CRATE:

A Utility for modifying POLYRATE for use with CHARMMRATE

CRATE

Version 8.1.1

Cristobal Alhambra,[a] José Corchado,[b] María Luz, Sánchez,[b] J. Villà,[b]
Jiali Gao,[a] and Donald G. Truhlar[b]

[a] Department of Chemistry, State University of New York at Buffalo, Buffalo, NY 14260, U.S.A.
[b] Department of Chemistry and Supercomputer Institute, University of Minnesota, Minneapolis, MN 55455-0431, U.S.A.

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Note: The version number of CRATE is 8.1.1. This means that CRATE–version 8.1.1 is based on POLYRATE–version 8.1.1.

CRATE abstract

CRATE (pronounced as "see-rate") is a utility to prepare POLYRATE for use with the CHARMMRATE module of CHARMM. The standard POLYRATE program requires modifications to make it compatible with CHARMM. Modifications are made for efficient transfer of information between CHARMM and POLYRATE and to eliminate conflicts and other problems during compilation.

The files ef.src, energetics.src, fromblas.src, interface.src, polyag.src, polyrr.src, and polysz.src are modified by a script called install_cr.com that is provided as part of the CRATE utility. In particular, subroutine names are modified to remove conflicts with the CHARMM libraries, an additional keyword is added to the input read options in subroutine read5, some statements are commented out because they call ACES routines that are not part of POLYRATE, some subroutines are commented because they will never be used, all tab characters are removed to allow the CHARMM preprocessor to process the code properly, and all source code files are given the extension required by CHARMM.

In addition, the CRATE utility contains (i) a subroutine called "maino", which replaces the POLYRATE main routine, (ii) a new set of “hooks” (interface subprograms) that are required to interface CHARMM with POLYRATE, and (iii) a version of the POLYRATE param.inc file that has dimensions large enough to run the CHARMMRATE test run.

Referencing CRATE

CRATE is a utility for preparing POLYRATE for use with CHARMMRATE. Since CHARMMRATE and CRATE were developed as a package, it is not necessary to reference CRATE if CHARMMRATE is referenced. The recommended referencing for CHARMMRATE is as follows:

A) J. Chem. Phys. format:

The rate constant (or reaction path or geometry optimization, etc.) calculations were carried out using the CHARMMRATE program.[1–3]

1. C. Alhambra, J. C. Corchado, M. L. Sánchez, J. Villà, J. Gao, and D. G. Truhlar, CHARMMRATE–version 1.0, University of Minnesota, Minneapolis, 1999, a module of CHARMM (Ref. 2) for interfacing it with POLYRATE (Ref. 3).
2. *Chemistry at HARvard Macromolecular Mechanics* (CHARMM) computer program, as described in B. R. Brooks, R. E. Bruccoleri, B. D. Olafson, D. J. States, S. Swaminathan, and M. Karplus, J. Comput. Chem. **4**, 187 (1983).
3. Y.-Y. Chuang, J. C. Corchado, P. L. Fast, J. Villà, W.-P. Hu, Y.-P. Liu, G. C. Lynch, C. F. Jackels, K. A. Nguyen, M. Z. Gu, I. Rossi, E. L. Coitiño, S. Clayton, V. S. Melissas, R. Steckler, B. C. Garrett, A. D. Isaacson, and D. G. Truhlar, POLYRATE–version 8.1.1, University of Minnesota, Minneapolis, 1999.

B) American Chemical Society format:

The rate constant (or reaction path or geometry optimization, etc.) calculations were carried out using the CHARMMRATE program.[1–3]

1. Alhambra, C.; Corchado, J.C.; Sánchez, M. L.; Villà, J.; Gao, J.; Truhlar, D. G. CHARMMRATE–version 1.0, University of Minnesota, Minneapolis, 1999, a module of the CHARMM computer program (Ref. 2) for interfacing it with the POLYRATE computer program (Ref. 3).
2. Brooks, B. R.; Bruccoleri, R. E.; Olafson, B. D.; States, D. J.; Swaminathan, S.; Karplus, M., *J. Comput. Chem*. **1983**, *4*, 187.

3. Chuang, Y.-Y.; Corchado, J. C.; Fast, P. L.; Villà, J.; Hu, W.-P.; Liu, Y--P.; Lynch, G. C.; Jackels, C. F.; Nguyen, K. A.; Gu, M. Z.; Rossi, I.; Coitiño, E. L.; Clayton, S.; Melissas, V. S.; Steckler, R.; Garrett, B. C.; Isaacson, A. D.; Truhlar, D. G. POLYRATE–version 8.1.1, University of Minnesota, Minneapolis, 1999.

Availability of CRATE

CRATE-version 8.1.1 is a utility for preparing POLYRATE for use with CHARMMRATE. It is available at http://comp.chem.umn.edu.

Contents

Description of CRATE

The CRATE utility will automatically make changes to the source code of POLYRATE to allow the interface between CHARMM and POLYRATE. When both CHARMM (with the CHARMMRATE module) and POLYRATE have been obtained, integration of the code into a single executable called CHARMMRATE is possible with the utility, CRATE, which is available from the University of Minnesota (http://comp.chem.umn.edu).

The CHARMMRATE interface for CHARMM and POLYRATE takes advantage of the modular nature of both programs, and, consequently, minimal modifications of CHARMM and POLYRATE were required. The CHARMM program is the main driver of the integrated program, which makes a FORTRAN call to the interface subprogram, CHARMMRATE, to initiate VTST calculations by POLYRATE. The energy and energy gradients for the primary-zone atoms required by POLYRATE are determined by CHARMM through the interface subprogram and are supplied to POLYRATE through a set of subroutines called the POLYRATE hooks. Efforts are being made to make all large arrays adjustable by CHARMM.

In general, all the standard CHARMM directives were followed to make CHARMMRATE possible. That means that specific modifications of the original POLYRATE program have been made for efficient transfer of information between CHARMM and POLYRATE. The CRATE utility will automatically make these modifications, which are accomplished in two ways:
(1) A subroutine called "maino", which replaces the POLYRATE main routine, and a new set of

POLYRATE hooks are provided as part of the CRATE utility. For further details of these modifications, see sections ***a*** and ***b*** below.

(2) Several other files, namely ef.src, energetics.src, fromblas.src, interface.src, polyag.src, polyrr.src and polysz are modified by the script file called install_cr.com that is provided as part of the CRATE utility. In particular, subroutine names are modified to remove conflicts with the CHARMM libraries, an additional keyword is added to the input read options in subroutine read5, some statements are commented out because they call ACES routines that are not part of POLYRATE, some subroutines are commented because they will never be used, all tab characters found in the source code and all characters beyond column 72 are removed to allow the CHARMM preprocessor to process the code properly, and all source code files are given the extension required by CHARMM. Further details of these changes are provided in parts ***c*** through ***h*** below.

In addition, the CRATE utility contains a version of the POLYRATE param.inc file that has dimensions large enough to run the CHARMMRATE test run.

Details:

a. main.src

a.1. At the beginning of the file, the POLYRATE main program is converted into a subroutine by adding the line: subroutine maino

a.2. The calls to open the files fu5 and fu6 have been commented since these units have already been opened by CHARMM.

```
call openfi(fu5....
call openfi(fu6....
```

a.3. For similar reasons the call to fiopen has been commented.

call fiopen

a.4. Any calls to fcrate and the subsequent stop statement have been deactivated. This allows control to return to CHARMM once the execution of POLYRATE is over.

a.5. call readic is replaced by call cr_readic.

a.6. A return statement is placed at the end of the routine.

b. hooks.src

In this file, there are two main changes: the ACES potential option has been deactivated to avoid problems during compilation, and the routines to setup and read the from file fu70 in version 0.1 of CHARMMRATE have been deactivated.

b.1. subroutine ehook

```
else if (ipot.eq.2) then
call acalc(1,fmat)
```

b.2. subroutine ghook

```
call acalc(2,fmat)
```

b.3. subroutine ohook

```
if(opt.eq.5) call gseta
```

The routine gseta is not present. Therefore, this line is commented out.

```
call acalc(4,fmat)
```

b.4. subroutine prep was deactivated.

b.5. subroutine prepj

```
call aceset(jtype)
```

b.6. subroutine hhook

```
call acalc(3,fmat)
```

b.7. subroutine surf

All additions in the version 0.1 of CHARMMRATE have been removed because system calls including read/write for communication between CHARMM and POLYRATE are no longer needed. Now, there is only one line necessary, a call to initiate the energy/gradient evaluation:

```
call cr_ener
```

b.8. subroutine setup was deactivated (used in version 0.1 to handle fu70).

b.9. subroutine read70 was deactivated (as above).

b.10. subroutine ratmq was deactivated (as above).

b.11. subroutine pdbchn was deactivated (as above).

c. interface.src

c.1. subroutine read5

The option *finish is added to terminate the command stream for POLYRATE from CHARMM. The following 3 lines are added:

```
C       Stop input stream from CHARMM file
        else if (string(j:j+5).eq.'finish') then
```

go to 1201
The next "call intab" was replaced by:
1201 call intab

c.2. subroutine renerg
The SPECBASIS options have been commented out since it is not available.

c.3. subroutine rline
The function case was changed to casito to avoid problems during the compilation.

c.4. subroutine readic was replaced by subroutine cr_readic.

d. energetics

d.1. subroutine deriv2 was deactivated to avoid problems during the compilation.
d.2. subroutine derv24 was deactivated to avoid problems during the compilation.

e. polyag

e.1. The function erf has been replaced by cr_erf.
e.2. call readic is replaced by call cr_readic.

f. polysz

f.1. The function erf has been replaced by cr_erf.

g. ef, fromblas, polyrr

g.1. All tqlrat were replaced by cr_tqlrat.
g.2. All tql2 were replaced by cr_tql2.

h. All source files must have the file extension `.src` and mustn't have more than 72 columns to be processed by CHARMM preprocessor during compilation.

For details about CRATE installation, see the CHARMMRATE manual.