Manual
JAGUARATE – version 2007

Jingjing Zheng and Donald G. Truhlar
Department of Chemistry and Supercomputing Institute
University of Minnesota, Minneapolis, Minnesota 55455

Program version: 2007/P9.6-J6.5
Program version date: May 25, 2007
Manual version date: Jul. 31, 2021
Copyright 2007

Abstract:

JAGUARATE is a set of FORTRAN subroutines and Unix scripts for interfacing the POLYRATE and JAGUAR computer programs for the purpose of carrying out direct dynamics calculations of gas-phase chemical reaction rates of polyatomic species (and also atoms and diatoms as special cases) using the electronic structure methods available in JAGUAR to calculate the potential energy surface and POLYRATE for the dynamics. The interface is based on the POLYRATE hooks protocol. The dynamical methods used are variational or conventional transition state theory and multidimensional semiclassical approximations for tunneling and nonclassical reflection. Rate constants may be calculated by any of the methods available in the POLYRATE–version 9.6 program for canonical or microcanonical ensembles or for specific vibrational states of selected modes with translational, rotational, and other vibrational modes treated thermally. Bimolecular and unimolecular reactions are included. Both single-level and dual-level calculations may be carried out. In single-level mode, optimized geometries, potential energies, gradients, and Hessians can be calculated by any of the electronic structure methods in the JAGUAR packages. In dual-level mode, the lower-level data is calculated by JAGUAR, and the higher-level data is read in from an external file.

JAGUARATE–version 2007 provides an interface between two other programs:

POLYRATE–version 9.6, by 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, POLYRATE–version 9.6, University of Minnesota, Minneapolis, 2007.

and

JAGUAR, version 6.5, Schrödinger, LLC, New York, NY, 2005.

CONTENTS

1. LICENSING

JAGUARATE - version 2007 is licensed under the Apache License, Version 2.0.
The manual of *JAGUARATE* - version 2007 is licensed under CC-BY-4.0.

Publications of results obtained with the *JAGUARATE* - version 2007 software should cite the program and/or the article describing the program.

No guarantee is made that this software is bug-free or suitable for specific applications, and no liability is accepted for any limitations in the mathematical methods and algorithms used within. No consulting or maintenance services are guaranteed or implied.

The use of the *JAGUARATE* - version 2007 implies acceptance of the terms of the licenses.

2. REQUIRED REFERENCES

Publications based on results obtained with this computer code should include the following references:

1. J. Zheng and D. G. Truhlar, JAGUARATE –version 2007, University of Minnesota, Minneapolis, MN, 2007.

2. 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, POLYRATE–version 9.6, University of Minnesota, Minneapolis, 2007.

3. JAGUAR, version 6.5, Schrödinger, LLC, New York, NY, 2005.

Additional references are given in the documentation for POLYRATE and JAGUAR.

3. INTRODUCTION

JAGUARATE is a program for the analysis of reactants, products, and transition states of chemical reactions and for direct dynamics calculations of variational transition state theory (VTST) rate constants and multi-dimensional semiclassical tunneling probabilities using the electronic structure methods in the JAGUAR packages to represent the potential energy of interaction and its first and second derivatives with respect to nuclear coordinates whenever they are needed. This version, 2007/P9.6-J6.5, interfaces POLYRATE–version 9.6, which is a program for dynamical rate calculations, with the electronic structure program JAGUAR.

Using JAGUARATE presuppose that the user has both POLYRATE 9.6 and JAGUAR 6.5 on the same computer working properly before attempting to run JAGUARATE. No part of POLYRATE 9.6 or JAGUAR 6.5 is contained in JAGUARATE or needs to be modified for running this program.

This JAGUARATE manual covers only material that is not covered in the POLYRATE and JAGUAR manuals. The user of JAGUARATE should read those manuals first.

The interface between POLYRATE and JAGUAR is made by a series of FORTRAN subroutines included in the files `hooks_jr.f` and `hooks_mdep.f`, which are specialized versions of the routines in the `hooks.f` file in POLYRATE 9.6 and by a C shell script for running JAGUAR. This C shell scripts, named `jshuttle` and `jextract`, are called from inside JAGUARATE, and they has to be able to start running JAGUAR using an input file named as the first argument given to the scripts. It produces an output file named as the second argument given to the scripts. For the user's convenience, a well documented script is provided, and in most cases the user will only need to change one line, in order to set the *jaguarpath* and *SCHRODINGER* variable to the appropriate path where JAGUAR is located.

Note that running two JAGUARATE calculations in the same directory can cause problems due to overwriting of some of the temporary files.

JAGUARATE uses a subroutine usually included in libraries provided with FORTRAN compilers. This subroutine is called *system* on the IBM Regatta Power4, SGI Altix, and

IBM Netfinity with Pentium III computers. The prospective user of JAGUARATE should be aware that this utility program is needed for running JAGUARATE.

4. DISTRIBUTION

JAGUARATE is a set of subroutines for interfacing POLYRATE and JAGUAR. The user needs to obtain four items of code:

– POLYRATE: The POLYRATE code is a licensed code available from the University of Minnesota. Currently the license fee is waived for all users. For further information see:
```
http://comp.chem.umn.edu/polyrate
```

– JAGUAR: JAGUAR is a licensed code available from Schrödinger LLC. For further information see
```
http://www.schrodinger.com
```

– JAGUARATE: The JAGUARATE code is a licensed code available from the University of Minnesota. Currently the license fee is waived for all users. For further information see:
```
http://comp.chem.umn.edu/jaguarate
```

– *system*:   This utility code is also required. It is available in standard FORTRAN libraries.

The prospective user of JAGUARATE must obtain and install POLYRATE and JAGUAR before proceeding with JAGUARATE.

The JAGUARATE program is distributed as a compressed tar file named `jaguarate2007.tar.gz`. The distributed file (either one of the above files) should be uncompressed and untarred in the `polyrate9.6` directory. To uncompress, enter:

```
gunzip jaguarate2007.tar.gz
```

The uncompressed file will be named `jaguarate2007.tar`. After extracting the files from the tar file, which can be done with the command:

```
tar -xvf jaguarate2007.tar
```

a new directory, `jaguarate`, is created. This directory contains all the files included in the distribution package. If these instructions are followed correctly, the directory structure should be the following tree structure:

```
                          polyrate9.6
                               |
  -------------------------------------------------------------------
  |     |       |         |       |        |        |       |         |      |
 doc   exe  jaguarate    obj    poten   script    src    testo   testrun  util
              |
         ---------------------------------------
              |         |          |                      |
           script    source     testo                  testrun
                                                          |
                                                 -----------------
                                                 |      |      |       |
                                                ch5    h3    nh3    oh3
```
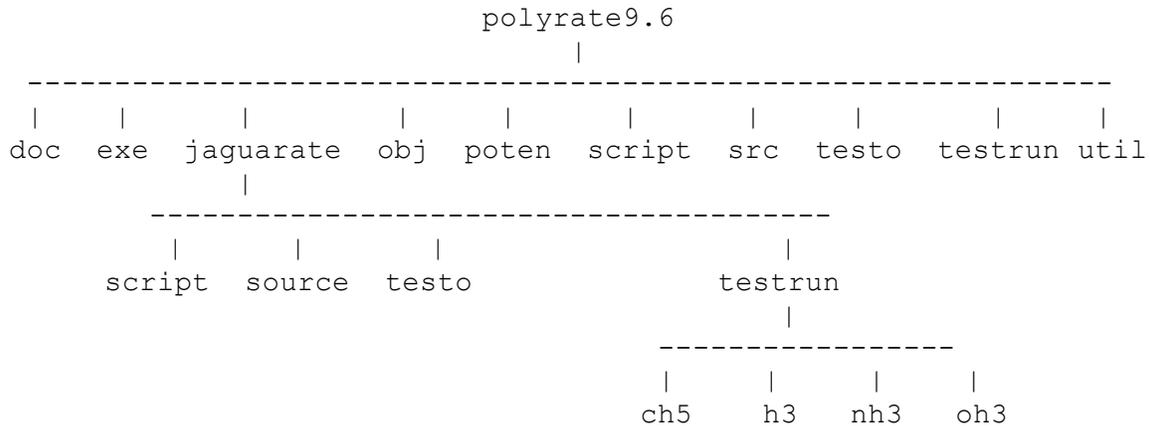
The files will be distributed among the directories as follows:

`jaussrate:` the C shell scripts `jshuttle,` `jextract` and five subdirectories:

`script:`   1 files: `jrcompile`

`source:`   4 files comprising the source code for JAGUARATE: `jaguarate.inc,` `head_jr.f`, `hooks_jr.f`, and `hooks_jr.wrk`

`testo:`   This directory contains the following output files of the test runs:
         10 files: `ch5tr1.fu15, ch5tr2.fu15, oh3tr1.fu15,` `oh3tr2.fu15, oh3tr3.fu15,` oh3tr4.fu15, `h3tr1.fu15, h3tr2.fu15, nh3tr1.fu15,` `nh3tr2.fu6`

`testrun:`   1 file: `run_all.jc,` and 3 subdirectories: `ch5,` `h3,` nh3 and `oh3` with the input files for the test calculations.

5. INSTALLATION

First the user should obtain licensed copies and install the POLYRATE and JAGUAR packages. Next the user should obtain a licensed copy of the JAGUARATE package. After downloading, uncompressing, and untarring the file, the JAGUARATE package should appear as a directory, as described in Section 4.

There are a few variables that have to be set large enough to accommodate the system or systems to be studied. These variables are set in the include file `param.inc` in the POLYRATE side of the interface. The user should consult the POLYRATE manual for additional details.

The installation of the JAGUARATE program is carried out by running the Perl script `configure`. The script will copy `hooks_jr.wks` to the `hooks_mdep.f`, will compile the POLYRATE 9.6 files substituting the `hooks.f` file of standard POLYRATE by `hooks_jr.f` and `hooks_mdep.f`, and will create the executable file `jaguarate.exe` in the `exe` subdirectory in the `polyrate9.6` directory. The executable `jaguarate.exe` will then be accessible for all the JAGUARATE calculations.

Before running JAGUARATE, one line of the C shell script `jshuttle` and `jextract` should be changed as described in Section 1., in order to set the *jaguarpath* and *SCHRODINGER* variable to the appropriate path where JAGUAR is located

6. PROGRAM DESCRIPTION

The JAGUARATE program follows the POLYRATE hooks protocol. This means that if energy, gradient, and/or Hessian calculations are needed by POLYRATE, the program calls the appropriate hooks subroutine that will return that information. (The user may read more about hooks in the POLYRATE manual.)

6.1.   Description of JAGUARATE subprograms

This is a brief description of JAGUARATE subprograms. In most of the cases, a more detailed description is given in the comment cards at the beginning of the FORTRAN code for each subprogram.

ehook   Equivalent to the *ehook* subroutine in the POLYRATE hooks. For a given set of coordinates, it calculates the energy using JAGUAR.

enatin   Calculates the energy for atomic systems.

escener   Carries out JAGUAR energy calculations.

escfirst   Carries our JAGUAR energy and first derivative calculations. First derivatives are also called gradients.

escsec   Carries out JAGUAR Hessian calculations. Hessian are also called second derivatives.

geoin   Carries out JAGUAR geometry optimizations.

ghook   Equivalent to the *ghook* subroutine in the POLYRATE hooks. For a given geometry, calculates the energy and first derivatives.

ginpene   Creates the JAGUAR input file for energy calculations.

ginpfrs   Creates the JAGUAR input file for gradient calculations.

ginpsec   Creates the JAGUAR input file for Hessian calculations.

goutsec	Reads the output and restart files generated by JAGUAR and extracts the geometry, energy, and first and second derivatives of the energy with respect to atomic coordinates.
grest	Reads and writes the information in the restart files of a JAGUARATE restart calculation.
headr	Prints out the program header.
hhook	Equivalent to the *hhook* subroutine in the POLYRATE hooks. For a given geometry, calculates the Hessian matrix using whether JAGUAR or POLYRATE methods.
ohook	Equivalent to the *ohook* subroutine in the POLYRATE hooks. Optimizes a given initial geometry, using either POLYRATE or JAGUAR methods.
prep	Prepares the calculation and, depending on the selected options, carries out certain geometry optimizations and Hessian calculations.
prepj	Initialize variables dependent on each stationary point.
rcodgr	Reads the input option for the JAGUAR runs from file `esp.fu70`.
redinf	Reads the information about reactants, products and saddle point calculated in the *prep* subroutine.
renergr	Reads the input options for JAGUAR energy calculations.
rfirstgr	Reads the input options for JAGUAR gradient calculations.
rgengr	Reads the options in the general section of the `esp.fu70` input file.
rinpgr	Reads the `esp.fu70` JAGUARATE input file.

rlingr	Utility program for reading in a line of the `esp.fu70` input file and parsing off comments and extra spaces.
rsecgr	Reads the input options for JAGUAR Hessian calculations.
rstatgr	Reads the input options given in the `esp.fu70` input file for the stationary points.
secin	Carries out JAGUAR Hessian calculations for stationary points.
setup	Initializes some variables and calls the subroutines for reading in the `esp.fu70` input file.
store	Stores some information that could be useful in future calculations in order to avoid duplicate JAGUAR calls.

Note that JAGUARATE does not use any of the utility routines (routines starting with *y*) of the generic hooks package of POLYRATE.

6.2.   Restarting a calculation

The JAGUARATE restart option should not be confused with the POLYRATE restart options (see Section 7.C of the POLYRATE manual). The POLYRATE restart options can be used with JAGUARATE, but JAGUARATE also has its own, unique restart capability. The rest of this section concerns this JAGUARATE restart capability.

The JAGUARATE restart option is controlled by the JRRESTART keyword in the JRGENERAL section of the unit `esp.fu70` input file. The JAGUARATE restart option is designed to take advantage of any previous calculations that may have been made on the same system, so that the number of JAGUAR calls is minimized. As long as the information on the stationary points from previous calculations is still applicable, a restart calculation can be made (if there is a change in any stationary point input or option, the program will not read this information, and the results of trying a restart calculation are unpredictable). This restart option allows the user to change any parameter related to the reaction path calculations using as much information as possible from previous calculations.

Two restart files are used in this kind of restart calculation: `esp.fu83`, which stores the information to be read, as originated in a previous JAGUARATE calculation, and `esp.fu84`, where the useful information read from `esp.fu83` is stored along with the information calculated for the first time in the present JAGUARATE run (`esp.fu84` is the file to be used for future restart runs). The `esp.fu84` file has to be created by JAGUARATE, so if the program finds that this file exists, it will stop, to prevent overwriting a restart file.

One important practical point related to this restart option is that, if one finds that the range of the reaction path calculated in a JAGUARATE run is not large enough to describe some effect (for example, tunneling), one can extend the calculated reaction path without repeating the calculation of the points included in the previous JAGUARATE run. One should rename the `esp.fu84` file provided by the first run as `esp.fu83` and then run again with JRRESTART on. In a similar way, if one finds problems in the SCF convergence at some points along the reaction path, one can repeat the calculation including some of the options for improving SCF convergence available in JAGUAR without recalculating the well converged points. Another possibility is computing one side of the reaction path with one computer (or one processor of a multiprocessor

computer) and the other side with a different computer (or different processor); a new restart file combining the information from both calculations can be constructed by just appending one restart file to the end of the other restart file, allowing a calculation using the whole reaction path with no duplication of effort, at least in principle; in practice, due to the different precision of two different machines and round-off errors, some recalculation might be needed. One should be aware, though, that if a calculation is made using a step-size that is too large, giving a non-converged reaction path, a restart calculation using a different step-size would probably be unsuccessful, since the points along the two reaction paths would be different.

There is only one parameter related to the path that should not be changed between an original calculation and a restart calculation, namely the value of SCALEMASS. Changing this parameter will cause a miscalculation of the frequencies. It is important to note that its default value is 1.0 amu, and this is the value assumed if no reaction path calculation is desired. Therefore, if a restart calculation including the reaction path is based on a restart file written by a TST-only calculation, SCALEMASS must be set to 1 amu in order to get the right frequencies. In general, we recommend always using a value of 1.0 amu for SCALEMASS in JAGUARATE.

A JAGUARATE restart run requires that all the information about all the stationary points be present on file `esp.fu83`, and this data cannot be updated in this kind of restart run. However, the use of the STATUS keyword in the REACT1, REACT2, PROD1, PROD2, WELLR, WELLP, and START sections of the POLYRATE `fu5` input file can alleviate this inconvenience. Thus, the user can calculate reactants and products separately and include the information obtained in the `fu5` input file.

The restart option works in the following way: when POLYRATE needs an energy, gradient, and/or Hessian for a given geometry, it first check if the geometry is stored in `esp.fu83`, and then it checks if the required information is stored in this same file. If one of these conditions is not fulfilled, a JAGUAR calculation is run to obtain the desired information. If both conditions are fulfilled, the information is read from `esp.fu83`, and no JAGUAR job is spawned. The geometry check is performed by comparing each of the Cartesian coordinates of the desired geometry with the Cartesian coordinates in `esp.fu83`. If the values differ by more than a criterion given by RSTTOL, the geometries are considered to be different. It is important to have an appropriate value for RSTTOL: if the criterion is too tight, the check might fail due to the numerical round-off and to the fact that the

precision of the written information is limited, and redundant calculations could be carried out, increasing unnecessarily the cpu time of the calculation. However, if this criterion is too loose, the check could be passed for two geometries that are only slightly different, and the restart option can be giving to JAGUARATE inaccurate information. The later case can be especially true when performing reaction-path calculations with very small step-sizes, numerical differentiations, or accurate geometry optimizations. Therefore, the user must be very careful about changing this parameter. The default value is `1.D-8`, which is somehow very conservative, but it is safe. For very expensive calculations, one might want to use a higher value, but a too high value can give unphysical results. If the user increases this parameter, he or she has to be very aware of the risk it posses in the calculation, and all the results must be carefully checked. Therefore, only experienced users are advised to change this parameter.

7. DESCRIPTION OF INPUT FILES

We will assume that the user knows how to use POLYRATE 9.6 and JAGUAR 6.5 and is familiar with all their keywords. Therefore, when talking about the common input files, we will only discuss the differences between running POLYRATE 9.6 and running JAGUARATE 2007

7.1. File usage

In addition to the POLYRATE 9.6 and JAGUAR 6.5 input files, JAGUARATE uses several files of its own for input data, for storing restart information, and for output. All these files have the name esp.fu#, where # denotes an integer.

esp.fu70   General JAGUARATE input data.

esp.fu71   JAGUAR input file for geometry optimization of reactant 1, if such optimization is going to be carried out.

esp.fu72   JAGUAR input file for geometry optimization of reactant 2, if the reaction studied is bimolecular and if such optimization is going to be carried out.

esp.fu73   JAGUAR input file for geometry optimization of product 1, if such optimization is going to be carried out.

esp.fu74   JAGUAR input file for geometry optimization of product 2, if the reaction studied has two products and if such optimization is going to be carried out.

esp.fu75   JAGUAR input file for geometry optimization of the saddle point or constrained optimization of a reaction path starting geometry, if such optimization is desired.

esp.fu76   reserved

esp.fu77   JAGUAR input file for geometry optimization of a well on the reactant side of the reaction path, if it exists and its optimization is going to be carried out.

esp.fu78   JAGUAR input file for geometry optimization of a well on the product side of the reaction path, if it exists and its optimization is going to be carried out.

esp.fu81   JAGUAR temporary input file, generated by JAGUARATE.

esp.fu82   JAGUAR temporary output file, generated by JAGUAR and *jextract* script . If the JAGUAR calculation fails, it can be examined in order to find out why the failure occurred.

esp.fu83   Restart file to be read during a restart calculation (see Section 6.1).

esp.fu84   Restart file to be written during a restart calculation (see Section 6.1).

esp.fu85   JAGUARATE uses the jextract script to get energy, Cartesian coordinates, and force from jaguar output and write these information to `Test.Fchk` so that FORTRAN code can read them from this file. JAGUARATE also copy the restart file generated by JAGUAR to `Test.rst` so that FORTRAN code can read Hessian from this formatted restart fiel. This file will not be removed after finishing a calculation, so if the JAGUAR calculation fails, it can be examined in order to find the cause of the failure.

Note that this file usage is consistent with Section 17 of the POLYRATE manual. Note also that `esp` stands for electronic structure package, and `fu` stands for FORTRAN unit. Finally note that `esp.fu76` is reserved for future use, but it is not used in this version.

7.2. Description of `fu5` unit

A JAGUARATE calculation requires some input from input units for POLYRATE. At the very least, an `fu5` input file is required for indicating several options such as electronic degeneracies, temperatures for the rate constant calculations, etc. Therefore, an `fu5` file must be written, precisely as if we were using an analytic potential energy surface. If the calculation requires some additional input files, the user must provide them, following the instructions in the POLYRATE 9.6 manual. It is important to clarify some points about preparing the input file for unit `fu5`:

RESTART

If a POLYRATE 9.5 restart run is selected (option *readfu1* or *readfu1&2* for the RESTART keyword in the GENERAL section), the program will not modify any characteristic of the calculated reaction path. We therefore advise the user to use only the restart option in JAGUARATE, controlled by the JRRESTART keyword in JRGENERAL section of the `esp.fu70` input file, until the reaction path calculation is completely converged and all the desired tunneling options are calculated. When no more electronic structure calculations are required, the POLYRATE restart is recommended, since it is faster than the JAGUARATE restart.

ATOMS

The ordering in the ATOMS keyword list of the GENERAL section of the input file for unit `fu5` must be consistent with the ordering in unit `fu75`, if this unit is used in the calculation.

NOSUPERMOL

Because of the way the interface is constructed, the NOSUPERMOL keyword is required (note that SUPERMOL is the default option). Therefore, it is recommended that only size-consistent methods should be used in JAGUARATE.

EZERO

Because of the way the interface is constructed, the user must choose the *calculate* option for the EZERO keyword of the ENERGETICS section, which is the default option.

POTENTIAL

The *hooks* option is required.

OPTTS and **OPTMIN**

In JAGUARATE there are two ways to optimize the geometries: by means of JAGUAR methods or by means of POLYRATE 9.6 methods. The choice between the two methods is done in the OPTIMIZATION section of the fu5 input file. Choosing the option *BFGS*, *NR*, or *EF*, for the OPTMIN or OPTTS keywords in the OPTIMIZATION section, will cause JAGUARATE to use the methods native to POLYRATE 9.6, using as starting geometries those in the fu5 input file and controlling the optimization procedure by means of the keywords selected in the OPTIMIZATION section of the fu5 input file. In these cases, the input files fu71 through fu75 will not be required. The INITGEO keyword needs to take the option *GEOM* in the REACT1, REACT2, PROD1, PROD2, WELLR, WELLP, and START sections of the fu5 input file.

If the option *OHOOK* is chosen for both the OPTTS and OPTMIN keywords in the OPTIMIZATION section of the fu5 input file, JAGUARATE will optimize the geometries of the stationary points using the JAGUAR program according to the options selected in the fu70 input file and the fu71-fu78 input files. The initial geometries for the optimization will be those indicated in the fu71-fu78 input files and the options selected in the OPTIMIZATION section in the fu5 input file will be ignored. INITGEO should take the value *HOOKS* in the REACT1, REACT2, PROD1, PROD2, WELLR, WELLP, and START sections of the fu5 input file.

If the user wishes to optimize the stationary points, we recommend the use of JAGUAR methods; in particular this is accomplished by using the *OHOOK* option for both the OPTMIN and the OPTTS keyword in the OPTIMIZATION section of the fu5 input file, using initial geometries given in the fu71 through fu75 input files, and setting

INITGEO equal to *HOOKS*. A further explanation of these keywords will be provided below.

SECOND

The calculation of the Hessian matrices can be done by numerical differentiation of the gradients, by means of the POLYRATE 9.6 methods, or by the JAGUAR methods, with the latter option strongly recommended. The choice is made by means of the *GHOOK* or *HHOOK* options in the HESSCAL keyword in the SECOND section of the `fu5` input file. If *HHOOK* is selected, the remaining keywords of the SECOND section are ignored and the Hessian, calculations will be controlled by the options selected in the `fu70` input file. If *GHOOK* is selected, the Hessian calculation will be carried out following the options indicated in the SECOND section, ignoring the options for the Hessian calculation selected in the `fu70` input file.

Although JAGUAR can perform Hessian calculations using any of the electronic structure methods available in JAGUAR, the option of performing the Hessian calculation using POLYRATE methods is implemented for completeness. However the user is advised for efficiency reasons against using POLYRATE for the Hessian calculations.

GEOM

The ordering of the atoms in the GEOM keyword in sections REACT1, REACT2, PROD1, PROD2, and START must be consistent with the ordering in units `fu71`, `fu72`, `fu73`, `fu74`, and `fu75`, when they are used; and also the ordering in `fu75` must be consistent with the one in ATOMS in the GENERAL section.

CONSTANT

If the user selects JAGUAR for optimizing the geometries (this is accomplishing with the *OHOOK* option for the OPTMIN and OPTTS keywords in the OPTIMIZATION section of the POLYRATE `fu5` input), the CONSTANT keyword in the REACT1, REACT2, PROD1, PROD2, WELLR, WELLP and START sections of the `fu5` input file is meaningless. The frozen parameters must be indicated in units `fu71-fu78`, according to the instructions explained in the JAGUAR manual. If a user selects POLYRATE 9.6 for optimizing the geometries, this keyword has the same function as in any other POLYRATE

calculation, fixing the value of the selected coordinates and avoiding their optimization, as explained in Section 11.A.6 of the POLYRATE 9.6 manual.

INITGEO and **STATUS**

There are two options for reading the initial geometries of reactants, products, wells, and saddle point: the first one is by means of units `fu71` through `fu78`, if a JAGUAR optimization is desired (*OHOOK* option for the OPTMIN and OPTTS keywords in the OPTIMIZATION section). In this case, the INITGEO keyword has to be set to *HOOKS*, and the files `fu71-fu78` should be the appropriate input files for a JAGUAR optimization. The second one is by means of the GEOM keyword, if a POLYRATE 9.6 optimization (*BFGS*, *NR*, or *EF* options in the OPTMIN or OPTTS keyword in the OPTIMIZATION section) or no optimization is going to be carried out. Then, the INITGEO keyword needs to be set to *GEOM*. Therefore, the initial geometry for the optimization of those systems that are going to be optimized using JAGUAR methods should be given in units `fu71-fu78` and the INITGEO keyword in the respective section has to be set to *HOOKS*, while the initial geometry for those systems which are to be set to *HOOKS*, while the initial geometry for those systems which are going to be optimized using POLYRATE methods or the optimized geometry of the systems which are not going to be further optimized should be given in unit `fu5` and the INITIGEO keyword in the respective sections has to be set to *GEOM*.

The combination of the keywords INITGEO, STATUS and OPTTS and OPTMIN, therefore, will indicate the procedure of the initial and/or optimized geometries for the stationary points. The combinations are:

– For optimizing the geometries using the methods in JAGUAR: OPTTS and OPTMIN in the OPIMIZATION section have to be set to *OHOOKS*, INITGEO has to be set to *HOOKS* and STATUS set to *0* in the corresponding REACT1, REACT2, PROD1, PROD2, WELLR, WELLP, and/or START sections. The initial geometry should be given in the files `fu71` through `fu78`.

– If the geometry optimization of one of the stationary points is not desired, the INITGEO keyword has to be set to *GEOM*, and the STATUS keyword should be set to an allowed value greater than zero in the corresponding REACT1, REACT2, PROD1,

PROD2, WELLR, WELLP, and START sections of the `fu5` input file. The optimized geometry will be read from the `fu5` input file.

– For optimizing the geometries using the methods in POLYRATE (not recommended): OPTTS and OPTMIN in the OPTIMIZATION section have to be set to *BFGS*, *NR* and/or *EF*, and INITGEO has to be set to *GEOM* and STATUS set to *0* in the corresponding REACT1, REACT2, PROD1, PROD2, WELLR, WELLP, and/or START sections of the `fu5` input file. The initial geometry will be given in the appropriate section of the `fu5` input file. If the geometry of one of the stationary points is already optimized, the only parameter that has to be changed is the value of the STATUS keyword in the corresponding section of the `fu5` input file.

A value greater than *0* for the STATUS keyword in any of the REACT1, REACT2, PROD1, PROD2 and/or START sections involves no optimization of the geometry input in the `fu5` file and, if a value greater than *2* is selected, no Hessian calculation. If STATUS is set to *4* in the START section of the `fu5` input file, the Hessian matrix as it appears in a JAGUAR restart file can be input, according to the instructions in the POLYRATE manual.

ANHARMONICITY

Although anharmonic calculations can be carried out, the user must keep in mind the extremely high cost of numerical third or fourth derivatives of the energy when using ab initio methods. With the anharmonicity options available in POLYRATE 9.6, this extra cost is not usually warranted. We therefore recommend not using anharmonic options in the REACT1, REACT2, PROD1, PROD2, WELLR, WELLP, and START sections when they require derivatives of order higher than two, at least until some later version of POLYRATE with better anharmonicity options becomes available. The only anharmonicity option that do not require derivatives higher than second are Morse I and hindered rotator.

In addition, when calculating second or higher order derivatives using the numerical methods of POLYRATE 9.6, JAGUAR is unable to successfully calculate some slightly distorted structures of linear molecules. Therefore, we recommend that Hessians be calculated with JAGUAR rather than with the methods native to POLYRATE.

SCALEMASS

If restart calculations are desired, the value of the SCALEMASS variable keyword must be the same for the whole series of calculations. Note that SCALEMASS is the reduced mass to which all isoinertial coordinates are scaled. See also the discussion of SCALEMASS in Section 6.2.

7.3. Description of `esp.fu71` through `esp.fu78` input files

The data files `esp.fu71` through `esp.fu78` are JAGUAR-type data files. They are used only as input files for JAGUAR optimization on reactants 1 and 2 (`esp.fu71` and `esp.fu72`, respectively), products 1 and 2 (`esp.fu73` and `esp.fu74`), of the well on the reactant side (`esp.fu77`), of the well on the product side (`esp.fu78`), and of the saddle point or other starting geometry (`esp.fu75`). If no optimization using JAGUAR is desired, these files are not needed.

For constructing these files, the user must check the JAGUAR manual. Any option available for JAGUAR can be used.

As mentioned above, when creating these files, the order of the atoms in unit `fu75` must be consistent with the order of the atoms input in the ATOMS keyword in the GENERAL section of the POLYRATE `fu5` input file, and the order of the atoms in units `fu71-fu78` must be consistent with the index specifications in the GEOM keyword in the REACT1, REACT2, PROD1, PROD2, WELLR, WELLP, and START sections of the `fu5` input file.

For the sake of consistency, the method chosen for the electronic structure calculations for a given reaction must be the same in all the `esp.fu71` through `esp.fu78` files representing the species for that reaction. Only if one of the species is the hydrogen atom and electronic correlation is included can the quantum methods be different (since no correlation energy can be calculated for the hydrogen atom). The electronic structure method must also be consistent with the options related to energy and first and second derivatives chosen in the `fu70` input file.

When studying a reaction with no saddle point, the user must insure that the optimization procedures chosen for the starting point will not lead the system to reactants or products. This can be accomplished by freezing the appropriate geometrical parameters. If no geometrical parameter is kept fixed, the optimization will lead to a point where the gradients are zero and the procedure for following the reaction path will not work successfully.

7.4. Description of `esp.fu70` input file

Along with the input `fu5` file, which controls the POLYRATE options, the `fu70` input file will control all of the JAUSSRATE options and some of the JAGUAR input options. The `fu70` input file is divided into sections which, like the `fu5` sections, are denoted by a header preceded by an asterisk (*). There are eight sections, each starting with JR in order to avoid confusion with similar sections in the `fu5` input file. These sections are JRGENERAL, JRCOMMON, JRREACT1, JRREACT2, JRPROD1, JRPROD2, JRWELLR, JRWELLP, JRSTART and JRPATH. In these sections, the appropriate keywords have to be specified.

Section name	Description
JRGENERAL	Restart options
JRCOMMON	JAGUAR options common to all the stationary points
JRREACT1	JAGUAR options specific to the first reactant
JRREACT2	JAGUAR options specific to the second reactant, if any
JRPROD1	JAGUAR options specific to the first product
JRPROD2	JAGUAR options specific to the second product, if any
JRWELLR	JAGUAR options specific to the reactant well, if any
JRWELLP	JAGUAR options specific to the product well, if any
JRSTART	JAGUAR options specific to the starting (or saddle) point
JRPATH	JAGUAR options common to all the nonstationary points along the reaction path

There are three type of keywords: switch (which does not have any argument), variable (which requires one argument following the keyword), and list (which requires a list of options, with an END line). See the POLYRATE manual for a more thorough discussion of the three types of keywords.

7.4.1. The GRGENERAL section

The JRGENERAL section controls JAGUARATE's own options. There are only three keywords allowed in this section, JRRESTART and NOJRRESTART, with JRRESTART being the default, and RSTTOL.

GRRESTART (NOGRRESTART)

This is a switch keyword that tells the program to check the restart file `esp.fu83` and search for information about the point to be calculated. If it finds the required information about that point, the program writes it in the `esp.fu84` file and uses the stored information instead of calculating it. If the information needed is not present in the `fu83` file, JAGUARATE runs JAGUAR and writes the JAGUAR output information to unit `fu84`. If NOJRRESTART is selected, neither reading file `fu83` nor writing file `fu84` will be performed.

RSTTOL

RSTTOL is a variable keyword that must be followed by a real number, which is the value of the tolerance in the comparison of geometries between the geometry currently used by JAGUARATE and the geometry found in a restart file `esp.fu83`. The meaning of this keyword is explained in detail in Section 6.2. The inexperienced user is not advise to change this value from its default value, *1.E-8*.

> *Example:*
> ```
>     RSTTOL        0.00000001
> ```

7.4.2. The JRCOMMON section

The JRCOMMON section reads the information common to all the JAGUAR calculations for the stationary points and points along the reaction path, excepting the JAGUAR geometry optimizations, which are totally controlled by the `fu71` through `fu78` input files. The options selected in this section will be applied to all the JAGUAR calculations unless a different keyword is specified in the section corresponding to a specific point. This section needs to precede the specific sections JRREACT1, JRREACT2, JRPROD1, JRPROD2, JRSTART, JRWELLR, JRWELLP, and JRPATH. The following keywords are allowed in the JRCOMMON section:

JRENER

This is a list type keyword and therefore it must include an END line to indicate the end of the list (see the POLYRATE manual for a description of list keywords). JRENER includes the keywords that JAGUAR will use for carrying out an energy calculation. The default for this keyword is *#&gen isymm=0 iunit=2 basis=STO-3G &*. In order to get the desired results, one particular keyword must always be supplied for this kind of calculation: *iunit=2* (or their equivalent JAGUAR keywords; see the JAGUAR manual for a discussion of alternative forms of JAGUAR keywords).

> *Example:*
> ```
> JRENER
> &gen isymm=0 iunit=2 basis=6-31G* iuhf=1 &
> END
> ```
The JAGUAR keywords line can also be written in a few separate lines.

JRFIRST

This accomplishes a similar purpose as the JRENER keyword, but it indicates the keywords to be used in gradient calculations. Again, *iunit=2* are required. The default is *&gen isymm=0 iunit=2 basis=STO-3G igeopt=-1 &*.

JRSEC

This keyword is only used when the *HHOOK* option is specified in the HESSCAL keyword of the SECOND section of the `fu5` input file. It accomplishes a purpose similar to the

JRENER and JRFIRST keywords, but indicating the options for a Hessian calculation. *iunit=2* and *igeopt=-1* are required, since JAGUAR will not give force information with the keyword *igeopt=-1*. The default is *&gen isymm=0 iunit=2 basis=STO-3G ifreq=1 igeopt=-1 &*.

7.4.3. The JRREACT1, JRREACT2, JRPROD1, JRPROD2, JRWELLR, JRWELLP, JRSTART, and JRPATH sections

In some cases, the options selected in the JRCOMMON section might not be the most useful for all the points to be calculated, especially when spin multiplicities are different for reactants, products, wells, and saddle point. Therefore these eight sections allow us to select different keywords for the energy, gradients, and Hessian calculations by means of the JRENER, JRFIRST, and JRSEC list keywords. The options for the first reactant should be specified in the JRREACT1 section; in the JRREACT2 the options for the second reactant, if it exists; in JRPROD1 and JRPROD2 the options for the first product and, if it exists, the second one; in JRWELLR the options for a well on the reactant side of the reaction path, if it exists; in JRWELLP the options for a well on the product side, if it exists; section JRSTART will indicate the options for the saddle point or starting geometry, and JRPATH will indicate the options for JAGUAR calculations on the non-stationary points along the reaction path. If no changes from the options selected in the JRCOMMON section are wanted, these sections can be skipped.

These sections can include one or more of the JRENER, JRFIRST, and JRSEC keywords explained above for the JRCOMMON section, with the same syntax that we explained in the previous section, and requiring the keywords *iunit=2* in all the inputs.

In order to avoid problems related to the reorientation of the systems that JAGUAR performs, in addition to *iunit=2*, the keyword *isymm=0* is strongly recommended for its use in the JRPATH section; otherwise, the results could be wrong even though they would seem reasonable and no error would be detected without a careful study of the directions of the gradients (see the POLYRATE manual for a more thorough discussion of reorientation problems and JAGUAR reorientation).

The *isymm=0* keyword is also recommended when third or fourth derivatives of the energy are needed(i.e., for anharmonic calculations or when using the cubic algorithm for starting the reaction path) and when the *HHOOK* option is selected for the HESSCAL keyword in the SECOND section of the fu5 input file is on, since for the numerical differentiation of the derivatives computed using JAGUAR it is necessary to have them oriented in a consistent way.

8. TESTING JAGUARATE

8.1. Tests performed

We tested version 2007 of JAGUARATE using version 9.6 of POLYRATE and the indicated release of JAGUAR 6.5 on the following machines (the operating system is indicated in parentheses):

1. IBM Regatta with Power4 processor (AIX 5.2); JAGUAR VERSION 6.5; release 112.

2. SGI Altix with Itanium 2 processor (SuSE Linux); JAGUAR VERSION 6.5; release 112.

3. IBM Netfinity with Pentium III (RedHat Enterprise Linux 3); JAGUAR VERSION 6.5; release 112.

The code is expected to work with all JAGUAR versions that use input files and scripts of extracting calculated values from output files with the same structure as the above mentioned versions.

8.2. Test suite

The purpose of the test suite is to provide some examples of the way JAGUARATE works, not to check all JAGUAR or POLYRATE 9.6 options. Therefore, the number of tests included is only seven, and the tests illustrate only the most basic features of JAGUARATE. The level of calculation, size of the systems, and computational requirements of the test runs have been chosen in such a way that running the whole suite does not consume an inordinate amount of computing time. All the test runs were run after compiling JAGUARATE using the `param4.inc` file.

The test suite is located in the `testrun` directory that contains several subdirectories. Each subdirectory contains one or more tests based on the same reaction. The summary output files for these test runs that are distributed in the current version of the program are located in the `testo` directory. (The output files were obtained in runs on a SGI Altix Itanium 2 machine.)

Each directory in `testrun` includes one or more tests based on one of the following reactions:

Reaction	Directory	Test names
$CH_3 + H_2 \rightarrow CH_4 + H$	ch5	ch5tr1, ch5tr2
$OH + H_2 \rightarrow H_2O + H$	oh3	oh3tr1, oh3tr2, oh3tr3, oh3tr4.
$H + H_2 \rightarrow H_2 + H$	h3	h3tr1, h3tr2
NH_3 inversion	nh3	nh3tr1, nh3tr2

The test runs are run in a subdirectory created for each run. This way, problems that could be caused when running other JAGUAR or JAGUARATE calculations in the same directory that JAGUARATE is using are avoided. After the test run is completed, the directory is removed and the temporary files created are moved to the `JRTEMPFILES` directory.

8.2.1. Test run `ch5tr1`

Tunneling:	SCT
Number of levels:	single level (UHF/3-21G)
Hindered rotation:	none

This sample run for the reaction $CH_3 + H_2 \rightarrow CH_4 + H$ performs calculations of the TST, CVT, and ICVT rate constants at the UHF/3-21G level, and it is based on following the reaction path using the Euler steepest descents method (also called Euler single-step method). For all the stationary points symmetry is employed in all the JAGUAR calculations (which is the default for JAGUAR calculations); nevertheless, this option is turned off when calculating points along the reaction coordinate in order to avoid possible problems due to the reorientation of the system. A restart file is created (JRRESTART keyword), and all the input of the geometries is done by means of files `fu71` through `fu75`, in order to allow JAGUAR to optimize the stationary points (*ohook* option in OPTTS and *optmin* in the OPTIMIZATION section of the `fu5` input file, and INITGEO set to *hooks* in the REACT1, REACT2, PROD1, PROD2, and START sections in the input file `fu5`).

JAGUARATE I/O files	JAGUARATE file names	
`ch5tr1.70`	`esp.fu70`	Input data for JAGUARATE
`ch5tr1.71`	`esp.fu71`	Input data for reactant 1
`ch5tr1.72`	`esp.fu72`	Input data for reactant 2
`ch5tr1.73`	`esp.fu73`	Input data for product 1
`ch5tr1.74`	`esp.fu74`	Input data for product 2
`ch5tr1.75`	`esp.fu75`	Input data for the saddle point
`ch5tr1.dat`	`poly.fu5`	Input data for POLYRATE
`ch5tr1.61`	`esp.fu61`	POLYRATE output file containing information about the stationary points
`ch5tr1.fu6`	`poly.fu6`	Long output file
`ch5tr1.fu15`	`poly.fu15`	Summary output file
`ch5tr1.rst`	`esp.fu84`	Restart file written by JAGUARATE

8.2.2. Test run `ch5tr2`

Tunneling: SCT
Number of levels: dual levels (UHF/3-21G and MP2/6-31G**)
Hindered rotation: none

This test run uses the restart file created by the previous run and performs a calculation using the ISPE technique by using ten MP2/6-31G** energies input in the `esp.fu51` input file. Of these ten energies, two are for products and the saddle point, and eight are for nonstationary points. Since the ISPE technique does not modify the reaction path, the calculation can be restarted successfully. The user must run the `ch5tr1` test run before running `ch5tr2`, in order to create the restart file to be read, `ch5tr2.rst`, which will be a copy of the `ch5tr1.rst` file generated by the previous run and located in the same directory.

JAGUARATE I/O files	JAGUARATE file names	
ch5tr2.51	poly.fu51	Input data for ISPE information
ch5tr2.70	esp.fu70	Input data for JAGUARATE
ch5tr2.71	esp.fu71	Input data for reactant 1
ch5tr2.72	esp.fu72	Input data for reactant 2
ch5tr2.73	esp.fu73	Input data for product 1
ch5tr2.74	esp.fu74	Input data for product 2
ch5tr2.75	esp.fu75	Input data for the saddle point
ch5tr2.dat	poly.fu5	Input data for POLYRATE
ch5tr2.61	esp.fu61	POLYRATE output file containing information about the stationary points
ch5tr2.fu6	poly.fu6	Long output file
ch5tr2.fu15	poly.fu15	Summary output file
ch5tr2.rst.old	esp.fu83	Restart file read by JAGUARATE
ch5tr2.rst	esp.fu84	Restart file written by JAGUARATE

8.2.3. Test run `oh3tr1`

Tunneling:	none
Number of levels:	single level (B3PW91/6-31G(d,p))
Hindered rotation:	none

This is a test run for a conventional TST calculation for the reaction $OH + H_2 \rightarrow H_2O +$ H. The geometries for the reactants and products are given (it is assumed that they already are fully optimized) in the `fu5` input file (INITGEO is set to *geom*, and STATUS set to *2* in the REACT1, REACT2, PROD1 and PROD2 sections of the `fu5` input file), while the saddle point optimization is carried out by means of JAGUAR, requiring, therefore, the `esp.fu75` input file, and STATUS set to *0* and the option *hooks* for the INITGEO keyword in the START section of the input file `fu5`. The JAGUARATE restart file `esp.fu84` is written. The level of electronic structure calculation used for this test run is B3PW91/6-31G(d,p).

JAGUARATE I/O files	JAGUARATE file names	
oh3tr1.70	esp.fu70	Input data for JAGUARATE
oh3tr1.75	esp.fu75	Input data for the saddle point
oh3tr1.dat	poly.fu5	Input data for POLYRATE
oh3tr1.61	esp.fu61	POLYRATE output file containing information about the stationary points
oh3tr1.fu6	poly.fu6	Long output file
oh3tr1.fu15	poly.fu15	Summary output file
oh3tr1.rst	esp.fu84	Restart file written by JAGUARATE

8.2.4. Test run `oh3tr2`

Tunneling: none
Number of levels: single level (B3PW91/6-31G(d,p))
Hindered rotation: none

This is a test run that, by making use of the `oh3tr1.rst` file previously written by the `oh3tr1` test run, restarts the calculation performed by the previous test run and makes a canonical variational theory (CVT) calculation, without tunneling, by following the reaction path using the variational reaction path algorithm based on the Euler method (*VRPE* option of RPM keyword) with a step size of 0.025 bohr. The reaction path is calculated between –0.3 bohr and +0.3 bohr. Nonredundant internal coordinates are used for describing the vibrations. The user must run the `oh3tr1` test run before running `oh3tr2`, since the restart file to be read, `oh3tr2.rst`, will be a copy of the `oh3tr1.rst` file generated by the previous run and located in the same directory. Otherwise, the `oh3tr2.rst` file will not exist, and the program will calculate the frequencies for all the stationary points and the optimum geometry for the saddle point instead of reading them from the restart file. It should be noted that the `fu75` file is required, and it is used by JAGUARATE although not by JAGUAR. At the end of the calculation, a new restart file, including the information calculated for the first time in the present run, will take the name of `oh3tr2.rst`, while the old restart file will be renamed as `oh3tr2.rst.old` (and this will be unchanged from what was in file `oh3tr1.rst` at the start of the present run).

JAGUARATE I/O files	JAGUARATE file names	
`oh3tr2.70`	`esp.fu70`	Input data for JAGUARATE
`oh3tr2.75`	`esp.fu75`	Input data for the saddle point
`oh3tr2.dat`	`poly.fu5`	Input data for POLYRATE
`oh3tr2.61`	`esp.fu61`	POLYRATE output file containing information about the stationary points
`oh3tr2.fu6`	`poly.fu6`	Long output file
`oh3tr2.fu15`	`poly.fu15`	Summary output file
`oh3tr2.rst.old`	`esp.fu83`	Restart file read by JAGUARATE
`oh3tr2.rst`	`esp.fu84`	Restart file written by JAGUARATE

8.2.5. Test run `oh3tr3`

Tunneling:	none
Number of levels:	single level (B3PW91/6-31G(d,p))
Hindered rotation:	none

This test run uses the `oh3tr2.rst` file written by the `oh3tr2` test run, copying it as `oh3tr3.rst`, and it performs the same calculation as the `oh3tr1` test. Since more information than is required for the calculation is stored in the `oh3tr2.rst` file, the restart file created by this test run, `oh3tr3.rst`, will be smaller than the file `oh3tr2.rst`. This is the reason why it is convenient to keep the file from which a restart calculation reads the information (in the executable scripts of these test runs, such files are renamed with the extension `old`). No JAGUAR calculations are needed for this test run, so it is the fastest test run of the suite.

JAGUARATE I/O files	JAGUARATE file names	
`oh3tr3.70`	`esp.fu70`	Input data for JAGUARATE
`oh3tr3.75`	`esp.fu75`	Input data for the saddle point
`oh3tr3.dat`	`poly.fu5`	Input data for POLYRATE
`oh3tr3.61`	`esp.fu61`	POLYRATE output file containing information about the stationary points
`oh3tr3.fu6`	`poly.fu6`	Long output file
`oh3tr3.fu15`	`poly.fu15`	Summary output file
`oh3tr3.rst.old`	`esp.fu83`	Restart file read by JAGUARATE
`oh3tr3.rst`	`esp.fu84`	Restart file written by JAGUARATE

8.2.6. Test run `oh3tr4`

Tunneling:	none
Number of levels:	single level (LMP2/3-21G*)
Hindered rotation:	none

This is a test run for a conventional TST calculation for the reaction $OH + H_2 \rightarrow H_2O +$ H. The geometries for the reactants, products and saddle point are optimized by means of JAGUAR, at LMP2/3-21G* level. Therefore, the initial geometries and keywords for the optimization are given in the input files `esp.fu71-75`, and INITGEO is set to *hooks* and STATUS to *0* in the REACT1, REACT2, PROD1, PROD2, and START sections of the `fu5` input file. The Hessian matrices are also calculated, using the methods in POLYRATE since jaguar can not calculate second derivatives at LMP2 level. The JAGUARATE restart file `esp.fu84` is written.

JAGUARATE I/O files	JAGUARATE file names	
`oh3tr4.70`	`esp.fu70`	Input data for JAGUARATE
`oh3tr4.71`	`esp.fu71`	Input data for reactant 1
`oh3tr4.72`	`esp.fu72`	Input data for reactant 2
`oh3tr4.73`	`esp.fu73`	Input data for product 1
`oh3tr4.74`	`esp.fu74`	Input data for product 2
`oh3tr4.75`	`esp.fu75`	Input data for the saddle point
`oh3tr4.dat`	`poly.fu5`	Input data for POLYRATE
`oh3tr4.61`	`esp.fu61`	POLYRATE output file containing information about the stationary points
`oh3tr4.fu6`	`poly.fu6`	Long output file
`oh3tr4.fu15`	`poly.fu15`	Summary output file
`oh3tr4.rst`	`esp.fu84`	Restart file written by JAGUARATE

8.2.7. Test run `h3tr1`

Tunneling:	none
Number of levels:	single level (UHF/6-31G**)
Hindered rotation:	none

This is a test run for the $H_2 + H \rightarrow H + H_2$ reaction. The geometries are optimized by means of JAGUAR methods at UHF/6-31G** level. Therefore, the initial geometries and keywords for the optimization are given in the input files `esp.fu71-75`, and INITGEO is set to *hooks* and STATUS to *0* in the REACT1, REACT2, PROD1, PROD2, and START sections of the `fu5` input file. The Hessian matrices are also calculated, as recommended, using the methods in JAGUAR. With the information for the stationary points obtained in this way, a conventional TST rate constant without tunneling is calculated. This test run demonstrates that a linear system may be calculated using JAGUARATE.

JAGUARATE I/O files	JAGUARATE file names	
`h3tr1.70`	`esp.fu70`	Input data for JAGUARATE
`h3tr1.71`	`esp.fu71`	Input data for reactant 1
`h3tr1.72`	`esp.fu72`	Input data for reactant 2
`h3tr1.73`	`esp.fu73`	Input data for product 1
`h3tr1.74`	`esp.fu74`	Input data for product 2
`h3tr1.75`	`esp.fu75`	Input data for the saddle point
`h3tr1.dat`	`poly.fu5`	Input data for POLYRATE
`h3tr1.61`	`esp.fu61`	POLYRATE output file containing information about the stationary points
`h3tr1.fu6`	`poly.fu6`	Long output file
`h3tr1.fu15`	`poly.fu15`	Summary output file

8.2.8. Test run `h3tr2`

Tunneling: none
Number of levels: single level (UHF/6-31G**)
Hindered rotation: none

This is a test run for the $H_2 + H \rightarrow H + H_2$ reaction in solvent using the JAGUAR's Poisson-Boltzmann solver. The solvent is water. The geometries are optimized by means of JAGUAR methods at UHF/6-31G** level. Therefore, the initial geometries and keywords for the optimization are given in the input files `esp.fu71-75`, and INITGEO is set to *hooks* and STATUS to *0* in the REACT1, REACT2, PROD1, PROD2, and START sections of the `fu5` input file. The Hessian matrices are also calculated, as recommended, using the methods in JAGUAR. With the information for the stationary points obtained in this way, a conventional TST rate constant without tunneling is calculated. This test run demonstrates that a linear system may be calculated using the solvation model found in JAGUARATE.

JAGUARATE I/O files	JAGUARATE file names	
h3tr2.70	esp.fu70	Input data for JAGUARATE
h3tr2.71	esp.fu71	Input data for reactant 1
h3tr2.72	esp.fu72	Input data for reactant 2
h3tr2.73	esp.fu73	Input data for product 1
h3tr2.74	esp.fu74	Input data for product 2
h3tr2.75	esp.fu75	Input data for the saddle point
h3tr2.dat	poly.fu5	Input data for POLYRATE
h3tr2.61	esp.fu61	POLYRATE output file containing information about the stationary points
h3tr2.fu6	poly.fu6	Long output file
h3tr2.fu15	poly.fu15	Summary output file

8.2.9. Test run `nh3tr1`

Tunneling: none
Number of levels: single level (GVB/6-31G*)
Hindered rotation: none

This is a test run for optimizing the planar geometry of NH_3 by treating it as the transition state for the $NH_3 \rightarrow NH_3$ inversion. The geometries are optimized by means of JAGUAR methods at GVB/6-31G* level. Therefore, the initial geometries and keywords for the optimization are given in the input files `esp.fu71`, `fu73`, and `fu75`, and INITGEO is set to *hooks* and STATUS to *0* in the REACT1, PROD1, and START sections of the `fu5` input file. The Hessian matrices are also calculated, as recommended, using the methods in JAGUAR. With the information for the stationary points obtained in this way, frequencies are calculated for both tetrahedral and planar ammonia. This test run demonstrates that a system may be calculated using GVB method implemented in JAGUAR.

Note that it does not make sense to speak about a rate constant for the NH_3 inversion because it is a coherent process. Therefore the TST rate constant printed in this run should be ignored.

JAGUARATE I/O files	JAGUARATE file names	
nh3tr1.70	esp.fu70	Input data for JAGUARATE
nh3tr1.71	esp.fu71	Input data for reactant 1
nh3tr1.73	esp.fu73	Input data for product 1
h3tr1.75	esp.fu75	Input data for the saddle point
nh3tr1.dat	poly.fu5	Input data for POLYRATE
nh3tr1.61	esp.fu61	POLYRATE output file containing information about the stationary points
nh3tr1.fu6	poly.fu6	Long output file
nh3tr1.fu15	poly.fu15	Summary output file

8.2.9. Test run `nh3tr2`

Tunneling:	none
Number of levels:	single level (GVB/6-31G*)
Hindered rotation:	none

This is a test run for the $NH_3 \rightarrow NH_3$ inversion. It is the restart calculation of nh3tr1 by using nh3tr.rst. MEPSAG (also called ZCT) and CD–SCSAG (also called SCT) tunneling probabilities are calculated, and they can be used to study the tunneling splitting in this reaction. The GVB option can be defined using either *igvball=1* keyword in the input file or *&gvb* section explicitly.

Note that it does not make sense to speak about a rate constant for the NH_3 inversion because it is a coherent process. However, one can use the table of tunneling probabilities as a function of energy to calculate θ, from which one can compute the tunneling splitting. See "Semiclassical Reaction-Path Methods Applied to Calculate the Tunneling Splitting in NH_3," F. B. Brown, S. C. Tucker, and D. G. Truhlar, Journal of Chemical Physics **83**, 4451-4455 (1985).

JAGUARATE I/O files	JAGUARATE file names	
nh3tr1.70	esp.fu70	Input data for JAGUARATE
nh3tr1.71	esp.fu71	Input data for reactant 1
nh3tr1.73	esp.fu73	Input data for product 1
h3tr1.75	esp.fu75	Input data for the saddle point
nh3tr1.dat	poly.fu5	Input data for POLYRATE
nh3tr1.61	esp.fu61	POLYRATE output file containing information about the stationary points
nh3tr1.fu6	poly.fu6	Long output file
nh3tr1.fu15	poly.fu15	Summary output file

8.3. Test run timings

Here are the timings for the test runs, in CPU seconds on a single processor of SGI Altix Itanium 2.

The following timings apply to version 2007/P9.6-J6.5.

	SGI Altix Itanium 2
Test run ch5tr1	3588.7
Test run ch5tr2	13.7
Test run oh3tr1	134.7
Test run oh3tr2	515.2
Test run oh3tr3	0.0
Test run oh3tr4	36378.0
Test run h3tr1	88.7
Test run h3tr2	454.1
Test run nh3tr1	1142.7
Test run nh3tr2	3084.4

9. COMPUTERS, OPERATING SYSTEMS, AND JAGUAR VERSIONS ON WHICH THE CODE HAS BEEN DEVELOPED AND TESTED

In each case we give the JAGUARATE version number, then the computers and operating system on which JAGUARATE was tested. For each computer and operating system we also specify the JAGUAR version that was used for testing.

JAGUARATE Version	Machine (Operating system)	JAGUAR Version
2007/P9.6-J6.5		
	IBM Regatta with Power4 processor (AIX 5.2)	6.5
	SGI Altix with Itanium 2 processor (SuSE Linux)	6.5
	IBM Netfinity with Pentium III (RedHat Enterprise Linux 3)	6.5

11.   VERSION INFORMATION

11.1.   JAGUARATE version numbers

JAGUARATE version numbers have the general form x.y.z/Px'.y'.z'-Jx'' where x.y.z is the overall version number, x'.y'.z' is the number of the version of POLYRATE on which it is based, and x'' is the number of the version of JAGUAR on which it is based. The part before the solidus, i.e., x.y.z, is unique, i.e., it changes if the interface changes, the POLYRATE version changes, or the JAGUAR version changes. Thus, the part after the solidus it is redundant information, and it may be omitted for simplicity if desired. In general, third-level revisions (z or z') are bug fixes (either to JAGUARATE itself or to one or more of the codes interfaced by JAGUARATE), and first and second level revisions (x,y,x', or y') are enhancements.

Note: we sometimes update one or more of the manuals without updating the version number. The manual version is determined by the date of its most recent change and is given on its first page. Any changes other than the manual(s) always involve a change in version number of the code.

11.2. JAGUARATE revision history

This section contains the revision history subsequent to version 2007 (May 2007), which was the first version of the code.

Version 2007/P9.6-J6.5 (May 2007)

1. This is the first version of JAGUARATE to interface POLYRATE and JAGUAR to do direct dynamic calculations.

12. ACKNOWLEDGMENTS