
This report shows the most relevant data predicted by AutoMeKin (using the PM7 semiempirical Hamiltonian) for the reaction mechanisms and kinetics of your selected system. It includes the following files and figures generated by the program:

**Convergence.txt**: list of the number of located transition states as a function of the number of trajectories and iteration.

**MINinfo**: list of minima (reactant and intermediate species). **Note**: this web interface has reduced capabilities and does not check whether the minimum structures are true minima. Geometries and frequencies are included in the "Data" zip file.

**TSinfo**: list of transition states.

**RXNet**: complete list of predicted elementary steps.

**RXNet.cg**: coupled set of elementary steps (reaction network). Here each family of conformers form a single state and only the minimum-energy structure of each family is considered. This is also shown as a graph (Complete Graph below).

**Complete Graph**: Graph displaying RXNet.cg reaction network. The nodes correspond to reactant, intermediates and products, and the widths of the edges are proportional to the number of paths connecting the corresponding nodes. The starting node is shown in red.

**Kinetics Graph**: Graph displaying only those nodes actively participating in the kinetics at the chosen temperature $T$ or energy $E$. Here, the widths of the edges are proportional to the total (forward + backward) flux in the kinetics simulations. The starting node is shown in red.

**Population vs time**: Plot showing the population of reactant, intermediates and products as a function of simulation time in the kinetics (at the chosen $T$ or $E$).

If you report results obtained with AutoMeKin, you should cite the following papers:
1) E. Martínez-Núñez, *Phys. Chem. Chem. Phys.* 2015, *17*, 14912–14921.
2) E. Martínez-Núñez, *J. Comput. Chem.* 2015, *36*, 222–234.
3) A. Rodríguez, R. Rodríguez-Fernández, S. A. Vázquez, G. L. Barnes, J. J. P. Stewart and E. Martínez-Núñez, *J. Comput. Chem*. 2018, *39*, 1922–1930.
4) MOPAC2016, Version: 16.307, J. J. P. Stewart, Stewart Computational Chemistry, web-site: HTTP://OpenMOPAC.net.