

Supporting Information for the Main Article
Manual for RAI Calculator (Version 1.0, July 24, 2025)

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1. Introduction

RAI Calculator is a free program for the calculation of our newly-developed reaction activity indexes (RAI^+ and RAI^-), which could be viewed as novel indexes for chemical reactivity based on the Fukui function (FF) and electrostatic potential (EP). Further detailed information has been given in the main article.

2. Operating System

Current software (*RAI.exe*) works in Windows 10 (64bit). You can use it in other operating systems after compiling the source file (*main.f90*) using FORTRAN compiler.

3. Installation and Compiling

Simply extract the program (*RAI.exe*) on Windows 10 (64-bit) and run it directly.

If you want to compile the source code, you can use the following commands:

Commands in Windows:

```
gfortran.exe -ffree-line-length-none main.f90 -o main.o
```

```
gfortran.exe -static main.o -o RAI.exe
```

(In this manual, white characters in black boxes, such as `abc123` means the inputting characters from keyboard.)

Commands in Linux:

```
gfortran -ffree-line-length-none main.f90 -o RAI
```

4. Usage

4.1. Gaussian calculation

As an example, three Gaussian inputting files are created as follows:

(1) Content in EthyleneKetene.gjf

```
%chk=EthyleneKetene.chk
#p opt 6-311+g(d,p) int=ultrafine um062x em=gd3

Neutral state for ethenone

0 1
C          -3.10669451    2.56276159    0.00000000
H          -2.57353077    1.63505667    0.00000000
H          -4.17669451    2.56276159    0.00000000
C          -2.43142021    3.73773889    0.00000000
O          -1.80437978    4.82878924   -0.00000000
```

(2) Content in EthyleneKetene+1ele.gjf

```
%oldchk=EthyleneKetene.chk
%chk=EthyleneKetene+1ele.chk
#p 6-311+g(d,p) int=ultrafine um062x em=gd3 guess=read geom=check

One electron is added into the neutral ethenone

-1 2
```

(3) Content in EthyleneKetene-1ele.gjf

```
%oldchk=EthyleneKetene.chk
%chk=EthyleneKetene-1ele.chk
#p 6-311+g(d,p) int=ultrafine um062x em=gd3 guess=read geom=check

One electron is removed from the neutral ethenone

1 2
```

Run this inputting file in Gaussian, and then we will get the Gaussian outputting files, including three .chk files and three .log/.out files. Then we use the commands of

```
formchk EthyleneKetene.chk
```

```
formchk EthyleneKetene+1ele.chk
```

```
formchk EthyleneKetene-1ele.chk
```

to convert .chk file to .fchk/.fch file. Now, we have three .fchk/.fch files and three .log/.out files. Normally speaking, the .fch/.out files appear in Window OS, while the .fchk/.log files in Linux OS.

4.2. Generation of .cube/.cube files

Here we provide two methods to get .cube/.cube files. These two methods are both convenient.

(1) Use Gaussian software, you can use the following commands:

```
cubegen 0 density EthyleneKetene.fchk EthyleneKetene.cube 0 h
```

```
cubegen 0 potential EthyleneKetene.fchk EthyleneKeteneesp.cube 0 h
```

```
cubegen 0 density EthyleneKetene+1ele.fchk EthyleneKetene+1ele.cube 0 h
```

```
cubegen 0 density EthyleneKetene-1ele.fchk EthyleneKetene-1ele.cube 0 h
```

(2) Use Multiwfn 3.8(dev) or other tools to get electron density and EP information from three .fchk files to .cube files. In this sample, please generate EthyleneKetene.cub and Ethyleneoxideesp.cub from EthyleneKetene.fchk, generate EthyleneKetene+1ele.cub from EthyleneKetene+1ele.fchk, and generate EthyleneKetene-1ele.cub from EthyleneKetene-1ele.fchk.

Table 1. The usage of four files generating in Section 4.2

EthyleneKetene.cub	Electron density of neutral ethenone
Ethyleneoxideesp.cub	Electrostatic potential of neutral ethenone
EthyleneKetene+1ele.cub	Electron density of negative ethenone with one more electron (total charge: -1)
EthyleneKetene-1ele.cub	Electron density of positive ethenone with one less electron (total charge: +1)

Copy all these four .cube files into your working directory.

4.3. Read first ionization energy and electron affinity energy

Please read the single point energies from EthyleneKetene.log, EthyleneKetene+1ele.log and EthyleneKetene-1ele.log, labeled as $E(N)$, $E(N+1)$ and $E(N-1)$, respectively.

In this sample:

- $E(N) = -152.58186653$ a.u.
- $E(N+1) = -152.52867014$ a.u.
- $E(N-1) = -152.21869465$ a.u.

Then calculate first ionization energy (IE) and electron affinity energy (EA) as follows:

- $IE = E(N-1) - E(N)$
- $EA = E(N+1) - E(N)$
- Calculate $(IE - EA)$ (in fact, this value could be atomically calculated when you use RAI.exe)

In this sample, $(IE - EA)$ is 0.30997549 a.u. Normally speaking, IE and $(IE - EA)$ are positive values. If you obtain a negative $(IE - EA)$ value, please check the total charge of the file in Section 4.1(1) (EthyleneKetene.gjf in this sample). If the the total charge is not zero, please add the counter-ions in order to ensure the total charge is zero and try to calculate the whole system again.

4.4. RAI Calculator

Run “RAI.exe”, the program will display the following text:

```
----- RAI(+) and RAI(-) Calculating Program (v 1.0) -----
```

Input the cube file name of negative charge file (-1 e) unit of length must be Bohr, the same below:

Then drag the .cub file with negative charge (N+1 electrons) into the program window or directly input the path to the file:

```
<your working directory>\EthyleneKetene+1ele.cub
```

In this way, the .cub file with negative charge (N+1 electrons) will be read by the program. Similarly, read remaining three .cub files to the prompt:

```
Input the cube file name of electron neutral file ( 0 e ):
```

`<your working directory>\EthyleneKetene.cub`

Input the cube file name of positive charge file (+1 e):

`<your working directory>\EthyleneKetene-1ele.cub`

Input the cube file name of electrostatic file (esp):

`<your working directory>\EthyleneKeteneesp.cub`

If the grid definitions are same among these four .cub files, you will found the following information in the screen:

Compare complete. the cubes definitions and molecular definitions are same for these files:

fn1 --> negative charge file (-1 e):

`<your working directory>\EthyleneKetene+1ele.cub`

fn2 --> electron neutral file (0 e):

`<your working directory>\EthyleneKetene.cub`

fn3 --> positive charge file (+1 e):

`<your working directory>\EthyleneKetene-1ele.cub`

fn4 --> electrostatic file (esp):

`<your working directory>\EthyleneKeteneesp.cub`

Each file involves these points:

5	-7.777579	-8.378920	-6.000000
85	0.186015	0.000000	0.000000
96	0.000000	0.186015	0.000000
66	0.000000	0.000000	0.186015

Total data point number: 538560

Cube File 1: Fukui_function_negative

Cube File 2: Fukui_function_zero

Cube File 3: Fukui_function_positive

Cube File 4: Corrected_ESP

Above files have been written into the working dir using the Gaussian-cube format.

Then the program will ask you to input the values of first ionization energy (IE) and electron affinity energy (EA) using the unit of a.u..

Now please input the value of IE (first ionization energy, unit: a.u.):

0.36317188

Now please input the value of EA (electron affinity energy, unit: a.u.):

0.05319639

One more step, input the path of ar.txt, which contains the full information of atomic radius. If you don't have ar.txt, input the path of your working directory, the program will use the built-in radius values, and generate the final result to your working directory.

Please input the location of ar.txt e.g:D:\RAI-102\examples\H2O

<your working directory>

ar.txt not found. Now RAI program uses the built-in radius values.

Information from FORTRAN: Cannot open file '<your working directory>\ar.txt': No such file or directory

At last, the program will output two final result files:

- EthyleneKetene.cubRAI_minus.cube
- EthyleneKetene.cubRAI_plus.cube

And the following information will appear in the screen:

Cube File 5: Rai_function_positive

Cube File 6: Rai_function_negative

Above files have been written into the working dir using the Gaussian-cube format.

PAUSE

To resume execution, type go. Other input will terminate the job.

Using Gaussview (or other GUI programs for the grid files), open these two files, EthyleneKetene.cubRAI_minus.cube and EthyleneKetene.cubRAI_plus.cube.

4.5 Format of *ar.txt* file

The file containing the information of atomic radius, named as *ar.txt*, is mentioned in Section 4.4. Here, in order to facilitate users in changing the default atomic radius to a specified atomic radius, the structure of this file should be clearly explained.

The first 86 lines of this file contain all the valid data, in which the atomic radius of 86 elements (from H to Rn) are listed. All the data lines are written in the following manner (taking Line 52 as an example):

```
0.206    0.600 ! Te 52
```

The first float number 0.206 means that the atomic radii is 0.206 nm. All the atomic radius data are copied from the atomic radii settings in Multiwfn software (version 3.8dev). The second float number 0.600 is the radius scaling factor, which means that both of the RAI^+ and RAI^- values are set to -10.0 a.u. in the spherical space with a distance of less than $0.600 \times 0.206 = 0.124$ nm from the atomic nucleus. If you need other atomic radii and scaling factors, you can change the data in this file. The comments “! Te 52” means that this line is used to define the 52th element, tellurium (Te).