> Users often are the first to spot surprising behavior, which may indicate a bug. We try very hard to fix bugs as soon as we know about them, and then post the latest MultiWell release on the website.   THANK YOU, USERS, FOR REPORTING BUGS!

NEW IN VERSION 2008.2 (March 2008):

1. A few minor cosmetic bugs were fixed, including a problem with Thermo, which did not print data for hindered internal rotations in the output file (thermo.out). Computed output was not affected by these minor bugs.

NEW IN VERSION 2008.1 (January 2008):

2. We have changed the version numbering scheme to make it more informative. From now on, all of the codes in each distribution will be given the new distribution number, even if some of them have not been revised. The distribution number will consist of the year and the release number for that year (since there may be more than one release each year), e.g. "2008.1" is the first release of 2008.

3. Previously, error messages that were written in the DOS window (when executing with Windows) were not readable, because the DOS window closed too quickly. This problem with the Windows version has been fixed.

4. MultiWell: extension: at the request of some users, the default numbers of wells (MaxWell), product sets (MaxProd), and reactions (MaxRxn) have been increased to 50, 50, and 100, respectively. The defaults can be changed easily by revising file src/multiwell/declare1.inc and recompiling the code.

5. MultiWell: extension: it is now possible for a user to easily change the output filenames when running multiwell. If this option is not exercised, the output files are still named "multiwell.xxx" where xxx = "out", etc., just as in previous versions. See Section 2.5 of the latest MultiWell User Manual for details.

6. MultiWell: Bug-Fix: the lower energy limits of the numerical integrations for kinf and k0 (high and low pressure limiting rate constants) were Egrain1 in energy below the correct values. This caused very small errors (typically <0.5%) in the calculated values for the limiting rate constants.

7. Thermo: new feature: introduction of new types of degrees of freedom, "gor" and "fit", enables Thermo to find the hindered Gorin model that fits a user-supplied recombination rate constant. Three new examples illustrating the use of this feature were added to directory examples/thermo-examples. See the User Manual for details.

8. DenSum: Bug-Fix: when quantized rotation   ("qro") was selected, DenSum incorrectly neglected all rotor levels except the zero point level in the lowest

energy bin (densities of states in all other energy bins were correct). This error has been fixed.

9. DenSum: Bug-Fix: for Morse oscillators, the quantum number for the highest bound state was erroneously calculated to be about one state higher than it should have been. This bug had only a small effect at high energies and probably was negligible in most applications. In addition, there was a bug in the way anharmonicity was included. For strongly anharmonic molecules, this bug may have resulted in errors in the sums of states of as much as 5-10% at energies near and above the dissociation limit. These bugs have been fixed.

10. DenSum: new feature: a new type of degree of freedom ("kro") has been defined in order to calculate sums and densities of states when the K-rotor is included as an active quantized degree of freedom. According to this feature, the K quantum number is restricted to the 2J+1 values in the range from -J to +J for a specified value of J. [Normally, we recommend the pragmatic approximation that the K-rotor be treated as an ordinary (quantized or classical) 1-D rotor with quantum number K that is restricted only by conservation of energy.]

11. DenSum: new feature: the "_____.dens" output file, which is used as input by MultiWell, has been modified to include a succinct summary of the input data and the DenSum version number. This helps users keep a better record of the vibrational assignments used to generate sums and densities of states. This new version of the MultiWell master equation module is compatible with both the old format and this new one.

12. DenSum: new feature: It is now possible to run DenSum in a batch mode, in which calculations can be carried out all at one time for multiple species with a minimum amount of effort. This feature is useful when changing the energy grain or array boundaries for a complicated chemical system. See the MultiWell User Manual for details.

NEW IN VERSION 2.08 (February 2007):

a. Gauss2Multi: Bug-Fix: when compiled with older versions of the GNU GCC compiler, this module sometimes did not execute correctly. This bug has been corrected.

b. MultiWell: Bug-Fix: Previously, the tunneling correction was not correct when the energy grain size was not an integer multiple of 1.0 (e.g. 1.0, 3.0. 10.0, etc.). This error only affected k(E) significantly in the lower portion of the double array when Egrain1 was not an integer (e.g if Egrain1 = 2.45, then the value was truncated to 2.0 before calculating the tunneling correction). This bug has been fixed.

2. MultiWell: Bug-Fix: Previously, in simulations at zero pressure (zero collision frequency), an error could occur if the energy in a well was below all of the reaction thresholds for that well (zero rates of reaction). For this condition, the sum of the rates of all processes is equal to zero, but MultiWell would erroneously report reaction via the channel with the lowest index number. This error probably affected very few users. This bug has been fixed.

3. MultiWell: enhancement: This version of the MultiWell Suite should give the same results as v.2.07, but it is now much simpler to change Isize (the dimension of the double arrays) in MultiWell, since it is no longer necessary to recompile the code in order to do so. Now, Isize can be set at any value up to 20000 array elements. This makes it possible to use a very small grain size up to high energies. The only drawback to using very large numbers of array elements is that the execution time increases as more energy grains have to be visited (via collisions) in the lower half of the double array. *Note that Egrain1, Imax1, and Isize must still be identical for all of the wells and transition states in a given model, just as in previous versions of MultiWell.*

4. MultiWell: enhancement: The multiwell.out and multiwell.sum output formats have been changed slightly. The fractional abundance of each well is now reported with 4 significant digits instead of 3, while the statistical errors are now reported with 2 significant digits instead of 3.

5. MultiWell: enhancement: lower-case "time" and "coll" keywords are now accepted.

6. DenSum: enhancement: this version now lists (in densum.out) the lowest values of Imax1 (index number of the highest element in the lower portion of double arrays) and corresponding energy where the maximum relative fluctuations in state density are always below 1%, 2%, 3%, 4%, and 5%. If the fluctuations are not small, the extrapolation and interpolation routines are not accurate. Relative fluctuations are defined by the following, where ρ_i and ρ_{i+1} are adjacent elements in the array of densities of states:

$$\text{i.} \quad \frac{\Delta \rho_i}{\rho_i} = \frac{|\rho_i - \rho_{i+1}|}{\rho_i}$$

b. This version automatically gives a non-fatal warning on the terminal screen and in the title line of the "species.dens" output file if you choose a value for Imax1 where the density of states fluctuations are greater than 5% (the "species.dens" output file can still be used as input for MultiWell, whether or not a warning is issued). This feature gives helpful guidance regarding the choice of Imax1 when changing energy grain sizes (since the choice of Imax1 depends on the grain size), and when setting up a model for the first time. **All input and output files are completely compatible with previous versions; all sums and densities of states are the same as in v. 2.07.**

7. **NOTE: no other changes were made in this release.** Thus MomInert and Thermo are still version 2.06.

NEW IN VERSION 2.07 (February 2007):

1. MultiWell: Bug-Fix: In versions 2.05 and 2.06, an error occurred when the reaction critical energy (Eo) was lower than Emax1 when CHEMACT was selected. Essentially, when k(E) = 0 in some energy grains, part of the initial population distribution was erroneously placed in those energy grains. This could lead to calculating yields of stabilized product that are too high. The magnitude of this error depends on temperature and on the size of the excited reactant molecule. For ClOOCl and ClONO at 250 K, the erroneous excess yield was of the order of 1.e-03. This bug has been fixed. The revised version gives results for the cases when Eo > Emax1 that are almost indistinguishable from those obtained using version 2.06. When Eo < Emax1, the revised version no longer places initial population in energy grains where k(E) = 0.

2. **NOTE: no other changes were made in this release.** Thus DenSum, Mominert, Thermo, and Gauss2Multi are still version 2.06.

NEW IN VERSION 2.06 (January 2007):

1. **MultiWell: Bug-Fix:** An indexing error in multiwell-2.05 resulted in erroneous identification of the reaction channel in some multi-channel simulations. This bug was not present in previous versions and had no effect on single-channel reactions, but it could have affected some multi-channel simulations.

NEW IN VERSION 2.05 (December 2006):

2. **MultiWell: Bug-Fix:** A subtle error became apparent when using "chemact" at very low pressures in MultiWell. The error was due to an array element index error that in effect shifted the initial energy distribution to lower energy by an amount equal to Egrain1. In tests using models of the Cl + NO$_2$ and ClO + ClO recombination reactions at 300 K, this resulted in about 0.01% of the initial energies being selected erroneously below the dissociation energy of the reaction forming the chemically activated intermediate. The error first became noticeable at k/k$_\infty$ ≤ 10^{-3} and resulted in k/k$_\infty$ approaching a constant value at very low pressures. It is possible that this bug has lurked in the bowels of MultiWell since its early days. It has now been fixed. In addition, the rate constants at energies in the lower half of the double array are now treated as constant within each energy grain (Egrain1), instead of using linear interpolation within the grain. Linear Interpolation is still used at energies in the upper half of

the double array. For $k/k_\infty > 10^{-3}$, this bug fix is expected to affect results by no more than 10%-25% in most models (the relative effects are larger at $k/k_\infty < 10^{-3}$).

3. **MultiWell: Revision:** because densities of states are not calculated at reactant active energies greater than Emax2 and densities at higher energies are obtained by extrapolation, the k(E) values at the higher energies are not accurate. Previously, the higher energy k(E) values were printed in the output file. To eliminate the chance that the inaccurate k(E) values at high energy might be taken seriously, the output has been revised so that k(E) is not calculated at energies higher than is the reactant state density, but is instead set equal to 1.e-20. This revision will have no effect on any aspect of the calculations, other than the listing of k(E) in the "multiwell.array" output file.

NEW IN VERSION 2.04 (December 2006):

1. **DenSum: Bug-Fix:** Previously, the "qro" (quantum rotations) option worked properly for 2-D rotors, but not for other dimensions. Essentially, instead of the correct symmetry number, sig was replaced by sig^(d/2), where d=rotor dimension. The effect of this error depends on the symmetry number and on the dimensionality of the rotor. For a 3-fold, 1-D internal rotation, it gave sums and densities of states that were only 58% of the correct values. This error has been now been fixed.

2. **DenSum: revision:** Previously, classical rotations and translations were treated using a semi-classical approximation, where the sum of states at E=0 was set to unity. This has been changed so that they are treated as purely classical (the sum of states is zero at E=0.) This revision will have negligible effects for most users.

3. **MultiWell: revision:** subroutines Colnorm and Colstep were revised to improve accuracy of collisional energy transfer at low energies. The revised subroutines are less unstable and produce thermal energy distributions that are more accurate than previous versions. This revision is expected to affect unimolecular decay constants and fractional yields by up to 10-20%, depending on the system.

4. **MultiWell: revision:** when tunneling or slow IVR are not invoked, the k(E) array at energies below the critical energy and the IVR coefficient array are empty (set equal to zero). The empty portions of these arrays are no longer included in the output files, since they were just a waste of space.

5. **Gauss2Multi: Bug Fix:** the code has been revised so that it now works properly for atoms and linear molecules, as well as for non-linear polyatomics.

NEW IN VERSION 2.03 (August 2006):

1. **MultiWell: Bug-Fix:** (in ratearray.f) The barrier to reaction in the reverse direction was improperly calculated in the last version. This only affected simulations that calculated tunneling corrections to k(E).

2. **MultiWell: revision:** (in ratearray.f) The calculation of k(E) was modified when the density of states of the reactant is less than a fixed constant (DScrit = 0.000001/Egrain1). Thus in the sparse density of states regime, if an energy grain does not contain a reactant state, k(E) is set to zero. This change applies for k(E) calculated using both the tunneling and the non-tunneling subroutines. It protects against numerical overflow and unrealistic values for k(E) in reactions that have low energy barriers and very sparse densities of states.

3. **MultiWell: maintenance:** (in ratearray.f) The calculation of the reverse reaction rate constant was changed when tunneling is used so that the tunneling-modified sum of states of the transition state calculated for the forward direction is stored in an array and not re-calculated when computing the reverse reaction rate. This reduces execution times.

4. **MultiWell: maintenance:** (in multiwell.f) A fatal error is now returned when the CENT and TUN keywords are used simultaneously. This is because the tunneling subroutine is implemented only for reactions without centrifugal corrections. This change will have little practical effect in simulations, since tunneling is important only for tight transition states (where centrifugal corrections are not important) and centrifugal corrections are important only for loose transition states (where tunneling is not important). In a multichannel model, it is still possible to designate centrifugal corrections (keyword CENT) for some reactions (e.g. barrier-less reactions), while designating no centrifugal corrections (keyword NOCENT) for others.

NEW IN VERSION 2.0 (March 2006) - 2.03 (August 2006)

This is a major upgrade. We recommend that all users stop using older versions and use the latest version, even though it may require revising some input data files. The items marked with an asterisk (*) have necessitated changes in the input data files. See the *MultiWell Program Suite User Manual* for details.

Please use the following citations to acknowledge results obtained using this version of the MultiWell Program Suite:

a) MultiWell-2.03 Software, 2006, designed and maintained by John R. Barker with contributions from Nicholas F. Ortiz, Jack M. Preses, Lawrence L. Lohr, Andrea Maranzana, and Philip J. Stimac; University of Michigan, Ann Arbor, MI; http://aoss.engin.umich.edu/multiwell/.

b) John R. Barker, Int. J. Chem. Kinetics, 33, 232-45 (2001).

VERSION 2.02 (July 2006):

1. **MultiWell: Bug-Fix:** modified subroutine eckart.f so that tunneling corrections to k(E) terminate properly for both endothermic and exothermic reactions and for reactions with very low barriers. This error significantly affected the k(E) calculated for low barrier reactions. This bug had no effect when tunneling was not chosen.

2. **MultiWell: Bug-Fix:** corrected error in calculated reverse reaction threshold energy in subroutine ratearray.f. This error affected the magnitude of the tunneling transmission coefficients calculated in eckart.f. The magnitude of the difference in the transmission coefficient between the new version and the earlier version depends on the enthalpy of the reaction and the reaction threshold energy. This bug had no effect when tunneling was not chosen.

3. **Gauss2Multi: Bug-Fix:** minor bug fix to account properly for the Gaussian key word "RESTART".

VERSION 2.01 (April 2006):

1. **MultiWell: Bug-Fix:** corrected error in calculated strong-collider low pressure rate constant.

2. **MultiWell: maintenance:** modified subroutines colnorm.f and colstep.f to improve their accuracy when exceptionally large energy transfer step sizes are specified. These changes will result in small changes in the calculated pressure-dependence for all step sizes.

VERSION 2.0 (March 2006):

3. **MultiWell Program Suite User Manual**: **New:** the README files for the four components of the MultiWell program Suite and the Frequently Asked Questions (FAQ) have been consolidated in a User Manual (distributed as a pdf file).

4. **New: gauss2multi: New:** this new code (contributed by Andrea Maranzana) reads GAUSSIAN output files and automatically stes up data files for MomInert, DenSum, Thermo, and MultiWell. See the *MultiWell Program Suite User Manual* for details.

5. *** MultiWell**: **New:** *quantum mechanical tunneling* transmission coefficients for the Eckart unsymmetrical barrier can now be included in k(E). The data file (multiwell.dat) format has been revised and a KEYWORD is used for this purpose.

6. *** MultiWell: New:** The enthalpy of final products is now entered in the data file. This feature is used with the new tunneling feature.

7. *** MultiWell: New:** The effects of slow *intramolecular vibrational energy redistribution (IVR)* on k(E) can now be included.

8. **MultiWell: New:** Two new collision models have been added, see *MultiWell Program Suite User Manual* for info:
   a. Exponential Model with Alpha(E) = linear + exponential
   b. Exponential Model with alpha(E) switching function

9. **MultiWell: Maintenance Revision:** Subroutine qkinf.f was revised to improve its accuracy in calculating k(infinity).

10. **MultiWell: Maintenance Revisions:** subroutines Estart, Pdown, Colnorm, and Colstep were revised to improve accuracy of the initial distribution and of energy transfer at low energies. The revisions also ensure that the selected energies are aligned with energy grains at energies below Emax1.

11. **MultiWell: Maintenance Revisions:** subroutine qudint.f: converted to linear (instead of quadratic) interpolation in order to improve stability in Colnorm.f and Colstep.f numerical integrations.

12. **MultiWell: Bug-Fix:** the conversion factor for converting kcal/mole to kJ/mole was corrected from 4.1855 (international calorie) to 4.184 (thermochemical calorie). This correction also affected conversion from kcal/mole to cm^{-1} units.

13. *** MultiWell: Deleted:** option to use the Whitten-Rabinovitch method for calculating sums and densities of states within MultiWell. It is still possible to use DenSum to calculate sums and densities of states via the W-R approximation, if desired. In short, parameters related to the Whitten-Rabinovitch method for calculating densities of states are no longer input.

14. *** MultiWell: Deleted:** the un-tested feature that was intended to enable one to include elastic collisions has been removed because it did not work correctly.

15. **DenSum: New:** added the capability to calculate sum and density of *translational states* (new type of degree of freedom: "`trn`"). This enables one to use Densum to calculate microcanonical k(E)'s for *bimolecular* reactions, which can, in turn, generate microcanonical pseudo-first order reactions for use in MultiWell. See the *MultiWell Program Suite User Manual* for details.

16. **DenSum: Maintenance Revision:** Densities of states are now calculated using double-sided numerical finite differences, instead of the single-sided differences used earlier (originally described by Stein and Rabinovitch). This change does not affect the sums of states, but may affect calculated densities of states by 1-2%.

17. **Thermo: New:** a new chemical species type ("`ctst`", designating canonical transition state) enables direct calculation of *Canonical Transition State Theory rate constants*. See the *MultiWell Program Suite User Manual* for details.

18. *** Thermo: New:** electronic states and degeneracies are now listed explicitly. This change improves accuracy for species with low energy excited electronic states. [Note that there is no provision for changes in vibrational frequencies and moments of inertia for the excited electronic states.]

19. *** Thermo: New:** added provision for reading a comment line (up to 50 characters) for each chemical species.

20. **Thermo: Improvement:** parameters for van't Hoff expression of equilibrium constants $[K_{equil}(T) = A*exp(-B/T)]$ and rate constant Arrhenius parameters $[k_{TST}(T) = A*exp(-B/T)]$ are now obtained using an improved numerical derivative.

21. **Thermo: Bug-Fix:** the conversion factor for converting kcal/mole to kJ/mole was corrected from 4.1855 (international calorie) to 4.184 (thermochemical calorie). This correction also affected conversion from kcal/mole to cm^{-1} units.

22. **Thermo: Bug-Fix:** for anharmonic oscillators, the vibrational partition function, entropy, heat capacity, and enthalpy functions were not being calculated correctly. This error was greatest at high temperature for low frequency, highly anharmonic vibrations.

23. **MomInert: New:** from a single input file, the code now will calculate reduced moments of inertia for multiple torsions, instead of just one at a time.

NEW IN VERSION 1.4.1 (September 2004)

1. Please use the following citations to acknowledge results obtained using
   this version of MultiWell:
   a) John R. Barker, Nicholas F. Ortiz, Jack M. Preses, and Lawrence L. Lohr,
      MultiWell-<version> software, http://aoss.engin.umich.edu/multiwell/
      (<date>).
      [N.B. insert current <version> and <date>]
   b) John R. Barker, Int. J. Chem. Kinetics, 33, 232-45 (2001).
2. MINOR REVISION: MultiWell: when establishing the maximum length of a simulated
   time period according to the number of collisions, the collision frequency is
   now based on the collision rate constant of the initial well, and not necessarily
   on that of well #1.
3. BUG FIX: Thermo: fixed bug which produced incorrect values for A and B in the
   temperature-dependent expression for Kequil when MCC units were selected. The
   values of Kequil were correct, but the values for A and B were not.
4. BUG FIX: Estart: fixed bug that affected Pstart for thermal distribution with
   non-zero energy offset. The effect of the bug was to produce an un-shifted
   thermal distribution (Pstart) with Pstart=0 at energies less than the energy
   offset (i.e. with just the tail of the distribution above the energy offset).

NEW IN VERSION 1.3.3 (October 2003)

1. BUG FIX: MultiWell: when state densities are very sparse and hence some energy
   grains do not contain states, population could get trapped in the empty grains.
   This error (in subroutine colstep.f) affected calculations only at very low
   energies and therefore did not affect most users.
2. BUG FIX: MultiWell: an error in lower array bounds affected Estart (subroutine
   estart.f).
3. BUG FIX: DenSum: a bug that prevented use of the Whitten-Rabinovitch option
   in DenSum was fixed.
4. ANNOUNCEMENT: MultiWell: the MultiWell option to use the Whitten-Rabinovitch
   method for calculating sums and densities of states within MultiWell no longer
   works and is going to be eliminated. It will still be possible to use DenSum to
   calculate sums and densities of states via the W-R approximation.

NEW IN VERSION 1.3.2 (July 2003)

(Thanks go to Colleen Shovelin for assistance with this distribution)

1. NEW FEATURE: MultiWell: now can enter total concentration (molecule/cc) in
   place of total pressure [use Punit key word 'MCC'].
2. NEW FEATURE: Densum and Thermo: now can enter non-symmetric hindered
rotors.
   For symmetrical hindered rotors, the data file format is unchanged. For each
   unsymmetrical hindered rotor, a new line is inserted in the data file. See
   README.densum and README.thermo for details.
3. BUG FIX: Thermo: For vibrations with large negative anharmonicity, the energy
   could become negative and the summation used in calculating the partition
   function would not converge at high temperature. This summation is now
   terminated at the quantum number of the highest bound level [i.e. at
   vmax = -we/(2*xe) - 1/2].
4. MINOR FORMAT CHANGES: MultiWell: minor changes were made to the output file
   with the aim of making the debugging of data files easier. Specifically, the
   input for energy transfer parameters and reaction channels is echoed more
   closely in the multiwell.out output file. This will be helpful in spotting
   errors in the multiwell.dat input file.

NEW IN VERSION 1.3.1 (JAN 2003)

1. BUG FIX: Thermo: vibrational state degeneracies were not handled correctly
   when not equal to unity. This produced errors in the thermodynamic quantities.
2. BUG FIX: in Thermo: fixed bug that erroneously multiplied by the particle-in-
   a-box partition function when IDOF = "vib". This caused errors in entropy and
   heat capacities that varied with temperature. The magnitude of the error was
   largest for low frequency vibrations. This error affected versions 1.2.1,
   1.2.2, and 1.2.3.
3. ENHANCEMENT: MultiWell: In previous versions when using the ILT

method for k(E) and simultaneously including centrifugal corrections, the
A-factor for k(infinity) was equal to A(inf) = A*TSmom/MolMom, where A is
the A-factor from the input and TSmom and MolMom are the moments of inertia
of transition state and molecule, respectively. Thus the A-factor in the
data file did not correspond numerically to A(inf).
   TO IMPROVE CONVENIENCE, the code was revised so that the A-factor in the
data file should now be set equal to A(inf).
4. MINOR FORMAT CHANGES: MultiWell: the moment of inertia for the 2-dimensional
adiabatic external rotation has been re-labeled in the output files in order
to avoid confusion with the rotational quantum number.
5. MORE EXAMPLES: more examples have been included. Test data sets for DenSum
(taken from the literature) have been added to the examples directory.

NEW IN VERSION 1.2.3 (SEP 2002)

1. BUG FIX: in MultiWell: fixed bug in bookkeeping subroutine that gave
anomalous reaction at very short times when the collision frequency was much
smaller than all of the k(E)'s. This bug may have had a small effect on low
pressure fall-off calculations.
2. BUG FIX: in Densum: fixed bug that prevented calculation using Whitten-
Rabinovitch approximation. This bug was probably introduced in version 1.1.2.
It had no effect on the exact count option.
3. BUG FIX: in MultiWell: fixed bugs related to reading a file containing Pstart,
the initial cumulative energy distribution function.

NEW IN VERSION 1.2.2 (MAY 2002)

1. BUG FIX: Revised averaging of kuni so that only one sample per time bin per
trial is included in the average. The previous algorithm resulted in
over-weighting faster k(E)'s and gave erroneously high average kuni
values reported in multiwell.out.

NEW IN VERSION 1.2.1 (MARCH 2002)

1. BUG FIX: in Thermo, vibrational state degeneracies were not handled correctly
when not equal to unity. This produced errors in the thermodynamic quantities.
This bug has been fixed
2. NEW FEATURE: in DenSum and in Thermo, particle-in-a-box energy levels can be
selected by specifying 'box' for the type of degree of freedom; see README
files.
3. NEW NOTE: rotational and external symmetries can be handled in various ways
in MultiWell, Densum, and Thermo. To clarify the recommended way of handling
symmetry numbers, a new "NOTE ON SYMMETRY NUMBERS" has been added to
the
README files.
4. ENHANCED OUTPUT: a) the number of significant digits was increased for some

output quantities; b) zero point energies and energy differences are listed in Thermo output (this is helpful for hindered rotors and it facilitates isotopic substitution simultions).

NEW IN VERSION 1.2.0 (JANUARY 2002)

1. BUG FIX: the previous version applied the centrifugal corrections inconsistently when calculating Arrhenius parameters. k(inf) was correct, however, and no other parts of the calculation were affected. This bug has been fixed.
2. NEW FEATURE: can choose to apply or not apply the centrifugal corrections for any choice of k(E) model. Thus the corrections can be applied even when using the Inverse Laplace Transform version of k(E). This also allows centrifugal corrections be be calculated externally and then the corrected k(E) or sums of states can be read from an external file. NOTE: THIS NEW FEATURE AFFECTS DATA FILE FORMAT AS FOLLOWS: A NEW FLAG (ncen) MUST BE ADDED TO LINE #15 FOR EACH FORWARD REACTION.

NEW IN VERSION 1.1.3 (NOVEMBER 2001)

1. BUG FIX: minor bugs in the hindered rotor subroutines were fixed in Thermo and in DenSum. The bugs prevented execution on some platforms. MultiWell itself was not affected.

NEW IN VERSION 1.1.2 (SEPTEMBER 2001)

1. For convenience, input and output file names were changed to all lower case.
2. NEW OPTION (MultiWell and Thermo): energies can be read in units of cm-1, kJ/mole, or kcal/mole. Previous versions were only capable of reading the latter two units.
3. NEW OPTION (MultiWell): the maximum time simulated can be specified directly, or it can be specified as a maximum number of collisions (key-word: 'TIME' or 'COLL'. This feature is particularly useful for efficient calculation of fall-off curve and other pressure-dependent quantities. NOTE: THIS NEW OPTION AFFECTS THE LAST LINE OF THE DATA FILE.
4. NEW FEATURE (MultiWell): output file multiwell is generated that gives all of the header material in the full output file, but instead of the time-dependent results, gives only the final results of each simulation in the form of a summary table. This feature is particularly convenient for calculating fall-off curves and other pressure-dependent quantities.
5. NEW OPTION (DenSum and Thermo): by specifying a key word ('HAR' or 'OBS'), vibrational frequencies can be input as harmonic, or as observed 0-1 transition frequencies. This feature is useful when using observed fundamental frequencies

and estimated anharmonicities. NOTE: THIS NEW OPTION AFFECTS ONE LINE OF THE
   DATA FILE.
6. BUG FIX (MultiWell): the centrifugal corrections to k(E) and k(inf) were revised.
   They now correspond to Equations (4.31) and (4.30) respectively, in P. J. Robinson
   & K. A. Holbrook, "Unimolecular Reactions" (Wiley, London, 1972). The threshold
   energy including the centrifugal correction for each reaction is listed in file
   multiwell.array above the column of k(E) values for each reaction: "Eo+Rot: ...".
   A future version will incorporate a more accurate representation of centrifugal
   effects.
7. BUG FIX (DenSum and Thermo): bugs were fixed in the sums and densities
   of rotational and hindered-rotor states, and the corresponding partition
   functions.

NEW IN VERSION 1.1.1 (JULY 2001)

Note that all revised codes are compatible with the previous data file formats.

BUG FIXES

1. Collision frequency error of 0.6% in MultiWell.f.
2. Chemical activation option in MultiWell.f.

ENHANCEMENTS

MultiWell

1. Numerous minor output format revisions were made to improve clarity and
   convenience.
2. The vibrational population distribution that is output in file MultiWell.DIST
   was revised to give instantaneous "snapshots" of the population distribution.
   Previously, the distribution was obtained by averaging over the entire time-
   bin. The revised version gives the exact time-behavior, but a larger number of
   stochastic trials may be needed in order to achieve the desired precision.
3. A new output file, MultiWell.FLUX, is included. This file gives a record of
   the reactive flux for each reaction. It is useful for tracing reaction
   pathways and for identifying quasi-equilibration, etc.

DenSum

1. A good approximation for hindered rotor energies was added. Three convenient
   input formats can be chosen that are very convenient for using harmonic
   vibrational frequencies calculated by quantum chemistry programs.

MomInert

1. Subroutine Rotate.f was revised to eliminate the errors that occurred for some molecular geometries.

Thermo

1. Several portions of the code were re-written to make them more accurate.
2. The hindered rotor options that were added to DenSum were also added to Thermo.