

Contents

Thom H. Dunning, Jr.: Contributions to chemical theory and computing.....	1
Angela K. Wilson, Kirk A. Peterson, David E. Woon	
The nature of the SO bond of chlorinated sulfur–oxygen compounds.....	5
Beth A. Lindquist, Thom H. Dunning Jr.	
Correlation consistent, Douglas–Kroll–Hess relativistic basis sets for the 5<i>p</i> and 6<i>p</i> elements.....	19
David H. Bross, Kirk A. Peterson	
Improved accuracy benchmarks of small molecules using correlation consistent basis sets.....	31
David Feller, Kirk A. Peterson, Branko Ruscic	
Accurate ab initio potential energy curves and spectroscopic properties of the four lowest singlet states of C₂	47
Jeffery S. Boschen, Daniel Theis, Klaus Ruedenberg, Theresa L. Windus	
Comparative bonding analysis of N₂ and P₂ versus tetrahedral N₄ and P₄	59
P. Jerabek, G. Frenking	
Accurate first principles calculations on chlorine fluoride ClF and its ions ClF[±].....	69
Athanasios A. Vassilakis, Apostolos Kalemos, Aristides Mavridis	
Negative electron affinities from conventional electronic structure methods	85
Kenneth D. Jordan, Vamsee K. Voora, Jack Simons	
The <i>V</i> state of ethylene: valence bond theory takes up the challenge.....	101
Wei Wu, Huaiyu Zhang, Benoît Braïda, Sason Shaik, Philippe C. Hiberty	
Comparison of multireference configuration interaction potential energy surfaces for H + O₂ → HO₂: the effect of internal contraction	115
Lawrence B. Harding, Stephen J. Klippenstein, Hans Lischka, Ron Shepard	
Modern valence-bond description of aromatic annulene ions.....	123
Peter B. Karadakov, David L. Cooper	
Bonding in PF₂Cl, PF₃Cl, and PF₄Cl: insight into isomerism and apicophilicity from ab initio calculations and the recoupled pair bonding model	131
Jeff Leiding, David E. Woon, Thom H. Dunning Jr.	
MULTIMODE calculations of the infrared spectra of H₇⁺ and D₇⁺ using ab initio potential energy and dipole moment surfaces.....	141
Chen Qu, Rita Prossmiti, Joel M. Bowman	
Properties of local vibrational modes: the infrared intensity	149
Wenli Zou, Dieter Cremer	
The infrared spectra of C₉₆H₂₅ compared with that of C₉₆H₂₄	165
Charles W. Bauschlicher Jr., Alessandra Ricca	

The mechanism of the cycloaddition reaction of 1,3-dipole molecules with acetylene: an investigation with the unified reaction valley approach	173
Marek Freindorf, Thomas Sexton, Elfi Kraka, Dieter Cremer	
Active Thermochemical Tables: dissociation energies of several homonuclear first-row diatomics and related thermochemical values	191
Branko Ruscic, David Feller, Kirk A. Peterson	
Transition metal atomic multiplet states through the lens of single-reference coupled-cluster and the equation-of-motion coupled-cluster methods.....	203
Varun Rishi, Ajith Perera, Rodney Bartlett	
Molecular orbital interpretation of the metal–metal multiple bonding in coaxial dibenzene dimetal compounds of iron, manganese, and chromium	213
Hui Wang, Dong Die, Hongyan Wang, Yaoming Xie, R. Bruce King, Henry F. Schaefer III	
All electron ab initio calculations on the ScTi molecule: a really hard nut to crack.....	223
Apostolos Kalamos, Aristides Mavridis	
Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods	233
Manoj K. Kesharwani, Jan M. L. Martin	
Simulating Cl K-edge X-ray absorption spectroscopy in MCl_6^{2-} ($M = U, Np, Pu$) complexes and $UOCl_5^-$ using time-dependent density functional theory	247
Niranjan Govind, Wibe A. de Jong	
Accurate atomization energies from combining coupled-cluster computations with interference-corrected explicitly correlated second-order perturbation theory	255
Konstantinos D. Vogiatzis, Robin Haunschild, Wim Klopper	
On the mutual exclusion of variationality and size consistency	267
So Hirata, Ireneusz Grabowski	
Accurate quadruple-ζ basis-set approximation for double-hybrid density functional theory with an order of magnitude reduction in computational cost.....	277
Bun Chan, Leo Radom	
A perspective on the localizability of Hartree–Fock orbitals	287
Ida-Marie Høyvik, Kasper Kristensen, Thomas Kjærgaard, Poul Jørgensen	
Computing optical rotation via an N-body approach	297
Taylor J. Mach, T. Daniel Crawford	
Quantitative estimation of uncertainties from wavefunction diagnostics	307
Matthew K. Sprague, Karl K. Irikura	
What makes differences between intra- and inter-molecular charge transfer excitations in conjugated long-chained polyene? EOM-CCSD and LC-BOP study.....	319
Jong-Won Song, Kimihiko Hirao	
Unimolecular and hydrolysis channels for the detachment of water from microsolvated alkaline earth dication (Mg^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}) clusters.....	329
Evangelos Miliordos, Sotiris S. Xantheas	

Stacking of the mutagenic DNA base analog 5-bromouracil.....	341
Leo F. Holroyd, Tanja van Mourik	
Quantum Monte Carlo investigation of the H-shift and O₂-loss channels of <i>cis</i>-2-butene-1-peroxy radical.....	355
Zhiping Wang, Dmitry Yu Zubarev, William A. Lester Jr.	