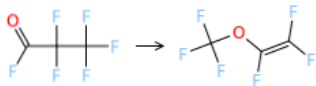


#### 4 reactions matched to 1,3\_sigmatropic\_rearrangement

index: 68

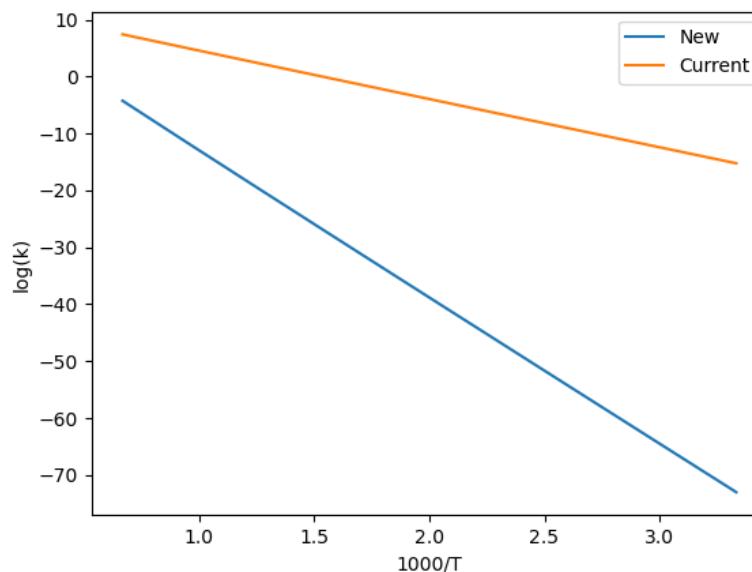


##### New Kinetics:

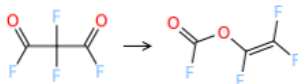
Arrhenius( $A=(7.89e+07, 's^{-1}')$ ,  $n=1.5$ ,  $E_a=(116144, 'cal/mol')$ ,  $T_0=(1, 'K')$ )

##### Current Kinetics

ArrheniusBM( $A=(9.39365e+11, 's^{-1}')$ ,  $n=0.324012$ ,  $w_0=(707, 'kJ/mol')$ ,  $E_0=(160.927, 'kJ/mol')$ ,  $T_{min}=(300, 'K')$ ,  $T_{max}=(2000, 'K')$ ,  $uncertainty=RateUncertainty(mu=0.014478493324023197, var=15.997960675483611, T_{ref}=1000.0, N=8, data\_mean=0.0, correlation='Root\_N-1R!H-inRing\_Ext-4R!H-R')$ ,  $comment=""$ Estimated from node Root\_N-1R!H-inRing\\_Ext-4R!H-R""")



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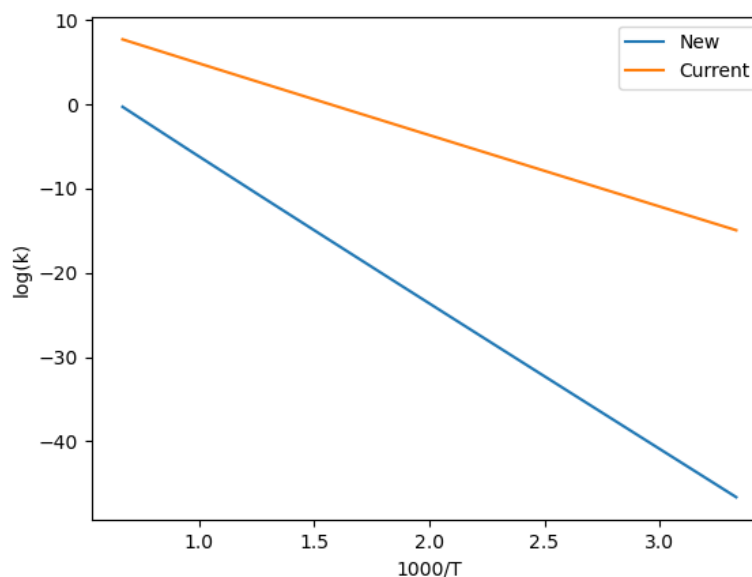


##### New Kinetics:

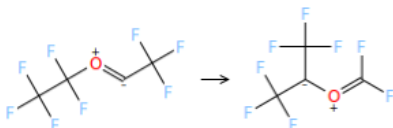
Arrhenius( $A=(4.5e+06, 's^{-1}')$ ,  $n=1.38$ ,  $E_a=(77809.6, 'cal/mol')$ ,  $T_0=(1, 'K')$ )

##### Current Kinetics

ArrheniusBM( $A=(1.87873e+12, 's^{-1}')$ ,  $n=0.324012$ ,  $w_0=(707, 'kJ/mol')$ ,  $E_0=(160.927, 'kJ/mol')$ ,  $T_{min}=(300, 'K')$ ,  $T_{max}=(2000, 'K')$ ,  $uncertainty=RateUncertainty(mu=0.014478493324023197, var=15.997960675483611, T_{ref}=1000.0, N=8, data\_mean=0.0, correlation='Root\_N-1R!H-inRing\_Ext-4R!H-R')$ ,  $comment=""$ Estimated from node Root\_N-1R!H-inRing\\_Ext-4R!H-R Multiplied by reaction path degeneracy 2.0""")



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132

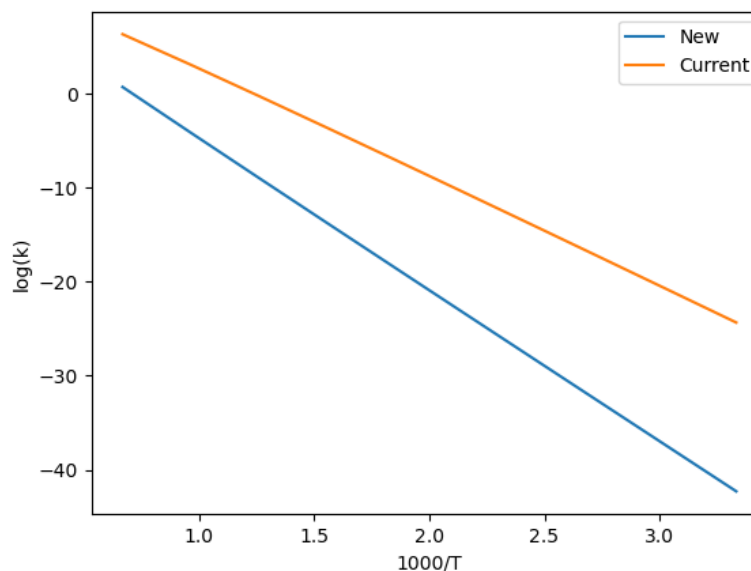


##### New Kinetics:

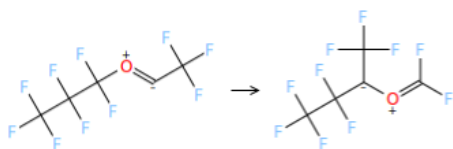
Arrhenius( $A=(1.83\text{e}+08,\text{'s}^{-1}\text{'})$ ,  $n=0.97$ ,  $E_a=(72710,\text{'cal/mol}\text{'})$ ,  $T_0=(1,\text{'K}\text{'})$ )

### Current Kinetics

ArrheniusBM( $A=(4.62709\text{e}+20,\text{'s}^{-1}\text{'})$ ,  $n=-1.9758$ ,  $w_0=(661.267,\text{'kJ/mol}\text{'})$ ,  $E_0=(230.31,\text{'kJ/mol}\text{'})$ ,  $T_{\min}=(300,\text{'K}\text{'})$ ,  $T_{\max}=(2000,\text{'K}\text{'})$ ,  $\text{uncertainty}=\text{RateUncertainty}(\mu=0.1791595854394145$ ,  $\text{var}=100.97114496904264$ ,  $T_{\text{ref}}=1000.0$ ,  $N=30$ ,  $\text{data\_mean}=0.0$ ,  $\text{correlation}=\text{'Root'}$ ,),  $\text{comment}=\text{"\"\"\"Estimated from node Root\"\"\"}"$ )



index:  
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### New Kinetics:

Arrhenius( $A=(302000,\text{'s}^{-1}\text{'})$ ,  $n=1.52$ ,  $E_a=(74068.3,\text{'cal/mol}\text{'})$ ,  $T_0=(1,\text{'K}\text{'})$ )

### Current Kinetics

ArrheniusBM( $A=(4.62709\text{e}+20,\text{'s}^{-1}\text{'})$ ,  $n=-1.9758$ ,  $w_0=(661.267,\text{'kJ/mol}\text{'})$ ,  $E_0=(230.31,\text{'kJ/mol}\text{'})$ ,  $T_{\min}=(300,\text{'K}\text{'})$ ,  $T_{\max}=(2000,\text{'K}\text{'})$ ,  $\text{uncertainty}=\text{RateUncertainty}(\mu=0.1791595854394145$ ,  $\text{var}=100.97114496904264$ ,  $T_{\text{ref}}=1000.0$ ,  $N=30$ ,  $\text{data\_mean}=0.0$ ,  $\text{correlation}=\text{'Root'}$ ,),  $\text{comment}=\text{"\"\"\"Estimated from node Root\"\"\"}"$ )

