AUTOF Manual

INTRODUCTION

The **AUTOF** program calculates the Turnover Frequency (TOF) of a catalytic reaction from energy data typically obtained by computational chemistry. Additionally it analyses the states limiting the TOF. Optionally one can analyse the effect of the reactant and product concentrations. The **AUTOF** program is based on the energetic span model[1-3] and can be used free of charge after signing the license agreement appended to this manual and sending it to the authors. For any questions and to obtain the program contact Andreas Uhe (uhe@itmc.rwth-aachen.de) Sebastian Kozuch (sebastian.kozuch@weizmann.ac.il) or Sason Shaik (sason@yfaat.ch.huji.ac.il).

THE INPUT FILE

An example file is distributed along with the program and this manual, but it can easily be created using the text editor of your choice or by exporting a spreadsheed as text file. The first line contains the temperature and the second line contains the number of steps in the cycle. Each of the following lines contains the information belonging to one step in the given order, i.e. intermediate and following transition state, concentration of a reactant entering the cycle in this step and concentration of a product leaving the cycle in this step. If no reactant enters and no product leaves the cycle, an x has to be entered instead of the respective concentration. If no concentrations shall be taken into account as in the initial version of the energetic span model[1] one has to enter an x for every concentration. Following the information of each step the net reaction energy should be given in kcal/mol, i.e. energies of all products minus the energies of all reactants. The values within one line can be seperated by space or tab and should be given in kcal/mol and mol/l, respectively. The number of steps that is read in is determined by the number of steps given in line 2.

# of line	*data*	*unit*	*format*
1	temperature	K	real
2	# of steps		integer
3 to (# of steps + 2)	energies and concentrations of each step	kcal/mol, kcal/mol, mol/L, mol /L	real
# of steps +3	net reaction energy	kcal/mol	real

RUNNING THE PROGRAM

You have to enter the following in your command line:

AUTOF.exe *input_file* [idthl]

where AUTOF.exe is the executable and *input_file* stands for the input file as described above. To remove parts of the output you can optionally write some letters behind the input file when you execute the program:

i - remove the input repetition
d - remove the degrees of TOF control
t - remove the TOF
h - remove the headers with all the exclamation marks
l - remove the licence and program information

You can combine all the letters in any way you want. The order of the letters is not important and you can – but need not – put blanks between them. So for example:
AUTOF.exe *input_file* iah
would output just the degrees of TOF control and the TOF without the headers.

REFERENCES

[1] S. Shaik, S. Kozuch, *J. Am. Chem Soc.* **2006**, *128*, 3355 - 3365.
[2] S. Kozuch, S. Shaik, *J. Phys. Chem. A* **2008**, *112*, 6032 - 6041.
[3] A. Uhe, S. Kozuch, S. Shaik, *J. Comp. Chem.* **2010**, submitted.

AUTOF User License

AUTOF users must agree to the following conditions:

1. Results obtained with AUTOF and published in the scientific literature must reference to
    a) S. Kozuch, S. Shaik, *A Combined Kinetic-Quantum Mechanical Model for Assessment of Catalytic Cycles: Application to Cross Coupling and Heck Reaction*, *J. Am. Chem. Soc.* **2006**, *128*, 3355-3365;
    b) S. Kozuch, S. Shaik, *Kinetic-Quantum Chemical Model for Catalytic Cycles: The Haber Bosch Process and the Effect of concentration*, *J. Phys. Chem. A* **2008**, *112*, 6032-6041;
    c) A. Uhe, S. Kozuch, S. Shaik, *Automatic Analysis of Computed Catalytic Cycles*, *J. Comput. Chem.* **2010**, submitted".
    It is the users responsibility to check for the current state of publication c).

2. The authors disclaim all warranties on the use of AUTOF program. The publication of results obtained by the use of the program is absolute responsibility of the users, and not of the authors.

3. The AUTOF program is provided directly to a research group. Anyone associated with the group can use and copy the program without limitations. Sharing the program outside the group is forbidden. The person signing the license must inform every user in his group about this license.

4. The users may change the AUTOF program freely, as long as he/she reports those changes to the original authors of the program. Whenever results obtained in a modified version of the program are published, these changes must be stated in the manuscript.

I accept all the previous conditions,

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