaction energy studies of 8-azapurine during transcription. *Journal of Computational Chemistry*, 8(3):272–280, April 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sanyal:1986:IESc

[SORT86] Nitish K. Sanyal, Rajendra Prasad Ojha, M. Roychoudhury, and S. N. Tiwari. Interaction energy studies of pyrrolopyrimidine nucleoside antibiotics: Sangivamycin. *Journal of Computational Chemistry*, 7(1):30–34, February 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schlick:1987:ASE

[SPBO87] Tamar Schlick, Charles Peskin, Suse Broyde, and Michael Overton. An analysis of the structural and energetic properties of deoxyribose by potential energy methods. *Journal of Computational Chemistry*, 8(8):1199–1224, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sanyal:1987:CSS

[SRKT87] Nitish K. Sanyal, M. Roychoudhury, Kavita R. Ruhela (Km), and Sugriva Nath Tiwari. Configurational specificity of stacking interactions in DNA base pairs: a computational analysis. *Journal of Computational Chemistry*, 8(5):604–617, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Scarsdale:1988:MMN

[SRPY88] J. N. Scarsdale, P. Ram, J. H. Prestegard, and R. K. Yu. A molecular mechanics-NMR pseudoenergy approach to the solution conformation of glycolipids. *Journal of Computational Chemistry*, 9(2):133–147, March 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sapse:1981:ISG

[SS81] A. M. Sapse and A. Santoro. An ab initio study of the guanidinium fragments in tetrodotoxin and saxitoxin. *Journal of Computational Chemistry*, 2(4):363–367, Winter 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Szamosi:1984:TMD

[SS84] Janos Szamosi and Z. A. Schelly. Treatment of multiexponential decay data by the method of zero determinants. *Journal of Computational Chemistry*, 5(2):182–185, April 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Scarsdale:1982:ISS

[SSSA82] J. N. Scarsdale, H. L. Sellers, Lothar Schäfer, and Norman L. Allinger. Ab initio studies of structural features not easily amenable to experiment. 22. Structural aspects of a long-chain hydrocarbon (n-nonane) and a study of the transferability of electronic effects through C — C single bonds. *Journal of Computational Chemistry*, 3(2):269–272, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schweig:1980:CHC

[ST80] Armin Schweig and Walter Thiel. The C_4H_4CO potential surface. Reactions involving bicyclo[2.1.0]pentenone. *Journal of Computational Chemistry*, 1(2):129–133, Summer 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shillady:1982:SSA

[ST82] Donald D. Shillady and David B. Talley. Spherically symmetric axial Gaussian lobe $3d$ and $4f$ orbitals. *Journal of Computational Chemistry*, 3(2):130–134, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schwenke:1987:CCR

[ST87] David W. Schwenke and Donald G. Truhlar. Converged calculations of rotational energy transfer in HF HF collisions. *Journal of Computational Chemistry*, 8(4):282–290, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sabio:1989:VTG

[ST89] Michael Sabio and Sid Topiol. 3*s*- versus 1*s*-type Gaussian primitives: Modifications of the 3-21G(*) basis set for the sulfur atom. *Journal of Computational Chemistry*, 10(5):660–672, July 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stewart:1989:OPSa

[Ste89a] James J. P. Stewart. Optimization of parameters for semiempirical methods I. Method. *Journal of Computational Chemistry*, 10(2):209–220, March 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stewart:1989:OPSb

[Ste89b] James J. P. Stewart. Optimization of parameters for semiempirical methods II. Applications. *Journal of Computational Chemistry*, 10(2):221–264, March 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sakai:1981:SPNa

[STH81a] Yoshiko Sakai, Hiroshi Tatewaki, and Sigeru Huzinaga. A systematic preparation of new contracted Gaussian-type orbital sets. V. From Na through Ca. *Journal of Computational Chemistry*, 2(1):100–107, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sakai:1981:SPNb

[STH81b] Yoshiko Sakai, Hiroshi Tatewaki, and Sigeru Huzinaga. A systematic preparation of new contracted Gaussian-type orbital sets. VI. Ab initio calculation on molecules containing Na through Cl. *Journal of Computational Chemistry*, 2(1):108–125, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sakai:1982:SPN

[STH82] Yoshiko Sakai, Hiroshi Tatewaki, and Sigeru Huzinaga. A systematic preparation of new contracted Gaussian-type orbital sets. VIII. MINI-1 and MIDI-1 sets for Ga through Cd. *Journal of Computational Chemistry*, 3(1):6–13, Spring 1982.

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Streitwieser:1985:BRB

[Str85] A. Streitwieser Jr. Book review: *Ab initio molecular orbital calculations for chemists*, by W. G. Richards and D. L. Cooper, 2nd ed., Clarendon, Oxford, 1983. *Journal of Computational Chemistry*, 6(1):76, February 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sprague:1987:MCM

[STYA87] Joseph T. Sprague, Julia C. Tai, Young Yuh, and Norman L. Allinger. The MMP2 calculational method. *Journal of Computational Chemistry*, 8(5):581–603, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stankevitch:1988:CMA

[STZ88] M. I. Stankevitch, S. S. Tratch, and N. S. Zefirov. Combinatorial models and algorithms in chemistry. Search for isomorphisms and automorphisms of molecular graphs. *Journal of Computational Chemistry*, 9(4):303–314, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schafer:1981:ISS

[SVS+81] Lother Schäfer, C. Van Alsenoy, J. N. Scarsdale, V. J. Klimkowski, and J. D. Ewbank. Ab initio studies of structural features not easily amenable to experiment. 18. Conformational analysis and molecular structure of glycine methyl ester. *Journal of Computational Chemistry*, 2(4):410–413, Winter 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Spangler:1983:DCT

[SWM83] Dale Spangler, Ian Henderson Williams, and Gerald M. Maggiora. Determination and characterization of a transition structure for water–formaldehyde addition. *Journal of Computational Chemistry*, 4(4):524–541, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Szoke:1987:OME

[Szö87] J. Szöke. Optimized method for the evaluation of the convolutionally distorted decay curves. *Journal of Computational*

Chemistry, 8(2):95–106, March 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tai:1981:CAS

[Tai81] Julia C. Tai. The conformation of alkyl sulfoxides. *Journal of Computational Chemistry*, 2(2):161–167, Summer 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tatewaki:1985:SPN

[Tat85] Hiroshi Tatewaki. A systematic preparation of new contracted Gaussian-type orbitals. IX [54/5], [64/5], [64/6], [74/6], [74/7] and MAXI-1–MAXI-5 from Li to Ne. *Journal of Computational Chemistry*, 6(3):237–248, June 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Taylor:1984:AME

[Tay84] Peter R. Taylor. Analytical MCSCF energy gradients: Treatment of symmetry and CASSCF applications to propadienone. *Journal of Computational Chemistry*, 5(6):589–597, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Taylor:1987:MC

[Tay87] Keith F. Taylor. On Madelung's constant. *Journal of Computational Chemistry*, 8(4):291–295, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Takada:1983:MSI

[TDK83] Toshikazu Takada, Michel Dupuis, and Harry F. King. Molecular symmetry. IV. The coupled perturbed Hartree–Fock method. *Journal of Computational Chemistry*, 4(2):234–240, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Thomson:1983:ISR

[TG83] Colin Thomson and Christopher Glidewell. An ab initio study of the relative stabilities of the isomers of CH_2N_2 and SiH_2N_2. *Journal of Computational Chemistry*, 4(1):1–8, Spring 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tinker:1986:CSM

[TG86] John F. Tinker and Herbert Gelernter. Computer simulation of metabolic transformation. *Journal of Computational Chemistry*, 7(5):657–665, October 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tatewaki:1980:SPN

[TH80] Hiroshi Tatewaki and Sigeru Huzinaga. A systematic preparation of new contracted Gaussian-type orbital sets. III. Second-row atoms from Li through ne. *Journal of Computational Chemistry*, 1(3):205–228, Autumn 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tseng:1980:AXC

[THW80] T. J. Tseng, S. H. Hong, and M. A. Whitehead. Atomic X_α calculations based on E^{HFS} $(\alpha) = E^{exp}$. *Journal of Computational Chemistry*, 1(1):88–93, Spring 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tinker:1981:CSA

[Tin81] John F. Tinker. A computerized structure–activity correlation program for relating bacterial mutagenesis activity to chemical structure. *Journal of Computational Chemistry*, 2 (3):231–243, Autumn 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Teleman:1986:VGP

[TJ86] Olle Teleman and Bo Jönsson. Vectorizing a general purpose molecular dynamics simulation program. *Journal of Computational Chemistry*, 7(1):58–66, February 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Takeuchi:1989:PPS

[TKI89] Kei Takeuchi, Chiaki Kuroda, and Masaru Ishida. Prolog program for subgraph enumeration and calculation of molecular connectivity indexes. *Journal of Computational Chemistry*, 10(3):380–385, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Theodorakopoulos:1981:MBS

[TKK+81] G. Theodorakopoulos, Á. Kucsman, I. Kapovits, G. Náray-Szabó, and I. G. Csizmadia. Minimal basis study of innershell ionization potentials for molecules containing sulfur: S,S-Diphenyl-N–p-Tolylsulfonyl-Sulfilimine. *Journal of Computational Chemistry*, 2(2):212–217, Summer 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tai:1989:MMM

[TLA89] Julia C. Tai, Jenn-Huei Lii, and Norman L. Allinger. A molecular mechanics (MM2) study of Furan, Thiophene, and related compounds. *Journal of Computational Chemistry*, 10 (5):635–647, July 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tewari:1984:DET

[TM84] R. D. Tewari and P. C. Mishra. A directing effect of n–π^* transitions on electronic charges. *Journal of Computational Chemistry*, 5(3):225–229, June 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Throckmorton:1985:SET

[TM85] Linda Throckmorton and Dennis S. Marynick. Systematic errors in the total energy of molecular wave functions calculated within the PRDDO approximations. *Journal of Computational Chemistry*, 6(6):652–655, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Topiol:1985:CSM

[TMOW85] S. Topiol, G. Mercier, R. Osman, and H. Weinstein. Computational schemes for modeling proton transfer in biological systems: Calculations on the hydrogen bonded complex $[CH_3OH \cdot H \cdot NH_3]^+$. *Journal of Computational Chemistry*, 6 (6):581–586, December 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tonge:1988:DMS

[TMrGM88] Alan P. Tonge, Peter Murray-rust, William A. Gibbons, and Lesley K. McLachlan. Determination of the major solution conformation of tyrocidine A, using molecular mechanics energy minimization and NMR-derived distance and torsion angle constraints. *Journal of Computational Chemistry*, 9(5): 522–538, July 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Topiol:1987:CUM

[Top87] Sid Topiol. Comparison of the use of the MNDO and MINDO/3 methods with ab initio methods to study tautomerism in histamine, 2- and 4-methylhistamine. *Journal of Computational Chemistry*, 8(2):142–148, March 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tosi:1984:QMS

[Tos84] Camillo Tosi. A quantum mechanical study of the equilibrium between 1,4- and 1,6-dialkylcyclooctatetraenes. *Journal of Computational Chemistry*, 5(3):248–251, June 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Trindle:1982:BRB

[Tri82] Carl O. Trindle. Book review: *An introduction to PASCAL for scientists*, James W. Cooper (Wiley-Interscience, New York, 1981). *Journal of Computational Chemistry*, 3(2):273, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Trindle:1984:MAI

[Tri84] Carl Trindle. Microcomputer-aided instruction and research in group theory. *Journal of Computational Chemistry*, 5(2): 162–169, April 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Trindle:1987:AMC

[Tri87] Carl Trindle. Application of the MuMATH computer algebra system to sets of first order kinetic equations of significance in chemistry. *Journal of Computational Chemistry*, 8(4):442–447, June 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Trindle:1988:QMP

[Tri88] Carl Trindle. Quantum mechanics of pseudorotation in ring systems: an application of the MuMATH symbolic algebra system. *Journal of Computational Chemistry*, 9(4):336–342, June 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Titchener:1983:DEA

[TS83] M. R. Titchener and R. M. Stimpfle. Digital emulation of analog computer techniques for the solution of kinetic systems. *Journal of Computational Chemistry*, 4(1):58–67, Spring 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tatewaki:1981:SPNa

[TSH81a] Hiroshi Tatewaki, Yoshiko Sakai, and Sigeru Huzinaga. A systematic preparation of new contracted Gaussian-type orbital sets. IV. The effect of additional $3s$ functions introduced by the use of the six-membered $3d$ GTOs. *Journal of Computational Chemistry*, 2(1):96–99, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tatewaki:1981:SPNb

[TSH81b] Hiroshi Tatewaki, Yoshiko Sakai, and Sigeru Huzinaga. A systematic preparation of new contracted Gaussian-type orbital sets. VII. MINI-3, MINI-4, MIDI-3, and MIDI-4 sets for transition metal atoms. *Journal of Computational Chemistry*, 2(3):278–286, Autumn 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tse-Tsai:1981:SMC

[TTZWGQKC81] Li Tse-Tsai, Shi Zheng-Wen, Zhou Guo-Qiang, and Chou Kuo-Chen. A semianalytic method for computing the concentration distribution in enzyme–substrate fast reaction systems. *Journal of Computational Chemistry*, 2(3):273–277, Autumn 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tseng:1981:SXS

[TW81] T. J. Tseng and M. A. Whitehead. SCF–Xα-SW calculation on the molecule N_2 using theoretical α_{ta}. *Journal of Computational Chemistry*, 2(1):38–40, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tseng:1982:LMO

[TW82] T. J. Tseng and M. A. Whitehead. Localized molecular orbital energies within the CNDO /BW formulation. *Journal of Computational Chemistry*, 3(4):552–555, Winter 1982. CO-

DEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

VanAlsenoy:1988:ICL

[Van88] C. Van Alsenoy. Ab initio calculations on large molecules: the multiplicative integral approximation. *Journal of Computational Chemistry*, 9(6):620–626, September 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Venanzi:1989:MMA

[VCZB89] Carol A. Venanzi, Preston M. Canzius, Zhifeng Zhang, and Jeffrey D. Bunce. A molecular mechanics analysis of molecular recognition by cyclodextrin mimics of α-chymotrypsin. *Journal of Computational Chemistry*, 10(8):1038–1052, December 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vedani:1986:EPF

[VDD86] Angelo Vedani, Max Dobler, and Jack D. Dunitz. An empirical potential function for metal centers: Application to molecular mechanics calculations on metalloproteins. *Journal of Computational Chemistry*, 7(6):701–710, December 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

vandeGraaf:1984:LMM

[vdGB84] B. van de Graaf and J. M. A. Baas. The Lagrange multiplier method for manipulating geometries. Implementation and applications in molecular mechanics. *Journal of Computational Chemistry*, 5(4):314–321, August 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vedani:1988:YIM

[Ved88] Angelo Vedani. YETI: an interactive molecular mechanics program for small-molecule protein complexes. *Journal of Computational Chemistry*, 9(3):269–280, April 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Verwoerd:1982:MCS

[Ver82] W. S. Verwoerd. MNDO calculations of silicon-containing molecules. *Journal of Computational Chemistry*, 3(3):445–

450, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Voets:1989:TSP

[VFM+89] R. Voets, J.-P. François, J. M. L. Martin, J. Mullens, J. Yperman, and L. C. Van Poucke. Theoretical study of the proton affinities of 2-, 3-, and 4-monosubstituted pyridines in the gas phase by means of MINDO/3, MNDO, and AM1. *Journal of Computational Chemistry*, 10(4):449–467, June 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

vanGunsteren:1984:SNC

[vGBC+84] W. F. van Gunsteren, H. J. C. Berendsen, F. Colonna, D. Perahia, J. P. Hollenberg, and D. Lellouch. On searching neighbors in computer simulations of macromolecular systems. *Journal of Computational Chemistry*, 5(3):272–279, June 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

VanGunsteren:1980:MCE

[VK80] W. F. Van Gunsteren and M. Karplus. A method for constrained energy minimization of macromolecules. *Journal of Computational Chemistry*, 1(3):266–274, Autumn 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

VanAlsenoy:1989:GOG

[VLG89] C. Van Alsenoy, A. T. H. Lenstra, and H. J. Geise. The gradient-optimized geometry of haloperidol at the 4-21G level. *Journal of Computational Chemistry*, 10(3):302–308, April 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Viswanadhan:1986:CAS

[VM86] V. N. Viswanadhan and Wayne L. Mattice. Conformational analysis of the sixteen C(4)–C(6) and C(4)–C(8) linked dimers of (+)-catechin and (-)-epicatechin. *Journal of Computational Chemistry*, 7(6):711–717, December 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Viruela-Martin:1986:MSR

[VMNGTVM86] P. M. Viruela-Martín, I. Nebot-Gil, F. Tomás, and R. Viruela-Martín. MINDO/3 study of the rearrangement of 1-methylcyclohexyl cation to 1,2-dimethylcyclopentyl cation. *Journal of Computational Chemistry*, 7(4):417–427, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schleyer:1986:BRA

[vRS86] Paul von Ragué Schleyer. Book review: Archives, bibliographies, and data bases: How to search the ab initio quantum chemistry literature. *Journal of Computational Chemistry*, 7 (3):380–383, June 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schleyer:1986:RSL

[vRSSRH86] Paul von Ragué Schleyer, Andrzej Sawaryn, Alan E. Reed, and Pavel Hobza. The remarkable structure of lithium cyanide/isocyanide. *Journal of Computational Chemistry*, 7 (5):666–672, October 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

VanAlsenoy:1982:ISS

[VSS82] C. Van Alsenoy, J. N. Scarsdale, and Lothar Schäfer. Ab initio studies of structural features not easily amenable to experiment. 17. The molecular structures of some strained cyclic hydrocarbons and estimates of their strain energies. *Journal of Computational Chemistry*, 3(1):53–61, Spring 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Viers:1984:MSR

[VSSS84] Jimmy W. Viers, John C. Schug, Michael D. Stovall, and Jeffrey I. Seeman. MNDO study of reaction pathways for S_N2 reactions. Menschutkin reaction potential energy surfaces. *Journal of Computational Chemistry*, 5(6):598–605, December 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Venkatachalam:1983:TCA

[VU83] C. M. Venkatachalam and D. W. Urry. Theoretical conformational analysis of the Gramicidin a transmembrane channel.

I. Helix sense and energetics of head-to-head dimerization. *Journal of Computational Chemistry*, 4(4):461–469, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Venkatachalam:1984:TAG

[VU84] C. M. Venkatachalam and D. W. Urry. Theoretical analysis of gramicidin A transmembrane channel. II. Energetics of helical librational states of the channel. *Journal of Computational Chemistry*, 5(1):64–71, February 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Venanzi:1988:CSB

[VV88] Thomas J. Venanzi and Carol A. Venanzi. A conformational study of a biologically active conjugated syn-oxime. *Journal of Computational Chemistry*, 9(1):67–74, January 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

VanHemelrijk:1981:AMS

[VVVG81] D. Van Hemelrijk, W. Versichel, C. Van Alsenoy, and H. J. Geise. On the applicability of the MINDO /3 method in studies of molecular structures in the vapor phase. Geometries, conformational energies, and vibrational amplitudes of alkenes and chloroalkanes. *Journal of Computational Chemistry*, 2(1):63–72, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wirth:1980:TCC

[WB80] David Wirth and Nathan L. Bauld. A theoretical comparison of cationic and anionic homoaromaticity: Reinforcement of cationic homoaromaticity by σ-nonclassical effects. *Journal of Computational Chemistry*, 1(2):189–191, Summer 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Watts:1988:PCM

[WD88] John D. Watts and Michel Dupuis. Parallel computation of the Møller–Plesset second-order contribution to the electronic correlation energy. *Journal of Computational Chemistry*, 9(2):158–170, March 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wenzel:1982:CIC

[Wen82] Klaus B. Wenzel. Configuration interaction (CI): Approximate inclusion of fourfold and threefold excitations, an application of knowledge engineering. *Journal of Computational Chemistry*, 3(2):191–207, Summer 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wertz:1982:BRB

[Wer82] David H. Wertz. Book review: *Distance geometry and conformational calculations*, G. M. Crippen. Research Studies Press, Chichester, New York, 1981, 58 pp. *Journal of Computational Chemistry*, 3(4):603, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wako:1987:ARC

[WG87] Hiroshi Wako and Nobuhiro Gō. Algorithm for rapid calculation of Hessian of conformational energy function of proteins by supercomputer. *Journal of Computational Chemistry*, 8 (5):625–635, July 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Williams:1989:GTR

[WG89] Martin L. Williams and Jill E. Gready. Guanidinium-type resonance stabilization and its biological implications. I. the guanidine and extended-guanidine series. *Journal of Computational Chemistry*, 10(1):35–54, January 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wiberg:1984:GEC

[Wib84] Kenneth B. Wiberg. Group equivalents for converting ab initio energies to enthalpies of formation. *Journal of Computational Chemistry*, 5(2):197–199, April 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wiberg:1986:BRB

[Wib86] Kenneth B. Wiberg. Book review: *Ab Initio Molecular Orbital Theory*, by W. J. Hehre, L. Radom, P. v. R. Schleyer, and J. A. Pople, John Wiley, New York, 548pp. Price: $79.95 (1986). *Journal of Computational Chemistry*, 7(3):379, June 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Williams:1988:RME

[Wil88] Donald E. Williams. Representation of the molecular electrostatic potential by atomic multipole and bond dipole models. *Journal of Computational Chemistry*, 9(7):745–763, October 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weiner:1981:AAM

[WK81] Paul K. Weiner and Peter A. Kollman. AMBER: Assisted model building with energy refinement. A general program for modeling molecules and their interactions. *Journal of Computational Chemistry*, 2(3):287–303, Autumn 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weiner:1986:AAF

[WKNC86] Scott J. Weiner, Peter A. Kollman, Dzung T. Nguyen, and David A. Case. An all atom force field for simulations of proteins and nucleic acids. *Journal of Computational Chemistry*, 7(2):230–252, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Whiteside:1980:SEC

[WKP+80] Robert A. Whiteside, Raghavachari Krishnan, John A. Pople, Mary-Beth Krogh-Jespersen, Paul von Ragúe Schleyer, and Gottfried Wenke. Small elemental clusters. I. The structures of Be_2, Be_3, Be_4, and Be_5. *Journal of Computational Chemistry*, 1(4):307–322, Winter 1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wiberg:1987:NIA

[WM87] Kenneth B. Wiberg and Mark A. Murcko. Nonbonded interactions. 1. Anisotropic hydrogen-hydrogen interactions. *Journal of Computational Chemistry*, 8(8):1124–1130, December 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wiberg:1988:BRA

[WM88] Kenneth B. Wiberg and Mark A. Murcko. Barriers to rotation adjacent to double bonds. 4. Effect of basis set on structures, and of electron correlation on relative energies. *Journal* of *Computational Chemistry*, 9(5):488–494, July 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Waldman:1989:AED

[WM89] Marvin Waldman and Brian B. Masek. Analytical energy derivatives and normal modes in force fields employing lone-pair pseudoatoms. *Journal of Computational Chemistry*, 10 (6):856–860, September 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Watowich:1988:SRC

[WMHJ88] Stanley J. Watowich, Eric S. Meyer, Ray Hagstrom, and Robert Josephs. A stable, rapidly converging conjugate gradient method for energy minimization. *Journal of Computational Chemistry*, 9(6):650–661, September 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Warner:1982:SES

[WP82] Philip M. Warner and Stephen Peacock. Strain energies of some bridgehead olefins as calculated with the MM 2 force field. *Journal of Computational Chemistry*, 3(3):417–420, Autumn 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Waite:1983:EBC

[WP83] J. Waite and M. G. Papadopoulos. Extended basis CNDO calculations of linear and nonlinear electric susceptibilities of some molecular dianions and carbonions using coupled Hartree–Fock perturbation theory. *Journal of Computational Chemistry*, 4(4):578–584, Winter 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wright:1988:ISG

[WSP88] Gregory M. Wright, Richard J. Simmonds, and David E. Parry. Ab initio studies of the ground-state potential energy surface of formamide. *Journal of Computational Chemistry*, 9(6):600–603, September 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wiberg:1981:ENC

[WW81] Kenneth B. Wiberg and John J. Wendoloski. The electrical nature of C — H bonds and its relationship to infrared intensities. *Journal of Computational Chemistry*, 2(1):53–57, Spring 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xie:1986:CFC

[XB86] Yaoming Xie and James E. Boggs. The computed force constants and vibrational spectra of toluene. *Journal of Computational Chemistry*, 7(2):158–164, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yip:1989:CLN

[YE89] Virginia Yip and Ron Elber. Calculations of a list of neighbors in Molecular Dynamics simulations. *Journal of Computational Chemistry*, 10(7):921–927, October 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yeh:1986:SRC

[YF86] You-Hsing Yeh and William H. Fink. A strategy for the regional characterization of potential energy surfaces. *Journal of Computational Chemistry*, 7(4):539–546, August 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yoon:1986:CST

[YJ86] Chang No Yoon and Mu Shik Jhon. Conformational study of the trinucleotide CpGpCp-pentapeptide Gly_5 complex: the important role of bridging water in the complex formation. *Journal of Computational Chemistry*, 7(2):189–200, April 1986. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yamamoto:1988:DPM

[YNAK88] Shigeyoshi Yamamoto, Umpei Nagashima, Tomoo Aoyama, and Hiroshi Kashiwagi. Development of a program for MCSCF calculations with large basis sets. *Journal of Computational Chemistry*, 9(6):627–635, September 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zuccarello:1980:SCS

[ZBR80] Felice Zuccarello, Giuseppe Buemi, and Antonio Raudino. Spectroscopic CNDO /CI study of some cyclic polyenes. *Journal of Computational Chemistry*, 1(4):341–347, Winter

1980. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zuccarello:1987:TVO

[ZD87] Felice Zuccarello and Giuseppe Del Re. Towards a valence-orbital/bond-orbital description of biochemical H-bonds from ab initio calculations. *Journal of Computational Chemistry*, 8(6):816–825, September 1987. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zielinski:1983:UHT

[Zie83] Theresa Julia Zielinski. Uracil–4-hydroxyuracil tautomerism revisited. *Journal of Computational Chemistry*, 4(3):345–349, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zauhar:1988:RCM

[ZM88] R. J. Zauhar and R. S. Morgan. The rigorous computation of the molecular electric potential. *Journal of Computational Chemistry*, 9(2):171–187, March 1988. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zielinski:1984:EFF

[ZP84] Theresa Julia Zielinski and Raymond Alcide Poirier. Examination of formamide, formamidic acid, amidine dimers, and the double proton transfer transition states involving these dimers. *Journal of Computational Chemistry*, 5(5):466–470, October 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zakrzewska:1985:OME

[ZP85] Krystyna Zakrzewska and Alberte Pullman. Optimized monopole expansions for the representation of the electrostatic properties of polypeptides and proteins. *Journal of Computational Chemistry*, 6(4):265–273, August 1985. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhou:1989:CSA

[ZP89] Xue-Feng Zhou and Peter Pulay. Characters for symmetric and antisymmetric higher powers of representations: Application to the number of anharmonic force constants in symmetrical molecules. *Journal of Computational Chemistry*, 10

(7):935–938, October 1989. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zielinski:1982:ISC

[ZPCR82] Theresa Julia Zielinski, Michael R. Peterson, Imre G. Csizmadia, and Robert Rein. An ab initio study on the conformations of protonated, neutral, and deprotonated amidine. *Journal of Computational Chemistry*, 3(1):62–68, Spring 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zielinski:1982:CSP

[ZPPC82] Theresa Julia Zielinski, Raymond Alcide Poirier, Michael Roy Peterson, and Imre G. Csizmadia. Conformational study of protonated, neutral, and deprotonated formamide. *Journal of Computational Chemistry*, 3(4):477–485, Winter 1982. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zielinski:1983:WMT

[ZPPC83] Theresa Julia Zielinski, Raymond Alcide Poirier, Michael Roy Peterson, and Imre G. Csizmadia. A water-mediated tautomerism mechanism in formamide and amidine. An ab initio study. *Journal of Computational Chemistry*, 4(3):419–427, Autumn 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zaera:1981:MCS

[ZR81] F. Zaera and Isak Rusinek. Monte Carlo simulation for inhomogeneous chemical kinetics: Application to the Belousov–Zhabotinskii reaction. *Journal of Computational Chemistry*, 2(4):402–409, Winter 1981. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zeiss:1983:CRN

[ZW83a] G. D. Zeiss and M. A. Whitehead. Comparison of RHF, NDDO, and MOM molecular one-electron expectation values calculated using weighted and unweighted STO–NG(ω) basis functions. *Journal of Computational Chemistry*, 4(1):48–52, Spring 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zeiss:1983:SDR

[ZW83b] G. D. Zeiss and M. A. Whitehead. Standard deviation in reduced errors (SDRE): a criterion to assess the relative overall quality of approximate wavefunctions. *Journal of Computational Chemistry*, 4(2):150–153, Summer 1983. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zeiss:1984:CRN

[ZW84] G. D. Zeiss and M. A. Whitehead. Comparison of the RHF, NDDO, and MOM molecular one-electron expectation values calculated using minimum basis sets with Slater, Burns, Clementi, and BLMO exponents. *Journal of Computational Chemistry*, 5(2):207–215, April 1984. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).