

```
In [4]: using DifferentialEquations
using PyPlot
using ReactionMechanismSimulator
```

```
In [3]: import Pkg; Pkg.add("PyPlot")
```

```
Updating registry at `~/anaconda3/envs/rms_env/share/julia/site/registries/General`
Resolving package versions...
Updating `~/anaconda3/envs/rms_env/share/julia/site/environments/v1.6/Project.toml`
[d330b81b] + PyPlot v2.9.0
No Changes to `~/anaconda3/envs/rms_env/share/julia/site/environments/v1.6/Manifest.toml`
```

```
In [ ]: from diffeqpy import de
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
```

```
In [8]: phaseDict = readinput("rms/chem76.rms")
```

```
[12:48:22] WARNING: not removing hydrogen atom without neighbors
Warning: failed to generate molecular information from smiles for species site
└─ @ ReactionMechanismSimulator /home/keerths/anaconda3/envs/rms_env/share/julia/site/packages/ReactionMechanismSimulator/MW0YP/src/Parse.jl:257
MethodError: no method matching Species(; index=23, name="site", adjlist="1 X u0 p0 c0\n\n", radicalectrons=0, thermo=NASA{EmptyThermoUncertainty}
  polys: Array{NASAPolynomial}((2,))
  unc: EmptyThermoUncertainty EmptyThermoUncertainty()
, smiles="[Pt]")
Closest candidates are:
  Species(; name, index, inchi, smiles, thermo, atomnums, bondnum, diffusion, radius, radicalectrons) at /home/keerths/anaconda3/envs/rms_env/share/julia/site/packages/Parameters/cGriM/src/Parameters.jl:520 got unsupported keyword argument "adjlist"
  Species(::Species; kws...) at /home/keerths/anaconda3/envs/rms_env/share/julia/site/packages/Parameters/cGriM/src/Parameters.jl:530
  Species(::Species, ::Tuple{Symbol, Any}...) at /home/keerths/anaconda3/envs/rms_env/share/julia/site/packages/Parameters/cGriM/src/Parameters.jl:534 got unsupported keyword arguments "index", "name", "adjlist", "radicalectrons", "thermo", "smiles"
  ...
```

Stacktrace:

```
[1] kwerr(kw::NamedTuple{(:index, :name, :adjlist, :radicalectrons, :thermo, :smiles)}, Tuple{Int64, String, String, Int64, NASA{EmptyThermoUncertainty}, String}), args::Type)
  @ Base ./error.jl:157
[2] top-level scope
  @ none:1
[3] eval
  @ ./boot.jl:360 [inlined]
[4] eval
  @ ~/anaconda3/envs/rms_env/share/julia/site/packages/ReactionMechanismSimulator/MW0YP/src/ReactionMechanismSimulator.jl:1 [inlined]
[5] fcdict2obj(d::Dict{Any, Any}, ymlunitsdict::Dict{Any, Any})
  @ ReactionMechanismSimulator ~/anaconda3/envs/rms_env/share/julia/site/packages/ReactionMechanismSimulator/MW0YP/src/Parse.jl:193
[6] readinputyaml(fname::String)
  @ ReactionMechanismSimulator ~/anaconda3/envs/rms_env/share/julia/site/packages/
```

```
ReactionMechanismSimulator/MW0YP/src/Parse.jl:282
 [7] readinput(fname::String; spcdict::String, output::String)
      @ ReactionMechanismSimulator ~/anaconda3/envs/rms_env/share/julia/site/packages/
ReactionMechanismSimulator/MW0YP/src/Parse.jl:206
 [8] readinput(fname::String)
      @ ReactionMechanismSimulator ~/anaconda3/envs/rms_env/share/julia/site/packages/
ReactionMechanismSimulator/MW0YP/src/Parse.jl:204
 [9] top-level scope
      @ In[8]:1
 [10] eval
      @ ./boot.jl:360 [inlined]
 [11] include_string(mapexpr::typeof(REPL.softscope), mod::Module, code::String, fil
ename::String)
      @ Base ./loading.jl:1094
```

In []:

In []: