**MESMER examples**

- **AcetylO2**

  a) **Acetyl_O2_associationEx.xml** : General multiwell system including a barrierless reaction treated by **ILT** and barriered processes treated using **RRKM**. This input is related to results from the following publication: http://pubs.acs.org/doi/abs/10.1021/jp1099199

  b) *.log: Gaussian output files used to create the Acetyl input file as described in the tutorial on creating MESMER input files from Gaussian outputs.

- **AcetylPrior**

  a) **AcetylPrior.xml:** This input file demonstrates how to initialise a **prior distribution** of energy. In this case an excess energy of 200 kJ $mol^{-1}$ is distributed between $CH_3CO$ and $CH_3C(O)OH$ and the decomposition of the $CH_3CO$ is then modelled. This input is related to results from the following publication: http://pubs.acs.org/doi/abs/10.1021/jp404233b

- **Butyl_H_to_Butane**

  a) **Butyl_H_to_Butane.xml:** This example demonstrates how to define both **analytical** and **numerical hindered rotation** potentials in the Butane species. The ab initio **Hessian** is also defined in order to project out the defined torsions and then re-diagonalise to obtain a new set of vibrational frequencies.

- **DefinedTunnelingCoefficients**

  a) **OH+methanol.xml:** This example treats tunnelling in the OH + methanol reaction by inputting **tunnelling coefficients** from some previous calculation.

- **Ethyl_H_to_Ethane**

  a) **Ethyl_H_to_Ethane.xml:** This example demonstrates the treatment of **internal rotations** using an **ab initio potential**.

- **H2Ominimal**

  a) **H2Ominimal.xml:** This simple example demonstrates the use of the **librarymols.xml** file.

- **I-propyl**

  a) **Ipropyl_test.xml:** This file demonstrates how to **fit** master equation parameters to match experimental data using a **Powel** algorithm.

  b) **Ipropyl_LM.xml:** This file demonstrates how to run **a Levenberg Marquardt** fitting routine.

  c) **Ipropyl_2ContrBlks.xml:** This file demonstrates how to define to separate control blocks to specify in this case a fitting calculation followed by generating **a Chebyshev** polynomial representation of the resulting rate coefficients.

- **I-propyl-SA**

  a) **Ipropyl_SA.xml:** This file demonstrates how to run a **sensitivity analysis** of calculated rate coefficients to the master equation variables.

- **Methoxymethyl**

  a) **Chebyshev.xml:** This file models the $CH_3OCH_2 + O_2$ reaction, and demonstrates how to represent the resulting rate coefficients in terms of **Chebyshev polynomials**.

  b) **ChebyshevCK.xml:** This file is identical to the above other than the Chebyshev polynomials are output in a format consistent with **Chemkin** format. The Methoxymethyl system is related to results from a recent publication: http://pubs.acs.org/doi/abs/10.1021/jp505422e

- **Methyl_H_to_Methane**

  a) **Methyl_H_to_Methane.xml:** This file models the $CH_3 + H \rightarrow CH_4$ reaction and incorporates **fitting** to experimental data.

  b) **Methyl_H_to_Methane_FTST_rev.xml:** This file demonstrate how to input **transition state sums of states** from some prior calculation, into the MESMER input. In this case **energy and angular momentum resolved sums of states** from a flexible transition state theory calculations are used instead of an ILT method.

  c) **Methyl_H_to_Methane_FTST_irev.xml:** This file is similar to the above the system is defined as an irreversible dissociation rather then an association.

- **OH_NO_HONO**

  a) **OH_NO_HONO_3Blks.xml:** This file models the OH+NO-> HONO system and incorporates a number of different functionalities using **3 separate control blocks** to run a fitting routing, then to produce a **Chebyshev representation** and finally to produce a table of **thermodynamic properties.**

- **OH-acetylene**

  a) **OH-HCCH-irreversibleBim-publish.xml:** This file demonstrates how to treat irreversible bimolecular reactions for non-thermal species using a **bimolecular sink approach**. This system models the OH + HCCH $+O_2$ system from a recent publication: http://www.sciencemag.org/content/337/6098/1066.abstract

- **ReservoirSink**

  a) **reservoirSinkAcetylO2.xml:** This file models the acetyl+ $O_2$ reaction but demonstrates how to introduce a **reservoir state approximation** for a deep well.

- **Spin_forbidden_kinetics**

  a) **HCCH_methylene.xml:** This file demonstrates how to incorporates **spin forbidden** reactions in to MESMER using the HCCH + singlet methylene reaction as an example.

b) **LZ_test.xml:** The file demonstrates the **Landau Zener** approach treating spin forbidden processes

c) **WKB_test.xml:** This file demonstrates the **Wentzel–Kramers–Brillouin (WKB)** approach to treating spin forbidden processes

- **Tunnelling**

a) **H+H2,T+T2.xml:** This file demonstrates how to treat tunnelling using a **WKB** approach utilising an **ab initio potential**.