Theor Chem Acc (2012) 131:1074
DOI 10.1007/s00214-011-1074-x

EDITORIAL

Fifty years of TCA

Christopher J. Cramer

Published online: 13 January 2012

Most of us probably do not remember the appearance of Volume 1, Number 1 of *Theoretica Chimica Acta* (TCA); it was in 1962. The present editorial board members were all very young at that time, if they had even yet been born. TCA was the first journal devoted *exclusively* to theoretical chemistry. Since then many other theoretical chemistry journals have debuted, including *Int. J. Quantum Chem.*, *J. Comput. Chem.*, *Computational and Theoretical Chemistry* (formerly *Theochem*), and *J. Chem. Theory Comput.* Meanwhile, in 1996, TCA changed its name from the Latin *Theoretica Chimica Acta* to the English *Theoretical Chemistry Accounts*.

The golden jubilee of the first theoretical chemistry journal provides an occasion both to look back and to look forward. When TCA was inaugurated, quantum mechanics was 37 years old. Now, it is 87 years old. When TCA was inaugurated, *J. Chem. Phys.* was 29 years old, *Phys. Rev.* as a journal of the American Physical Society was 49 years old, and *J. Phys. Chem.* was 66 years old. In the most recent impact factors (those for 2010), *J. Chem. Phys.*, TCA, and *Phys. Rev. A* all have impact factors of 2.9, and *J. Phys. Chem. A* has an impact factor of 2.7. Of the 49 Nobel Prizes in chemistry since 1962 (the 2011 Prize has not been announced at the time we are putting this to press), theoretical chemists have shared or won six: Lars Onsager, William Lipscomb, Ilya Progogine, Kenichi Fukui and Roald Hoffman (shared), Rudy Marcus, and Walter Kohn and John Pople (shared). We feel safe predicting that theoretical chemists will take home more than six of the next 49.

Let's look back in two ways. First, we wish to thank all those who have contributed to TCA through editorial service or editorial advisory service. Second, we wish to single out the most highly cited papers in the history of TCA. Then, we will look forward by means of the rest of this special issue.

1 Editorial service

Here is a list of those who have provided editorial service to TCA and the capacities in which they served. On behalf of the entire theoretical chemistry community, we thank them for their service.

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Published as part of the special collection of articles celebrating the 50th anniversary of Theoretical Chemistry Accounts/Theoretica Chimica Acta.

C. J. Cramer (✉)
Department of Chemistry, University of Minnesota,
207 Pleasant Street SE, Minneapolis, MN 55455-0431, USA
e-mail: cramer@umn.edu

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Yarkony, David R.
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Zeng, Xiao Cheng
Zerner, Michael C.
Zhan, Chang-Guo
Zhang, John Z. H.

2 Highly cited papers

For each decade, the list contains the twelve most highly cited papers from that decade, as of the preparation of this editorial, with the most highly cited first. The lists contain many important contributors and many important contributions, and it is interesting to notice the evolution of topics represented therein. A key topic that has persisted on the lists for the full 50 years is basis sets, which have always been featured prominently in *TCA*.

2.1 First decade: 1962–1971 (Theoretica Chimica Acta)

- Some remarks on the Pariser-Parr-Pople method. Ohno, K. 1964. *Theoretica Chimica Acta* 2, pp. 219–227
- Possible "ferromagnetic states" of some hypothetical hydrocarbons. Mataga, N. *Theoretica Chimica Acta* 10 (4), pp. 372–376
- Recherches sur la géométrie de quelques hydrocarbures non-alternants: son influence sur les énergies de transition, une nouvelle définition de l'aromaticité. Julg, A., François, P. 1967 *Theoretica Chimica Acta* 8 (3), pp. 249–259
- Porphyrins XIV. Theory for the luminescent state in VO, Co, Cu complexes. Ake, R.L., Gouterman, M. 1969 *Theoretica Chimica Acta* 15 (1), pp. 20–42 60
- Gaussian basis set for molecular wavefunctions containing second-row atoms. Veillard, A. 1968 *Theoretica Chimica Acta* 12 (5), pp. 405–411

- SCFMO calculations of heteroatomic systems with the variable β approximation—I. Heteroatomic molecules containing nitrogen or oxygen atoms. Nishimoto, K., Forster, L.S. 1966 *Theoretica Chimica Acta* 4 (2), pp. 155–165
- Porphyrins—VIII. Extended Hückel calculations on iron complexes. Zerner, M., Gouterman, M., Kobayashi, H. 1966 *Theoretica Chimica Acta* 6 (5), pp. 363–400
- Porphyrins—IV. Extended Hückel calculations on transition metal complexes. Zerner, M., Gouterman, M. 1966 *Theoretica Chimica Acta* 4 (1), pp. 44–63
- Valence orbital ionization potentials from atomic spectral data. Basch, H., Viste, A., Gray, H.B. 1965 *Theoretica Chimica Acta* 3 (5), pp. 458–464
- Energy partitioning with the CNDO method. Fischer, H., Kollmar, H. 1970 *Theoretica Chimica Acta* 16 (3), pp. 163–174
- The continuation of the periodic table up to $Z = 172$. The chemistry of superheavy elements. Fricke, B., Greiner, W., Waber, J.T. 1971 *Theoretica Chimica Acta* 21 (3), pp. 235–260
- Electronic wave functions for atoms—II. Some aspects of the convergence of the configuration interaction expansion for the ground states of the He isoelectronic series. Bunge, C.F. 1970 *Theoretica Chimica Acta* 16 (2), pp. 126–144.

2.2 Second decade: 1972–1981 (Theoretica Chimica Acta)

- The influence of polarization functions on molecular orbital hydrogenation energies. Hariharan, P.C., Pople, J.A. 1973 *Theoretica Chimica Acta* 28 (3), pp. 213–222
- An intermediate neglect of differential overlap technique for spectroscopy: Pyrrole and the azines. Ridley, J., Zerner, M. 1973 *Theoretica Chimica Acta* 32 (2), pp. 111–134 1171
- Bonded-atom fragments for describing molecular charge densities. Hirshfeld, F.L. 1977 *Theoretica Chimica Acta* 44 (2), pp. 129–138
- On the calculation of bonding energies by the Hartree–Fock Slater method—I. The transition state method. Ziegler, T., Rauk, A. 1977 *Theoretica Chimica Acta* 46 (1), pp. 1–10
- Individualized configuration selection in CI calculations with subsequent energy extrapolation. Buenker, R.J., Peyerimhoff, S.D. 1974 *Theoretica Chimica Acta* 35 (1), pp. 33–58
- An intermediate neglect of differential overlap theory for transition metal complexes: Fe, Co and Cu chlorides. Bacon, A.D., Zerner, M.C. 1979 *Theoretica Chimica Acta* 53 (1), pp. 21–54
- Triplet states via intermediate neglect of differential overlap: Benzene, pyridine and the diazines. Ridley, J.E., Zerner, M.C. 1976 *Theoretica Chimica Acta* 42 (3), pp. 223–236
- On the calculation of multiplet energies by the Hartree–Fock-Slater method. Ziegler, T., Rauk, A., Baerends, E.J. 1977 *Theoretica Chimica Acta* 43 (3), pp. 261–271
- Energy extrapolation in CI calculations. Buenker, R.J., Peyerimhoff, S.D. 1975 *Theoretica Chimica Acta* 39 (3), pp. 217–228
- A theoretical method to determine atomic pseudopotentials for electronic structure calculations of molecules and solids. Durand, P., Barthelat, J.-C. 1975 *Theoretica Chimica Acta* 38 (4), pp. 283–302
- Approximate calculation of the correlation energy for the closed shells. Colle, R., Salvetti, O. 1975 *Theoretica Chimica Acta* 37 (4), pp. 329–334
- Multiplicity of the ground state of large alternant organic molecules with conjugated bonds—(Do Organic Ferromagnetics Exist?). Ovchinnikov, A.A. 1978 *Theoretica Chimica Acta* 47 (4), pp. 297–304.

2.3 Third decade: 1982–1991 (Theoretica Chimica Acta)

- Energy-adjusted ab initio pseudopotentials for the second and third row transition elements. Andrae, D., Häußermann, U., Dolg, M., Stoll, H., Preuß, H. 1990 *Theoretica Chimica Acta* 77 (2), pp. 123–141
- Density matrix averaged atomic natural orbital (ANO) basis sets for correlated molecular wave functions—I. First row atoms. Widmark, P.-O., Malmqvist, P.-Å., Roos, B.O. 1990 *Theoretica Chimica Acta* 77 (5), pp. 291–306
- Medium-size polarized basis sets for high-level-correlated calculations of molecular electric properties—II. Second-row atoms: Si through Cl, Sadlej, A.J. 1991 *Theoretica Chimica Acta* 79 (2), pp. 123–140
- Energy-adjusted pseudopotentials for the rare earth elements. Dolg, M., Stoll, H., Savin, A., Preuss, H. 1989 *Theoretica Chimica Acta* 75 (3), pp. 173–194
- Density matrix averaged atomic natural orbital (ANO) basis sets for correlated molecular wave functions—II. Second row atoms. Widmark, P.-O., Persson, B.J., Roos, B.O. 1991 *Theoretica Chimica Acta* 79 (6), pp. 419–432
- r_{12}-Dependent terms in the wave function as closed sums of partial wave amplitudes for large l. Kutzelnigg, W. 1985 *Theoretica Chimica Acta* 68 (6), pp. 445–469
- Orbital-invariant formulation and second-order gradient evaluation in Møller-Plesset perturbation theory. Pulay, P., Saebø, S. 1986 *Theoretica Chimica Acta* 69 (5–6), pp. 357–368

- A generalized restricted open-shell Fock operator. Edwards, W.D., Zerner, M.C. 1987 *Theoretica Chimica Acta* 72 (5–6), pp. 347–361
- Theoretical investigations of molecules composed only of fluorine, oxygen and nitrogen: determination of the equilibrium structures of FOOF, (NO)2 and FNNF and the transition state structure for FNNF cis–trans isomerization. Lee, T.J., Rice, J.E., Scuseria, G.E., Schaefer III, H.F. 1989 *Theoretica Chimica Acta* 75 (2), pp. 81–98
- An overview of coupled cluster theory and its applications in physics. Bishop, R.F. 1991 *Theoretica Chimica Acta* 80 (2–3), pp. 95–148
- Recursive intermediate factorization and complete computational linearization of the coupled-cluster single, double, triple, and quadruple excitation equations. Kucharski, S.A., Bartlett, R.J. 1991 *Theoretica Chimica Acta* 80 (4–5), pp. 387–405
- A comparison of variational and non-variational internally contracted multiconfiguration-reference configuration interaction calculations. Werner, H.-J., Knowles, P.J. 1990 *Theoretica Chimica Acta* 78 (3), pp. 175–187.

2.4 Fourth decade: 1992–2001 (Theoretica Chimica Acta and Theoretical Chemistry Accounts)

- Towards an order-*N* DFT method. Fonseca Guerra, C., Snijders, J.G., Te Velde, G., Baerends, E.J. 1998 *Theoretical Chemistry Accounts* 99 (6), pp. 391–403 1524
- Auxiliary basis sets for main row atoms and transition metals and their use to approximate Coulomb potentials. Eichkorn, K., Weigend, F., Treutler, O., Ahlrichs, R. 1997 *Theoretical Chemistry Accounts* 97 (1–4), pp. 119–124
- RI-MP2: First derivatives and global consistency. Weigend, F., Häser, M. 1997 *Theoretical Chemistry Accounts* 97 (1–4), pp. 331-340
- An efficient data compression method for the Davidson subspace diagonalization scheme Dachsel, H., Lischka, H. 1995 *Theoretica Chimica Acta* 92 (6), pp. 339–349
- An implementation of the conductor-like screening model of solvation within the Amsterdam density functional package. Pye, C.C., Ziegler, T. 1999 *Theoretical Chemistry Accounts* 101 (6), pp. 396–408
- Reparameterization of hybrid functionals based on energy differences of states of different multiplicity. Reiher, M., Salomon, O., Hess, B.A. 2001 Theoretical Chemistry Accounts 107 (1), pp. 48–55
- A combination of quasirelativistic pseudopotential and ligand field calculations for lanthanoid compounds. Dolg, M., Stoll, H., Preuss, H. 1993 Theoretica Chimica Acta 85 (6), pp. 441–450
- Density matrix averaged atomic natural orbital (ANO) basis sets for correlated molecular wave functions—III. First row transition metal atoms. Pou-Amérigo, R., Merchán, M., Nebot-Gil, I., Widmark, P.-O., Roos, B.O. 1995 Theoretica Chimica Acta 92 (3), pp. 149–181
- The singlet and triplet states of phenyl cation. A hybrid approach for locating minimum energy crossing points between non-interacting potential energy surfaces. Harvey, J.N., Aschi, M., Schwarz, H., Koch, W. 1998 Theoretical Chemistry Accounts 99 (2), pp. 95–99
- Internally contracted multiconfiguration-reference configuration interaction calculations for excited states. Knowles, P.J., Werner, H.-J. 1992 *Theoretica Chimica Acta* 84 (1–2), pp. 95–103
- Extensions and tests of "multimode": A code to obtain accurate vibration/rotation energies of many-mode molecules. Carter, S., Bowman, J.M., Handy, N.C. 1998 *Theoretical Chemistry Accounts* 100 (1–4), pp. 191–198
- The MIDI! basis set for quantum mechanical calculations of molecular geometries and partial charges. Easton, R.E., Giesen, D.J., Welch, A., Cramer, C.J., Truhlar, D.G. 1996 *Theoretical Chemistry Accounts* 93 (5), pp. 281–301.

2.5 Fifth decade: 2002–2011 (Theoretical Chemistry Accounts)

- The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: Two new functionals and systematic testing of four M06-class functionals and 12 other functionals. Zhao, Y., Truhlar, D.G. 2008 *Theoretical Chemistry Accounts* 120 (1–3), pp. 215–241
- Systematically convergent basis sets for transition metals. II. Pseudopotential-based correlation consistent basis sets for the group 11 (Cu, Ag, Au) and 12 (Zn, Cd, Hg) elements. Peterson, K.A., Puzzarini, C. 2005 *Theoretical Chemistry Accounts* 114 (4–5), pp. 283–296
- Quantum molecular dynamics: Propagating wavepackets and density operators using the multiconfiguration time-dependent Hartree method. Meyer, H.-D., Worth, G.A. 2003 *Theoretical Chemistry Accounts* 109 (5), pp. 251–267 188
- QM/MM: What have we learned, where are we, and where do we go from here? Lin, H., Truhlar, D.G. 2007 *Theoretical Chemistry Accounts* 117 (2), pp. 185–199
- Ab initio calculation of molecular chiroptical properties. Crawford, T.D. 2006 *Theoretical Chemistry Accounts* 115 (4), pp. 227–245

- Molecular potential-energy surfaces for chemical reaction dynamics. Collins, M.A. 2002 *Theoretical Chemistry Accounts* 108 (6), pp. 313–324
- Method of moments of coupled-cluster equations: A new formalism for designing accurate electronic structure methods for ground and excited states. Piecuch, P., Kowalski, K., Pimienta, I.S.O., Fan, P.-D., Lodriguito, M., McGuire, M.J., Kucharski, S.A., Kus, T., Musiał, M. 2004 *Theoretical Chemistry Accounts* 112 (5–6), pp. 349–393
- Investigation of the S0 → S1 excitation in bacteriorhodopsin with the ONIOM(MO:MM) hybrid method. Vreven, T., Morokuma, K. 2003 *Theoretical Chemistry Accounts* 109 (3), pp. 125–132
- Electron localization function for transition-metal compounds. Kohout, M., Wagner, F.R., Grin, Y. 2002 *Theoretical Chemistry Accounts* 108 (3), pp. 150–156
- Improper, blue-shifting hydrogen bond. Hobza, P., Havlas, Z. 2002 *Theoretical Chemistry Accounts* 108 (6), pp. 325–334
- The fundamental nature and role of the electrostatic potential in atoms and molecules. Politzer, P., Murray, J.S. 2002 *Theoretical Chemistry Accounts* 108 (3), pp. 134–142
- Similarities and differences in the structure of 3d-metal monocarbides and monoxides. Gutsev, G.L., Andrews, L., Bauschlicher Jr., C.W. 2003 *Theoretical Chemistry Accounts* 109 (6), pp. 298–308.

3 A glimpse of the future: the 50th anniversary issue

Each of our five guest editors has selected an important or emerging area of theoretical chemistry and has recruited experts to write about some key issues in that area. The five areas featured and their coordinators are:

- Electronic structure: present and future challenges (So Hirata)
- Relativistic quantum chemistry (Christoph van Wüllen)
- Reaction dynamics in gas phase and in solution (Hua Guo)
- Macromolecules and extended systems (Gino DiLabio)
- Spectroscopy, atmospheric chemistry, and thermochemistry (Fernando Ornellas)

We believe that the subjects of these featured articles encompass several areas that will be growing in importance over the next many years. We hope that you enjoy reading these contributions.