**Donald G. Truhlar**

***Distributed computer programs***

updated Dec. 28, 2011

***Abbreviations for distributors and distribution sites:***

| | |
|---|---|
| comp.chem.umn | Truhlar group Web site<br>http://comp.chem.umn.edu |
| CCP6 | Collaborative Computational Project No. 6 on Heavy Particle Dynamics, Daresbury Laboratory, Warrington, U.K. |
| CPC | Computer Physics Communications Program Library, Department of Applied Mathematics and Theoretical Physics, Queen's University, Belfast, Northern Ireland.<br>http://cpc.cs.qub.ac.uk |
| EMSL | Environmental Molecular Sciences Laboratory,<br>Pacific Northwest Laboratory, Richland, Washington<br>http://www.emsl.pnl.gov/docs/nwchem/ |
| Makolab | Makolab, Lodz, Poland<br>http://www.makolab.com/amsol/ |
| METECC | Methods and Techniques in Computational Chemistry project, 1993-present, Club Européen MOTECC, Namur, Belgium and CRS4, Cagliari, Italy (financed by the Commission of the European Communities). |
| MOTECC | Modern Techniques in Computational Chemistry project, 1989-91, IBM Corporation, Kingston, New York. |
| NRCC | National Resource for Computation in Chemistry, Lawrence Berkeley Laboratory, Berkeley, California. After NRCC closed the programs were transferred to the National Energy Software Center, Argonne National Laboratory, Argonne, Illinois and to QCPE. |
| OMG | Oxford Molecular Group, Beaverton, OR |
| QCPE | Quantum Chemistry Program Exchange, Chemistry Department, Indiana University, Bloomington, Indiana<br>http://qcpe.chem.indiana.edu/ |
| Semichem | Semichem, Inc., Kansas City, MO |
| www.sdsc | San Diego Supercomputer Center<br>http://www.sdsc.edu/Software/chemistry.html |

***Programs:***

*Many of the programs have multiple versions; only the first released version, versions with published documentation, versions with new or notable distribtuion arrangments, new catalog entries, or new author lists, and the most recent version are listed. In general, a more complete version history is in the manual of the given program. The first mention of a given program is bold.*

1. "**FDBVM**: Numerical Eigenvalues and Matrix Elements for the Quantum Mechanical Radial Equation," D. G. Truhlar, QCPE program no. 203. See QCPE Catalog, Vol. X (1974), p. 72.

   This program is described in "Finite Difference Boundary Value Method for Solving One-Dimensional Eigenvalue Equations," D. G. Truhlar, Journal of Computational Physics 10, 123-132 (1972).

2. "**NETI**," R. L. Smith and D. G. Truhlar, CPC Program Library catalogue no. AAGP, Aug. 1972.

   "**NETIX**," R. L. Smith and D. G. Truhlar, CPC Program Library catalogue no. AAGT, Aug. 1972.

   NETI and NETIX are described in "Program for Evaluation of Non-Exchange Type Integrals Required in Electron-Atom Scattering Theory Using Slater-Type Orbitals As Basis Functions," R. L. Smith and D. G. Truhlar, *Computer Physics Communications* **5**, 80-87 (1973). Erratum: **8**, 333-336 (1974).

   "NETI/ETI," J. Abdallah, Jr. and D. G. Truhlar, CPC Program Library catalogue no. AAGP 0001, Jan. 1975.

   NETI/NETIX is described in "Continuum Exchange Integrals for Algebraic Variational Calculations of Electron-Atom Scattering Using Slater-Type Orbitals as Basis Functions," J. Abdallah, Jr. and D. G. Truhlar, *Computer Physics Communications* **9**, 327-336 (1975).

3. "**DCS**," M. A. Brandt, D. G. Truhlar, and R. L. Smith, CPC Program Library catalogue no. ACRL, Oct. 1972.

   This program is described in "Program for Calculating Differential and Integral Cross Sections for Quantum Mechanical Scattering Problems from Reactance or Transition Matrices," M. A. Brandt, D. G. Truhlar, and R. L. Smith, *Computer Physics Communications* **5**, 456-477 (1973). Erratum and addendum: **7**, 177 (1974).

   "ACRL Adapted for IBM 360 or 370," M. A. Brandt, D. G. Truhlar, and R. L. Smith, CPC Program Library catalogue no. ACRL adaptation 0001, Jan. 1974.

   This program is described in "Program ACRL to Calculate Differential and Integral Cross Sections Adapted to Run on IBM Computers," M. A. Brandt, D. G. Truhlar, and R. L. Smith, *Computer Physics Communications* **7**, 172-173 (1974).

"**DCS2**," K. Onda, D. G. Truhlar, and M. A. Brandt,

distributed as: CPC Program Library catalogue no. AAJE;
and as: program 17 of the CCP6 program library.

DCS2 calculates differential and integral cross sections from T matrices. This program is described in "New Version of Program for Calculating Differential and Integral Cross Sections for Quantum Mechanical Scattering Problems from Reactance and Transition Matrices," K. Onda, D. G. Truhlar, and M. A. Brandt, *Computer Physics Communications* **21**, 97-108 (1980).

4. "**KAPPAS**," B. C. Garrett and D. G. Truhlar, NRCC Software Catalog, Vol. 1 (1980), p. 23, program KS01.

   This program is described in "Semiclassical Tunneling Calculations," B. C. Garrett and D. G. Truhlar, *Journal of Physical Chemistry* **83**, 2921-2926 (1979).

5. "**MNN**: Minnesota Numerov," M. A. Brandt, D. G. Truhlar, K. Onda, and D. Thirumalai, NRCC, Software Catalog, Vol. 1 (1980), p. 22, program KQ12.

   This program is described in "Applications of Close Coupling Algorithms to Electron-Atom, Electron-Molecule, and Atom-Molecule Scattering," D. G. Truhlar, N. M. Harvey, K. Onda, and M. A. Brandt, in *Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory,* Vol. 1, edited by L. Thomas (National Resource for Computation in Chemistry, Lawrence Berkeley Laboratory, Berkeley, California, 1979), pp. 220-289.

6. "**MORSEX**: Matrix Elements in a Basis of Morse-Oscillator Eigenfunctions," K. Onda and D. G. Truhlar, QCPE program no. 399.

   This program was announced in QCPE Newsletter **70**, 36 (1980). It is described in "Numerical Evaluation of Matrix Elements over Eigenfunctions of One-Dimensional Vibrational Problems," D. G. Truhlar and K. Onda, Phys. Rev. A **23**, 973-974 (1981) and in "A New Algorithm for Vibrational Matrix Elements," D. W. Schwenke and D. G. Truhlar, Quantum Chemistry Program Exchange Bulletin **4**, 100-101 (1984).

7. "**VTST**," B. C. Garrett and D. G. Truhlar, CCP6 Program Library, program 37, 1984.

   This program is version 5 of the program that later became ABCRATE. It performs variational transition state theory calculations of rate constants for three-atom reactions.

"**ABCRATE**-version 10.0," B. C. Garrett, G. C. Lynch, T. C. Allison, and Donald G. Truhlar, Oct. 1997.

distributed as: CPC Program Library program no. ADHL;
and at: comp.chem.umn.

The program is described in "ABCRATE: A Program for the Calculation of Atom-Diatom Reaction Rates," B. C. Garrett, G. C. Lynch, T. C. Allison, and D. G. Truhlar, Computer Physics Communications **109**, 47-54 (1998).

8. "**POLYRATE** (Version 1.1)," A. D. Isaacson, D. G. Truhlar, S. N. Rai, R. Steckler, G. C. Hancock, B. C. Garrett, and M. J. Redmon, CPC Program Library catalogue no. ABBD, Aug. 1987.

   This program is described in "POLYRATE: A General Computer Program for Variational Transition State Theory and Semiclassical Tunneling Calculations of Chemical Reaction Rates," A. D. Isaacson, D. G. Truhlar, S. N. Rai, R. Steckler, G. C. Hancock, B. C. Garrett, and M. J. Redmon, Computer Physics Communications **47**, 91-102 (1987). All versions of POLYRATE are also described in a manual.

   "POLYRATE—version 2.5," D.-h. Lu, T. N. Truong, B. C. Garrett, R. Steckler, A. D. Isaacson, S. N. Rai, G. C. Hancock, J. G. Lauderdale, T. Joseph, V. S. Melissas, and D. G. Truhlar, QCPE program 601, Dec. 1990.

   This version was announced in QCPE Bulletin **11**, 13-14 (1991).

   "POLYRATE—version 4.0," D.-h. Lu, T. N. Truong, V. S. Melissas, G. C. Lynch, Y.-P. Liu, B. C. Garrett, R. Steckler, A. D. Isaacson, S. N. Rai, G. C. Hancock, J. G. Lauderdale, T. Joseph, and D. G. Truhlar, QCPE program 601-version 4.0, March 1992.

   This version was announced in QCPE Bulletin **12**, 35-36 (1992).

   "POLYRATE—version 4.0.1," D.-h. Lu, T. N. Truong, V. S. Melissas, G. C. Lynch, Y.-P. Liu, B. C. Garrett, R. Steckler, A. D. Isaacson, S. N. Rai, G. C. Hancock, J. G. Lauderdale, T. Joseph, and D. G. Truhlar,

   CPC Program Library catalogue no. ACJC, March 1992;

   QCPE program 601, April 1992.

   This new version is described in "POLYRATE 4: A New Version of a Computer Program for the Calculation of Chemical Reaction Rates for Polyatomics," D.-h. Lu, T. N. Truong, V. S. Melissas, G. C. Lynch, Y.-P. Liu, B. C. Garrett, R. Steckler, A. D. Isaacson, S. N. Rai, G. C. Hancock, J. G. Lauderdale, T. Joseph, and D. G. Truhlar, *Computer Physics Communications* **71**, 235-262 (1992).

   "POLYRATE—version 5.0," Y.-P. Liu, G. C. Lynch, W.-P. Hu, V. S. Melissas, R. Steckler, B. C. Garrett, D.-h. Lu, T. N. Truong, A. D. Isaacson, S. N. Rai, G. C. Hancock, J. G. Lauderdale, T. Joseph, and D. G. Truhlar, QCPE program 601-version 5.0, April 1993.

   This version was announced in QCPE Bulletin **13**, 28-29 (1993).

   "POLYRATE-version 6.0," R. Steckler, W.-P. Hu, Y.-P. Liu, G. C. Lynch, B. C. Garrett, A. D. Isaacson, D.-h. Lu, V. S. Melissas, T. N. Truong, S. N. Rai, G. C. Hancock, J. G. Lauderdale, T. Joseph, and D. G. Truhlar, QCPE program 601-version 6.0, May 1994.

   "POLYRATE-version 6.5," R. Steckler, W.-P. Hu, Y.-P. Liu, G. C. Lynch, B. C. Garrett, A. D. Isaacson, V. S. Melissas, D.-h. Lu, T. N. Truong, S. N. Rai, G. C. Hancock, J. G. Lauderdale, T. Joseph, and D. G. Truhlar.

   distributed at www.sdsc, Jan. 1995;

   as QCPE program 601-version 6.5, April 1995;

   and as CPC program library catalogue number ADBN, April 1995.

   This version was announced in the QCPE Bulletin **15**, 40-41 (1995). A new version announcement appeared in Computer Physics Communications **88**, 341-343 (1995).

"POLYRATE–version 7.0," R. Steckler, Y.-Y. Chuang, E. L. Coitiño, W.-P. Hu, Y.-P. Liu, G. C. Lynch, K. A. Nguyen, C. F. Jackels, M. Z. Gu, I. Rossi, P. Fast, S. Clayton, V. S. Melissas, B. C. Garrett, A. D. Isaacson, and D. G. Truhlar.

distributed at comp.chem.umn, Aug. 1996,

and at www.sdsc, Sep. 1996;

"POLYRATE–version 7.1.1"-versions by R. Steckler, Y.-Y. Chuang, E. L. Coitiño, P. L. Fast, J. C. Corchado, W.-P. Hu, Y.-P. Liu, G. C. Lynch, K. A. Nguyen, C. F. Jackels, M. Z. Gu, I. Rossi, S. Clayton, V. S. Melissas, B. C. Garrett, A. D. Isaacson, and D. G. Truhlar.

distributed at comp.chem.umn, Mar. 1997

"POLYRATE-version 7.3.1," R. Steckler, Y.-Y. Chuang, P. L. Fast, E. L. Coitiño, J. C. Corchado, W.-P. Hu, Y.-P. Liu, G. C. Lynch, K. A. Nguyen, C. F. Jackels, M. Z. Gu, I. Rossi, S. Clayton, V. S. Melissas, B. C. Garrett, A. D. Isaacson, and D. G. Truhlar,

distributed at comp.chem.umn, July 1997;

also available from QCPE as program 601-version 7.3.1, July 1997.

The reference for the announcement is: "POLYRATE: A Computer Program for the Calculation of Chemical Reaction Rates for Polyatomics," R. Steckler, Y.-Y. Chuang, P. L. Fast, E. L. Coitiño, J. C. Corchado, W.-P. Hu, Y.-P. Liu, G. C. Lynch, K. A. Nguyen, C. F. Jackels, M. Z. Gu, I. Rossi, S. Clayton, V. S. Melissas, B. C. Garrett, A. D. Isaacson, and D. G. Truhlar, QCPE Bulletin **17**, 34-36 (1997).

"POLYRATE–version 7.8," J. C. Corchado, Y.-Y. Chuang, P. L. Fast, J. Villà, E. L. Coitiño, W.-P. Hu, Y.-P. Liu, G. C. Lynch, K. A. Nguyen, C. F. Jackels, M. Z. Gu, I. Rossi, S. Clayton, V. S. Melissas, R. Steckler, B. C. Garrett, A. D. Isaacson, and D. G. Truhlar.

distributed at comp.chem.umn, Dec. 1997

"POLYRATE-version 8.0," by Y.-Y. Chuang, J. C. Corchado, P. L. Fast, J. Villà, E. L. Coitiño, W.-P. Hu, Y.-P. Liu, G. C. Lynch, K. A. Nguyen, C. F. Jackels, M. Z. Gu, I. Rossi, S. Clayton, V. S. Melissas, R. Steckler, B. C. Garrett, A. D. Isaacson, and D. G. Truhlar.

distributed at comp.chem.umn, Aug. 1998

"POLYRATE–version 8.1" Y.-Y. Chuang, J. C. Corchado, P. L. Fast, J. Villà, W.-P. Hu, Y.-P. Liu, G. C. Lynch, K. A. Nguyen, C. F. Jackels, M. Z. Gu, I. Rossi, E. L. Coitiño, S. Clayton, V. S. Melissas, R. Steckler, B. C. Garrett, A. D. Isaacson, and D. G. Truhlar.distributed at comp.chem.umn,

distributed at comp.chem.umn, version 8.1, May 1999

"POLYRATE–version 8.4.1," Y.-Y. Chuang, J. C. Corchado, P. L. Fast, J. Villà, W.-P. Hu, Y.-P. Liu, G. C. Lynch, K. A. Nguyen, C. F. Jackels, M. Z. Gu, I. Rossi, E. L. Coitiño, S. Clayton, V. S. Melissas, B. Lynch, R. Steckler, B. C. Garrett, A. D. Isaacson, and D. G. Truhlar. distributed at comp.chem.umn,

istributed at comp.chem.umn, Mar. 2000

"POLYRATE–version 8.5," J. C. Corchado, Y.-Y. Chuang, P. L. Fast, J. Villà, W.-P. Hu, Y.-P. Liu, G. C. Lynch, K. A. Nguyen, C. F. Jackels, V. S. Melissas, B. J. Lynch, I. Rossi, E. L. Coitiño, A. Fernandez-Ramos, R. Steckler, B. C. Garrett, A. D. Isaacson, and D. G. Truhlar.

distributed at comp.chem.umn, Oct. 2000

"POLYRATE–version 8.6," by J. C. Corchado, Y.-Y. Chuang, P. L. Fast, J. Villà, W.-P. Hu, Y.-P. Liu, G. C. Lynch, K. A. Nguyen, C. F. Jackels, V. S. Melissas, B. J. Lynch, I. Rossi, E. L. Coitiño, A. Fernandez-Ramos, J. Pu, R. Steckler, B. C. Garrett, A. D. Isaacson, and D. G. Truhlar.

distributed at comp.chem.umn, Feb. 2001

"POLYRATE–version 8.9," J. C. Corchado, Y.-Y. Chuang, P. L. Fast, J. Villà, W.-P. Hu, Y.-P. Liu, G. C. Lynch, K. A. Nguyen, C. F. Jackels, V. S. Melissas, B. J. Lynch, I. Rossi, E. L. Coitiño, A. Fernandez-Ramos, J. Pu, T. V. Albu, R. Steckler, B. C. Garrett, A. D. Isaacson, and D. G. Truhlar.

distributed at comp.chem.umn, May 2002

"POLYRATE–version 9.3.1," J. C. Corchado, Y.-Y. Chuang, P. L. Fast, W.-P. Hu, Y.-P. Liu, G. C. Lynch, K. A. Nguyen, C. F. Jackels, A. Fernandez-Ramos, B. A. Ellingson, B. J. Lynch, V. S. Melissas, J. Villà, I. Rossi, E. L. Coitiño, J. Pu, T. V. Albu, R. Steckler, B. C. Garrett, A. D. Isaacson, and D. G. Truhlar.

distributed at comp.chem.umn, June 2005

"POLYRATE–version 9.6," J. C. Corchado, Y.-Y. Chuang, P. L. Fast, W.-P. Hu, Y.-P. Liu, G. C. Lynch, K. A. Nguyen, C. F. Jackels, A. Fernandez-Ramos, B. A. Ellingson, B. J. Lynch, J. Zheng, V. S. Melissas, J. Villà, I. Rossi, E. L. Coitiño, J. Pu, T. V. Albu, R. Steckler, B. C. Garrett, A. D. Isaacson, and D. G. Truhlar.

distributed at comp.chem.umn, Feb. 2007

"POLYRATE–version 2008," J. Zheng, S. Zhang, J. C. Corchado, Y.-Y. Chuang, P. L. Fast, W.-P. Hu, Y.-P. Liu, G. C. Lynch, K. A. Nguyen, C. F. Jackels, A. Fernandez-Ramos, B. A. Ellingson, V. S. Melissas, J. Villà, I. Rossi, E. L. Coitiño, J. Pu, T. V. Albu, R. Steckler, B. C. Garrett, A. D. Isaacson, and D. G. Truhlar.

distributed at comp.chem.umn, May 2009

"POLYRATE–version 2010," J. Zheng, S. Zhang, J. C. Corchado, Y.-Y. Chuang, P. L. Fast, W.-P. Hu, Y.-P. Liu, G. C. Lynch, K. A. Nguyen, C. F. Jackels, A. Fernandez-Ramos, B. A. Ellingson, V. S. Melissas, J. Villà, I. Rossi, E. L. Coitiño, J. Pu, T. V. Albu, R. Steckler, B. C. Garrett, A. D. Isaacson, and D. G. Truhlar.

distributed at comp.chem.umn, June 2010

9. "**VIBCI**," S. C. Tucker, T. C. Thompson, J. G. Lauderdale, and D. G. Truhlar, CPC Program Library catalogue no. ABDY.

   This program is described in "A Vibrational Configuration Interaction Program for Energies and Resonance Widths," S. C. Tucker, T. C. Thompson, J. G. Lauderdale, and D. G. Truhlar, *Computer Physics Communications* **51**, 233-256 (1988).

10. "**MORATE**-version 4.5," T. N. Truong, D.-h. Lu, G. C. Lynch, Y.-P. Liu, V. S. Melissas, J. J. P. Stewart, R. Steckler, B. C. Garrett, A. D. Isaacson, A. González-Lafont, S. N. Rai, G. C. Hancock, T. Joseph, and D. G. Truhlar, CPC Program Library catalogue no. ACLM. Oct. 1992.

    This program is described in "MORATE: A Program for Direct Dynamics Calculations of Chemical Reaction Rates by Semiempirical Molecular Orbital Theory," T. N. Truong, D.-h. Lu, G. C. Lynch, Y.-P. Liu, V. S. Melissas, J. J. P. Stewart, R. Steckler, B. C. Garrett, A. D. Isaacson, A. Gonzàlez-Lafont, S. N. Rai, G. C. Hancock, T. Joseph, and D. G. Truhlar, *Computer Physics Communications* **75**, 143-159 (1993).

    "MORATE-version 6.5," W.-P. Hu, G. C. Lynch, Y.-P. Liu, I. Rossi, J. J. P. Stewart, R. Steckler, B. C. Garrett, A. D. Isaacson, D.-h. Lu, V. S. Melissas, and D. G. Truhlar,

    QCPE catalog number 666, Apr. 1995,

    and CPC catalog number ADBO, Apr. 1995.

    This program was announced in the QCPE Bulletin **15**, 26-27 (1995) and again in the QCPE Bulletin **15**, 63-64 (1995). In addition a new version announcement appeared in Computer Physics Communications **88**, 344-346 (1995).

    "MORATE-version 7.2," Y.-Y. Chuang, W.-P. Hu, G. C. Lynch, Y.-P. Liu, and D. G. Truhlar.

    distributed at comp.chem.umn, Mar. 1997.

    "MORATE–version 7.4," Y.-Y. Chuang, P. L. Fast, W.-P. Hu, G. C. Lynch, Y.-P. Liu, and D. G. Truhlar.

    Version 8.5/P8.5.1-M5.09, Oct. 2000.

11. "**AMSOL** (version 1.0)," C. J. Cramer and D. G. Truhlar, QCPE program 606-original version, July 1991.

    This program was announced in QCPE Bulletin **11**, 57-58 (1991).

    "AMSOL," versions by C. J. Cramer, G. C. Lynch, and D. G. Truhlar,

    versions 3.0 and 3.0c, QCPE program 606-version 3.0, June 1992;

    versions 3.0.1 and 3.0.1c, QCPE program 606-version 3.0.1, Sep. 1992;

    Versions 3.0 and 3.0c were announced in QCPE Bulletin **12**, 62-63 (1992).

    The manual for versions 3.0 and 3.0c are also available as University of Minnesota Supercomputer Institute Research Report UMSI 92/124, June 1992.

    Versions 3.0.1 and 3.0.1c were announced in QCPE Bulletin **12**, 77 (1992), but the announcement had a printer's error. A corrected version of the announcement was published in QCPE Bulletin **13**, 9-10 (1993).

    "AMSOL," versions by C. J. Cramer, G. C. Lynch, G. D. Hawkins, D. G. Truhlar, and D. A. Liotard,

    version 3.5, QCPE program 606-version 3.5, June 1993;

    version 4.0, QCPE program 606-version 4.0, Nov. 1993;

    Version 3.5 was announced in QCPE Bulletin **13**, 55 (1993).

    Version 4.0 was announced in QCPE Bulletin **13**, 78 (1993).

"AMSOL-version 4.5," C. J. Cramer, G. D. Hawkins, G. C. Lynch, D. J. Giesen, D. G. Truhlar, and D. A. Liotard, QCPE program 606-version 4.5, Aug. 1994.

This version was announced in QCPE Bulletin **14**, 55-57 (1994).

"AMSOL," versions by C. J. Cramer, G. D. Hawkins, G. C. Lynch, D. J. Giesen, I. Rossi, J. W. Storer, D. G. Truhlar, and D. A. Liotard,

version 4.6, QCPE program 606-version 4.6, Aug. 1994;

version 5.0, QCPE program 606-version 5.0, Apr. 1995.

Version 5.0 was announced in QCPE Bulletin **15**, 41-43 (1995).

"AMSOL," versions by G. D. Hawkins, G. C. Lynch, D. J. Giesen, I. Rossi, J. W. Storer, D. A. Liotard, C. J. Cramer, and D. G. Truhlar,

version 5.2.1, QCPE program 606-version 5.2.1, Oct. 1995;

version 5.4, QCPE program 606-version 5.4, Dec. 1995;

Version 5.2.1 was announced in QCPE Bulletin **15**, 77-79 (1995).

Version 5.4 was announced in QCPE Bulletin **16**, 11-13 (1996).

"AMSOL-version 6.1.1," D. J. Giesen, G. D. Hawkins, C. C. Chambers, G. C. Lynch, I. Rossi, J. W. Storer, D. Rinaldi, D. A. Liotard, C. J. Cramer, and D. G. Truhlar,

distributed by OMG, Sep. 1997,

and by Makolab, Oct. 1997.

"AMSOL," versions by G. D. Hawkins, D. J. Giesen, G. C. Lynch, C. C. Chambers, I. Rossi, J. W. Storer, J. Li, D. Rinaldi, D. A. Liotard, C. J. Cramer, and D. G. Truhlar,

version 6.5, distributed by OMG, Feb. 1998;

version 6.5.1, distributed by OMG, Feb. 1998,

and by Makolab, Apr. 1998,

and at comp.chem.umn, Apr. 1998;

version 6.5.2, distributed at comp.chem.umn, July 1998,

and by OMG. Aug. 1998.

"AMSOL-version 6.5.3," G. D. Hawkins, D. J. Giesen, G. C. Lynch, C. C. Chambers, I. Rossi, J. W. Storer, J. Li, T. Zhu, D. Rinaldi, D. A. Liotard, C. J. Cramer, and D. G. Truhlar,

distributed by OMG, Oct. 1998,

distributed by Makolab, Nov. 1998

distributed at comp.chem.umn, Nov. 1998,

and distributed by Semichem, Mar. 1999.

"AMSOL," versions by G. D. Hawkins, D. J. Giesen, G. C. Lynch, C. C. Chambers, I. Rossi, J. W. Storer, J. Li, T. Zhu, P. Winget, D. Rinaldi, D. A. Liotard, C. J. Cramer, and D. G. Truhlar.

distributed at comp.chem.umn, version 6.6, Dec. 1999

"AMSOL," versions by G. D. Hawkins, D. J. Giesen, G. C. Lynch, C. C. Chambers, I. Rossi, J. W. Storer, J. Li, T. Zhu, J. D. Thompson, P. Winget, D. Rinaldi, D. A. Liotard, C. J. Cramer, and D. G. Truhlar.

distributed at comp.chem.umn, version 6.8, Sept. 2002

"AMSOL-version 7.0," G. D. Hawkins, D. J. Giesen, G. C. Lynch, C. C. Chambers, I. Rossi, J. W. Storer, J. Li, T. Zhu, J. D. Thompson, P. Winget, B. J. Lynch, D. Rinaldi, D. A. Liotard, C. J. Cramer, and D. G. Truhlar, distributed at comp.chem.umn, March 2003

"AMSOL-version 7.1," G. D. Hawkins, D. J. Giesen, G. C. Lynch, C. C. Chambers, I. Rossi, J. W. Storer, J. Li, T. Zhu, J. D. Thompson, P. Winget, B. J. Lynch, D. Rinaldi, D. A. Liotard, C. J. Cramer, and D. G. Truhlar.

distributed at comp.chem.umn, Dec. 2004

A process is underway by which commerical licenses can be distrbuted directly from the University of Minnesota Office for Technology Commercialization.

12. "**RMPROP**-version 1.0," M. J. Unekis, D. W. Schwenke, N. M. Harvey, and D. G. Truhlar, MOTECC-91 program library.

This program is described in "RMPROP: A Computer Program for Quantum Mechanical Close Coupling Calculations for Inelastic Collisions," M. J. Unekis, D. W. Schwenke, N. M. Harvey, and D. G. Truhlar, in *Modern Techniques in Computational Chemistry: MOTECC-91*, edited by E. Clementi (ESCOM, Leiden, 1991), pp. 749-772. Citation: Mod. Tech. Comput. Chem.: MOTECC-91, 749-72 (1991). All versions of RMPROP are also described in a manual.

"RMPROP-version 2.1.1," M. S. Reeves, M. J. Unekis, D. W. Schwenke, N. M. Harvey, and D. G. Truhlar, METECC-94 program library.

This program is described in "RMPROP-Version 2: A Computer Program for Quantum Mechanical Close Coupling Calculations for Inelastic Collisions," in *Methods and Techniques in Computational Chemistry: METECC-94*, edited by E. Clementi (STEF, Cagliari, Italy, 1993), Vol. C, pp. 1-46. It was submitted to the METECC library in Aug. 1994.

"RMPROP-version 2.1.2," M. S. Reeves, M. J. Unekis, D. W. Schwenke, W. C. Necoechea, N. M. Harvey, and D. G. Truhlar, Apr. 1995, distributed at comp.chem.umn beginning Jan. 2000.

13. **MOPAC**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 5.05mn | 7/94 | comp.chem.umn | J. J. P. Stewart, I. Rossi, W.-P. Hu, G. C. Lynch, Y.-P. Liu, and D. G. Truhlar |
| 5.08mn | 9/99 | comp.chem.umn | J. J. P. Stewart, I. Rossi, W.-P. Hu, G. C. Lynch, Y.-P. Liu, Y.-Y. Chuang, J. Li, C. J. Cramer, and D. G. Truhlar |
| 5.09mn | 10/99 | comp.chem.umn. | J. J. P. Stewart, I. Rossi, W.-P. Hu, G. C. Lynch, Y.-P. Liu, Y.-Y. Chuang, J. Li, C. J. Cramer, P. L. Fast, and D. G. Truhlar |

| | | | |
|---|---|---|---|
| 5.010mn | 11/03 | comp.chem.umn | J. J. P. Stewart, I. Rossi, W.-P. Hu, G. C. Lynch, Y.-P. Liu, Y.-Y. Chuang, J. Pu, J. Li, C. J. Cramer, P. L. Fast, and D. G. Truhlar |
| 5.011mn | 8/06 | comp.chem.umn | J. J. P. Stewart, J. Zheng, I. Rossi, W.-P. Hu, G. C. Lynch, Y.-P. Liu, Y.-Y. Chuang, J. Pu, J. Li, C. J. Cramer, P. L. Fast, and D. G. Truhlar |
| 5.013mn | 10/09 | comp.chem.umn | J. J. P. Stewart, L. Fiedler, J. Zheng, I. Rossi, W.-P. Hu, G. C. Lynch, Y.-P. Liu, Y.-Y. Chuang, J. Pu, J. Li, C. J. Cramer, P. L. Fast, and D. G. Truhlar |
| 5.015mn | 4/10 | comp.chem.umn | J. J. P. Stewart, L. Fiedler, P. Zhang, J. Zheng, I. Rossi, W.-P. Hu, G. C. Lynch, Y.-P. Liu, Y.-Y. Chuang, J. Pu, J. Li, C. J. Cramer, P. L. Fast, and D. G. Truhlar |
| 5.017mn | 10/10 | comp.chem.umn | J. J. P. Stewart, L. Fiedler, P. Zhang, J. Zheng, I. Rossi, W.-P. Hu, G. C. Lynch, Y.-P. Liu, Y.-Y. Chuang, J. Pu, J. Li, C. J. Cramer, P. L. Fast, J. Gao, and D. G. Truhlar |
| 5.018mn | 3/11 | comp.chem.umn | J. J. P. Stewart, L. Fiedler, P. Zhang, J. Zheng, I. Rossi, W.-P. Hu, G. C. Lynch, Y.-P. Liu, Y.-Y. Chuang, J. Pu, J. Li, C. J. Cramer, P. L. Fast, J. Gao, and D. G. Truhlar |

14. **GAUSSRATE**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 7.1 | 3/97 | comp.chem.umn | J. C. Corchado, Y.-Y. Chuang, E. L. Coitiño, and D. G. Truhlar |
| 9.5 | 1/07 | comp.chem.umn | J. C. Corchado, Y.-Y. Chuang, E. L. Coitiño, B. A. Ellingson, and D. G. Truhlar |
| 9.7 | 6/07 | comp.chem.umn | J. C. Corchado, Y.-Y. Chuang, E. L. Coitiño, B. A. Ellingson, J. Zheng, and D. G. Truhlar |
| 2008 | 5/09 | comp.chem.umn | J. Zheng, S. Zhang, J. C. Corchado, Y.-Y. Chuang, E. L. Coitiño, B. A. Ellingson, and D. G. Truhlar |
| 2009-A | 3/10 | comp.chem.umn | J. Zheng, S. Zhang, J. C. Corchado, Y.-Y. Chuang, E. L. Coitiño, B. A. Ellingson, and D. G. Truhlar |

15. **OMNISOL**

| version | date | distribution | authors |
|---|---|---|---|
| 1.0 | 8/97 | comp.chem.umn | G. D. Hawkins, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |
| 2.0 | 8/07 | comp.chem.umn | G. D. Hawkins, B. J. Lynch, C. P. Kelly, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |

16. **GAMESOL**

| version | date | distribution | authors |
|---|---|---|---|
| 1.0 | 12/97 | comp.chem.umn | J. Li, G. D. Hawkins, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |
| 2.0 | 10/98 | comp.chem.umn | J. Li, T. Zhu, G. D. Hawkins, D. A. Liotard, D. Rinaldi, C. J. Cramer, and D. G. Truhlar |
| 2.1 | 1/99 | comp.chem.umn | J. Li, T. Zhu, G. D. Hawkins, Y.-Y. Chuang, D. A. Liotard, D. Rinaldi, C. J. Cramer, and D. G. Truhlar |
| 2.2.1 | 4/99 | comp.chem.umn | J. Li, T. Zhu, G. D. Hawkins, Y.-Y. Chuang, P. L. Fast, D. A. Liotard, D. Rinaldi, C. J. Cramer, and D. G. Truhlar |
| 3.0 | 2/01 | comp.chem.umn | J. D. Xidos, J. Li, T. Zhu, G. D. Hawkins, Y.-Y. Chuang, P. L. Fast, D. A. Liotard, D. Rinaldi, C. J. Cramer, and D. G. Truhlar |
| 3.1 | 8/02 | comp.chem.umn | J. D. Xidos, J. Li, T. Zhu, G. D. Hawkins, J. D. Thompson, Y.-Y. Chuang, P. L. Fast, D. A. Liotard, D. Rinaldi, C. J. Cramer, and D. G. Truhlar |
| 3.9 | 4/03 | comp.chem.umn | " |

**GAMESSPLUS**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 4.0 | 9/03 | comp.chem.umn | J. D. Xidos, J. Li, T. Zhu, G. D. Hawkins, J. D. Thompson, Y.-Y. Chuang, P. L. Fast, D. A. Liotard, D. Rinaldi, C. J. Cramer, and D. G. Truhlar |
| 4.1 | 1/04 | comp.chem.umn | J. Pu, J. D. Thompson, J. D. Xidos, J. Li, T. Zhu, G. D. Hawkins, Y.-Y. Chuang, P. L. Fast, D. A. Liotard, D. Rinaldi, J. Gao, C. J. Cramer, and D. G. Truhlar |
| 4.4 | 12/04 | comp.chem.umn | J. Pu, J. D. Thompson, J. D. Xidos, J. Li, T. Zhu, G. D. Hawkins, Y.-Y. Chuang, P. L. Fast, B. J. Lynch, D. A. Liotard, D. Rinaldi, J. Gao, C. J. Cramer, and D. G. Truhlar |
| 4.8 | 5/06 | comp.chem.umn | A. C. Chamberlin, J. Pu, J. D. Thompson, J. D. Xidos, J. Li, T. Zhu, G. D. Hawkins, Y.-Y. Chuang, P. L. Fast, B. J. Lynch, D. A. Liotard, D. Rinaldi, J. Gao, C. J. Cramer, and D. G. Truhlar |
| 2008 | 4/08 | comp.chem.umn | M. Higashi, A. C. Chamberlin, J. Pu, J. D. Thompson, J. D. Xidos, J. Li, T. Zhu, G. D. Hawkins, Y.-Y. Chuang, P. L. Fast, B. J. Lynch, D. A. Liotard, D. Rinaldi, J. Gao, C. J. Cramer, and D. G. Truhlar |

| | | | |
|---|---|---|---|
| 2008-2 | 8/08 | comp.chem.umn | M. Higashi, A. V. Marenich, A. C. Chamberlin, J. Pu, J. D. Thompson, J. D. Xidos, J. Li, T. Zhu, G. D. Hawkins, Y.-Y. Chuang, P. L. Fast, B. J. Lynch, D. A. Liotard, D. Rinaldi, J. Gao, C. J. Cramer, and D. G. Truhlar |
| 2010-2 | 9/10 | comp.chem.umn | " |

17. **AMSOLRATE**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 7.9.1 | 4/98 | comp.chem.umn | Y.-Y. Chuang, Y.-P. Liu, and D. G. Truhlar |
| 8.6 | 10/00 | comp.chem.umn | " |

18. **HONDO/S**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 1.0 | 6/99 | comp.chem.umn | J. Li, G. D. Hawkins, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |
| 1.0.1 | 5/00 | comp.chem.umn | J. Xidos, J. Li, G. D. Hawkins, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |
| 3.0 | 5/01 | comp.chem.umn | J. Xidos, J. Thompson, J. Li, G. D. Hawkins, D. Rinaldi, T. Zhu, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |
| 3.1 | 5/01 | comp.chem.umn | J. Xidos, J. Thompson, G. D. Hawkins, J. Li, T. Zhu, B. J. Lynch, D. Rinaldi, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |
| 3.3 | 6/01 | comp.chem.umn | J. Xidos, J. Thompson, G. D. Hawkins, J. Li, T. Zhu, B. J. Lynch, Y. Volobuev, D. Rinaldi, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |
| 4.0 | 4/02 | comp.chem.umn | H. Nakamura, J. Xidos, J. Thompson, G. D. Hawkins, J. Li, T. Zhu, B. J. Lynch, Y. Volobuev, D. Rinaldi, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |
| 4.3 | 1/03 | comp.chem.umn | " |

**HONDOPLUS**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 4.3 | 4/03 | comp.chem.umn | H. Nakamura, J. Xidos, J. Thompson, G. D. Hawkins, J. Li, T. Zhu, B. J. Lynch, Y. Volobuev, D. Rinaldi, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |
| 4.7 | 7/05 | comp.chem.umn | H. Nakamura, J. Xidos, C. P. Kellly, J. Thompson, G. D. Hawkins, J. Li, T. Zhu, B. J. Lynch, Y. Volobuev, D. Rinaldi, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |
| 5.0 | 11/05 | comp.chem.umn | H. Nakamura, J. Xidos, A. C. Chamberlin, C. P. Kelly, J. Thompson, J. Li, G. D. Hawkins, T. |

| | | | |
|---|---|---|---|
| 5.1 | 2/07 | comp.chem.umn | Zhu, B. J. Lynch, Y. Volobuev, D. Rinaldi, D. A. Liotard, C. J. Cramer, and D. G. Truhlar H. Nakamura, J. Xidos, A. C. Chamberlin, C. P. Kelly, R. Valero, J. Thompson, J. Li, G. D. Hawkins, T. Zhu, B. J. Lynch, Y. Volobuev, D. Rinaldi, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |

19. **ZINDO**, version 99.1, M. C. Zerner, J. E. Ridley, A. D. Bacon, W. D. Edwards, J. D. Head, J. McKelvey, J. C. Culberson, P. Knappe, M. G. Cory, B. Weiner, J. D. Baker, W. A. Parkinson, D. Kannis, J. Yu, N. Roesch, M. Kotzian, T. Tamm, M. M. Karelson, X. Zheng, G. Pearl, A. Broo, K. Albert, J. M. Cullen, C. J. Cramer, D. G. Truhlar, J. Li, G. D. Hawkins and D. A. Liotard, Sept. 1999.

**ZINDO-MN**

| *version* | *date* | *authors* |
|---|---|---|
| 1.0.1 | 12/01 | M. C. Zerner, J. E. Ridley, A. D. Bacon, W. D. Edwards, J. D. Head, J. McKelvey, J. C. Culberson, P. Knappe, M. G. Cory, B. Weiner, J. D. Baker, W. A. Parkinson, D. Kannis, J. Yu, N. Roesch, M. Kotzian, T. Tamm, M. M. Karelson, X. Zheng, G. Pearl, A. Broo, K. Albert, J. M. Cullen, J. Li, G. D. Hawkins, J. D. Thompson, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |
| 1.2 | 11/05 | M. C. Zerner, J. E. Ridley, A. D. Bacon, W. D. Edwards, J. D. Head, J. McKelvey, J. C. Culberson, P. Knappe, M. G. Cory, B. Weiner, J. D. Baker, W. A. Parkinson, D. Kannis, J. Yu, N. Roesch, M. Kotzian, T. Tamm, M. M. Karelson, X. Zheng, G. Pearl, A. Broo, K. Albert, J. M. Cullen, J. Li, G. D. Hawkins, J. D. Thompson, C. P. Kelly, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |
| 2010 | 9/10 | M. C. Zerner, J. E. Ridley, A. D. Bacon, W. D. Edwards, J. D. Head, J. McKelvey, J. C. Culberson, P. Knappe, M. G. Cory, B. Weiner, J. D. Baker, W. A. Parkinson, D. Kannis, J. Yu, N. Roesch, M. Kotzian, T. Tamm, M. M. Karelson, X. Zheng, G. Pearl, A. Broo, K. Albert, J. M. Cullen, J. Li, G. D. Hawkins, J. D. Thompson, C. P. Kelly, D. A. Liotard, A. V. Marenich, C. J. Cramer, and D. G. Truhlar |
| 2011 | 4/11 | " |

21. **GAMESOLRATE**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 8.1.1 | 7/99 | comp.chem.umn | Y.-Y. Chuang, J. C. Corchado, and D. G. Truhlar |
| 8.5 | 10/00 | comp.chem.umn | " |

**GAMESSPLUSRATE**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 9.3 | 12/04 | comp.chem.umn | Y.-Y. Chuang, J. C. Corchado, J. Pu, and D. G. Truhlar |

21. **TINKERATE**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 8.4 | 12/99 | comp.chem.umn | J. C. Corchado, Y. Kim, J. Villa, J. Xing, and D. G. Truhlar |
| 8.5 | 11/00 | comp.chem.umn. | J. C. Corchado, Y. Kim, J. Villa, J. Xing, and D. G. Truhlar |

**MC-TINKERATE**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 8.8 | 3/02 | comp.chem.umn | T. V. Albu, J. C. Corchado, Y. Kim, J. Villa, J. Xing, and D. G. Truhlar |
| 9.1 | 12/03 | comp.chem.umn | T. V. Albu, J. C. Corchado, Y. Kim, J. Villa, J. Xing, H. Lin, and D. G. Truhlar |
| 2007 | 7/07 | comp.chem.umn | T. V. Albu, O. Tishchenko, J. C. Corchado, Y. Kim, J. Villa, J. Xing, H. Lin, and D. G. Truhlar |
| 2008 | 7/08 | comp.chem.umn | T. V. Albu, O. Tishchenko, J. C. Corchado, Y. Kim, J. Villa, J. Xing, H. Lin, M. Higashi, and D. G. Truhlar |
| 2010 | 10/10 | comp.chem.umn | " |

22. **MULTILEVEL**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 1.0 | 3/00 | comp.chem.umn | J. M. Rodgers, B. J. Lynch, P. L. Fast, Y.-Y. Chuang, and D. G. Truhlar |
| 2.1.1 | 11/00 | comp.chem.umn | J. M. Rodgers, B. J. Lynch, P. L. Fast, Y.-Y. Chuang, J. Pu, and D. G. Truhlar |
| 2.5 | 7/02 | comp.chem.umn. | J. M. Rodgers, B. J. Lynch, P. L. Fast, Y. Zhao, J. Pu, Y. -Y. Chuang, and D. G. Truhlar |
| 4.0 | 4/04 | comp.chem.umn. | Y. Zhao, J. M. Rodgers, B. J. Lynch, P. L. Fast, J. Pu, Y. -Y. Chuang, and D. G. Truhlar |
| 4.1 | 7/06 | comp.chem.umn. | Y. Zhao, J. M. Rodgers, B. J. Lynch, N. Gonzalez-Garcia, P. L. Fast, J. Pu, Y. -Y. Chuang, and D. G. Truhlar |
| 4.2 | 7/06 | comp.chem.umn. | Y. Zhao, J. M. Rodgers, B. J. Lynch, N. Gonzalez-Garcia, P. L. Fast, J. Pu, Y. -Y. Chuang, B. A. Ellingson, and D. G. Truhlar |

23. **CRATE**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 8.1.1 | 12/99 | comp.chem.umn | C. Alhambra, J. C. Corchado, M. L. Sanchez, J. Villa, J. Gao, and D. G. Truhlar |
| 9.0 | 2/03 | comp.chem.umn | M. Garcia-Viloca, C. Alhambra, J. C. Corchado, M. L. Sanchez, J. Villa, J. Gao, and D. G. Truhlar |
| 9.0.1 | 4/06 | comp.chem.umn | " |

24. **EHT**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 1.0 | 4/00 | comp.chem.umn | T. Liu and D. G. Truhlar |

25. **TB**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 1.0 | 4/00 | comp.chem.umn | T. Liu and D. G. Truhlar |
| 2.0 | 7/04 | comp.chem.umn | G. Staszewska and D. G. Truhlar |

**TBPAC**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 2007 | 9/07 | comp.chem.umn | M. A. Iron, G. Styaszewska, T. Liu A. W. Jasper, and D. G. Truhlar |

26. **MC-TINKER**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 1.0 | 3/02 | comp.chem.umn | T. V. Albu, J. C. Corchado, Y. Kim, J. Villa, J. Xing, and D. G. Truhlar |
| 1.0.1 | 12/03 | comp.chem.umn | T. V. Albu, J. C. Corchado, Y. Kim, J. Villa, J. Xing, H. Lin, and D. G. Truhlar |
| 2008 | 6/08 | comp.chem.umn | O. Tishchenko, M. Higashi, T. V. Albu, J. C. Corchado, Y. Kim, J. Villà, J. Xing, H. Lin, and D. G. Truhlar |
| 2009 | 3/09 | comp.chem.umn | " |

**MCSI**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 2009-1 | 12/09 | comp.chem.umn | O. Tishchenko, M. Higashi, T. V. Albu, J. C. Corchado, Y. Kim, J. Villà, J. Xing, H. Lin, and D. G. Truhlar |
| 2010 | 10/10 | comp.chem.umn | " |

27. **AMM**

AMM is the AMSOL Model Module (AMM) that was originally (in 2001) made available as an add-on to Semichem, Inc.'s AMPAC 7.0 package. Beginning with AMPAC 9 (in 2008), AMM became an integral part of Semichem's AMPAC, rather than an add-on.

28. **DIRDYVTST**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 1.0 | 5/02 | comp.chem.umn | B. C. Garrett, Y.-Y. Chuang , D. G. Truhlar, R. A. Kendall, B. C. Garrett, and T. L. Windus |

See http://www.emsl.pnl.gov/docs/nwchem/doc/user/node39.html#SECTION37.2

29. **CGPLUS**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 1.0 | 1/04 | comp.chem.umn | J. Pu, J. Gao, and D. G. Truhlar |
| 2008 | 4/08 | comp.chem.umn | J. Pu, M. Higashi, J. Gao, and and D. G. Truhlar |

30. **SMXGAUSS**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 1.0 | 5/04 | comp.chem.umn | J. D. Thompson, B. J. Lynch, J. D. Xidos, J. Li, G. D. Hawkins, T. Zhu, Y. Volobuev, M. Dupuis, D. Rinaldi, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |
| 3.0 | 7/05 | comp.chem.umn | C. P. Kelly, J. D. Thompson, B. J. Lynch, J. D. Xidos, J. Li, G. D. Hawkins, T. Zhu, Y. Volobuev, M. Dupuis, D. Rinaldi, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |
| 3.4 | 2/06 | comp.chem.umn | A. C. Chamberlin, C. P. Kelly, J. D. Thompson, B. J. Lynch, J. D. Xidos, J. Li, G. D. Hawkins, T. Zhu, Y. Volobuev, M. Dupuis, D. Rinaldi, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |
| 3.4.2 | 8/07 | comp.chem.umn | " |

31. **MLGAUSS**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 1.0 | 2/05 | comp.chem.umn | Y. Zhao and D. G. Truhlar |
| 2.0 | 7/06 | comp.chem.umn | " |

32. **QMMM**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 1.0 | 2/05 | comp.chem.umn | H. Lin and D. G. Truhlar |
| 1.1 | 5/06 | comp.chem.umn | H. Lin, Y. Zhang, and D. G. Truhlar |

| | | | |
|---|---|---|---|
| 1.3.8 | 2/11 | comp.chem.umn | H. Lin, Y. Zhang, S. Pezeshki, and D. G. Truhlar |

33. **ANT**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 07 | 3/07 | comp.chem.umn | Z. H. Li, A. W. Jasper, D. A. Bonhommeau, and D. G. Truhlar |
| 08 | 6/08 | comp.chem.umn | Z. H. Li, A. W. Jasper, D. A. Bonhommeau, R. Valero, and D. G. Truhlar |
| 09 | 12//09 | comp.chem.umn | " |

34. **JAGUARATE**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 2007 | 5/07 | comp.chem.umn | J. Zheng and D. G. Truhlar |

35. **NWCHEMRATE**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 2007 | 12/07 | comp.chem.umn | J. Zheng, M. A. Iron, B. A. Ellingson, J. C. Corchado, Y.-Y. Chuang, and D. G. Truhlar |

36. **GESOL**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 2008 | 11/08 | comp.chem.umn | A. V. Marenich, G. D. Hawkins, D. A. Liotard, C. J. Cramer, and D. G. Truhlar |

37. **MFM**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 1.0 | 12/08 | comp.chem.umn | Y. Zhao and D. G. Truhlar |
| 1.3 | 5/11 | comp.chem.umn | Y. Zhao, R. Pverati, and D. G. Truhlar |
| 1.6 | 12/11 | comp.chem.umn | " |

38. **AMBERPLUS**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 2008 | 7/08 | comp.chem.umn | M. Higashi and D. G. Truhlar |
| 2010 | 12/10 | comp.chem.umn | " |

39. **MSTor**

| *version* | *date* | *distribution* | *authors* |
|---|---|---|---|
| 2011 | 10/11 | comp.chem.umn | J. Zheng, S. L. Mielke, K. L. Clarkson, and D. G. Truhlar |
| 2011-2 | 11/11 | comp./chem.umn | " |

The *MSTor* program has been submitted to the CPC Library and it will appear there soon.