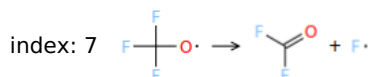


## 17 reactions matched to R\_Addition\_MultipleBond



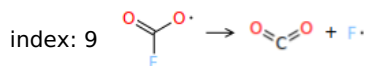
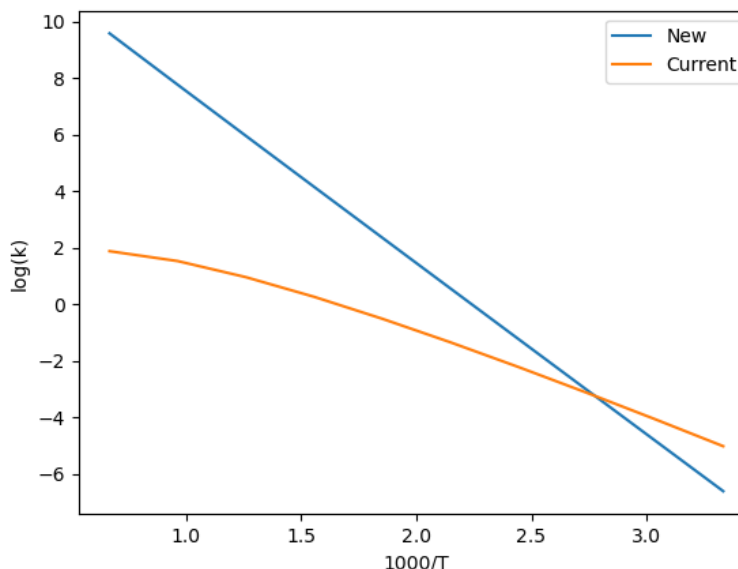
**Note: Training reaction written in opposite direction from reaction family.**

### New Kinetics:

Arrhenius( $A=(7.04e+12, 's^{-1}')$ ,  $n=0.23$ ,  $E_a=(27498.2, 'cal/mol')$ ,  $T_0=(1, 'K')$ )

### Current Kinetics

ArrheniusBM( $A=(4.08261e+20, 'm^3/(mol*s)')$ ,  $n=-5.07836$ ,  $w_0=(384, 'kJ/mol')$ ,  $E_0=(74.9893, 'kJ/mol')$ ,  $T_{min}=(300, 'K')$ ,  $T_{max}=(2000, 'K')$ ,  $uncertainty=RateUncertainty(\mu=0.0, var=33.13686319048999, T_{ref}=1000.0, N=1, data\_mean=0.0, correlation='Root\_N-3R-inRing\_N-3R->C\_N-1R!H->N\_2R!H->O')$ ,  $comment=""$ Estimated from node Root\_N-3R-inRing\_N-3R->C\_N-1R!H->N\_2R!H->O""")



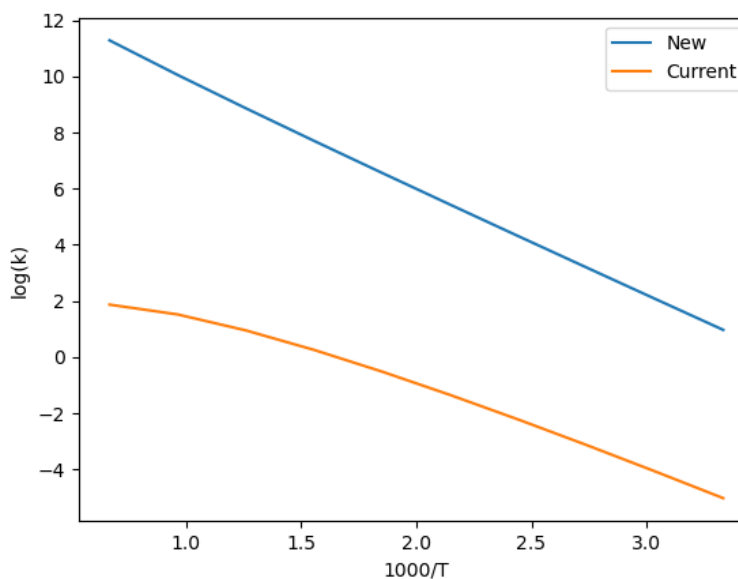
**Note: Training reaction written in opposite direction from reaction family.**

### New Kinetics:

Arrhenius( $A=(2.06e+10, 's^{-1}')$ ,  $n=1.06$ ,  $E_a=(16429.5, 'cal/mol')$ ,  $T_0=(1, 'K')$ )

### Current Kinetics

ArrheniusBM( $A=(4.08261e+20, 'm^3/(mol*s)')$ ,  $n=-5.07836$ ,  $w_0=(384, 'kJ/mol')$ ,  $E_0=(74.9893, 'kJ/mol')$ ,  $T_{min}=(300, 'K')$ ,  $T_{max}=(2000, 'K')$ ,  $uncertainty=RateUncertainty(\mu=0.0, var=33.13686319048999, T_{ref}=1000.0, N=1, data\_mean=0.0, correlation='Root\_N-3R-inRing\_N-3R->C\_N-1R!H->N\_2R!H->O')$ ,  $comment=""$ Estimated from node Root\_N-3R-inRing\_N-3R->C\_N-1R!H->N\_2R!H->O""")



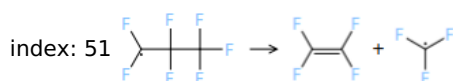
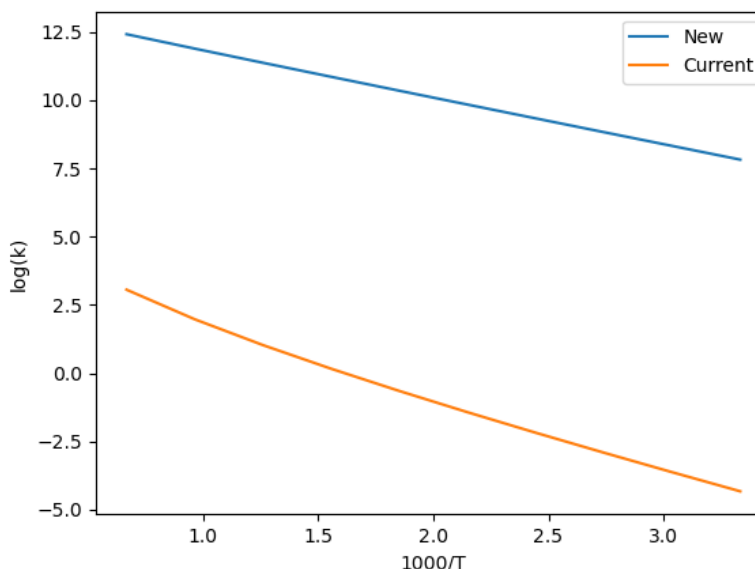
**Note: Training reaction written in opposite direction from reaction family.**

### New Kinetics:

Arrhenius( $A=(7.19e+12, 's^{-1}')$ ,  $n=0.21$ ,  $E_a=(7626.53, 'cal/mol')$ ,  $T_0=(1, 'K')$ )

### Current Kinetics

ArrheniusBM(A=(1.4291e-06,'m^3/(mol\*s)'), n=3.20779, w0=(393.5,'kJ/mol'), E0=(36.9032,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=0.0, var=33.13686319048999, Tref=1000.0, N=1, data\_mean=0.0, correlation='Root\_N-3R-inRing\_Ext-3R-R\_N-Sp-4R!H=3R\_3R->C\_Ext-1R!H-R\_N-5R!H-inRing\_Ext-1R!H-R\_N-2R!H->C\_N-5R!H-u1'), comment="" "Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_N-Sp-4R!H=3R\_3R->C\_Ext-1R!H-R\_N-5R!H-inRing\_Ext-1R!H-R\_N-2R!H->C\_N-5R!H-u1" ""



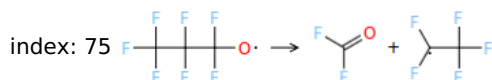
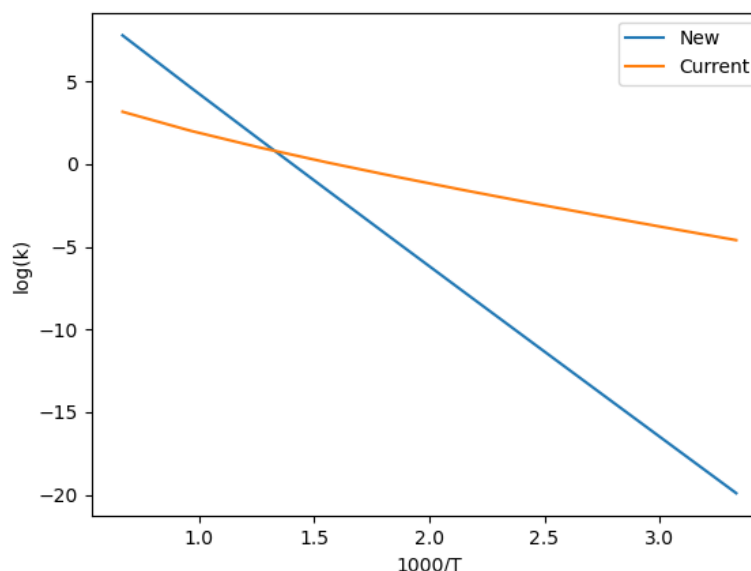
**Note: Training reaction written in opposite direction from reaction family.**

### New Kinetics:

Arrhenius(A=(3.33e+11,'s^-1'), n=0.95, Ea=(46364.6,'cal/mol'), T0=(1,'K'))

### Current Kinetics

ArrheniusBM(A=(1.89178e-07,'m^3/(mol\*s)'), n=3.53001, w0=(303.056,'kJ/mol'), E0=(38.0148,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=-0.4944253016374622, var=1.7828810760479818, Tref=1000.0, N=135, data\_mean=0.0, correlation='Root\_N-3R-inRing\_Ext-3R-R\_N-Sp-4R!H=3R\_3R->C\_Ext-1R!H-R\_N-5R!H-inRing\_Ext-1R!H-R'), comment="" "Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_N-Sp-4R!H=3R\_3R->C\_Ext-1R!H-R\_N-5R!H-inRing\_Ext-1R!H-R Multiplied by reaction path degeneracy 2.0" ""



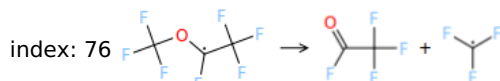
**Note: Training reaction written in opposite direction from reaction family.**

### New Kinetics:

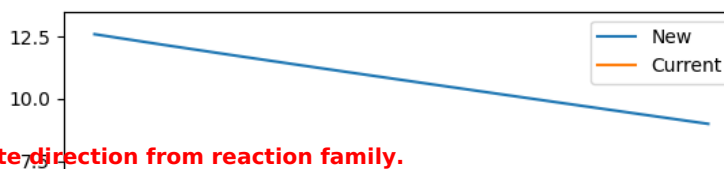
Arrhenius(A=(3.92e+12,'s^-1'), n=0.27, Ea=(5852.35,'cal/mol'), T0=(1,'K'))

### Current Kinetics

ArrheniusBM(A=(1.22525e-05,'m^3/(mol\*s)'), n=2.9005, w0=(393.5,'kJ/mol'), E0=(46.1097,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=0.0, var=33.13686319048999, Tref=1000.0, N=1, data\_mean=0.0, correlation='Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R\_N-Sp-5R!H=4R!H\_Sp-2R!H=1R!H\_Ext-4R!H-R\_N-2R!H->C'), comment="" "Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R\_N-Sp-5R!H=4R!H\_Sp-2R!H=1R!H\_Ext-4R!H-R\_N-2R!H->C" ""



**Note: Training reaction written in opposite direction from reaction family.**

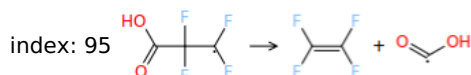
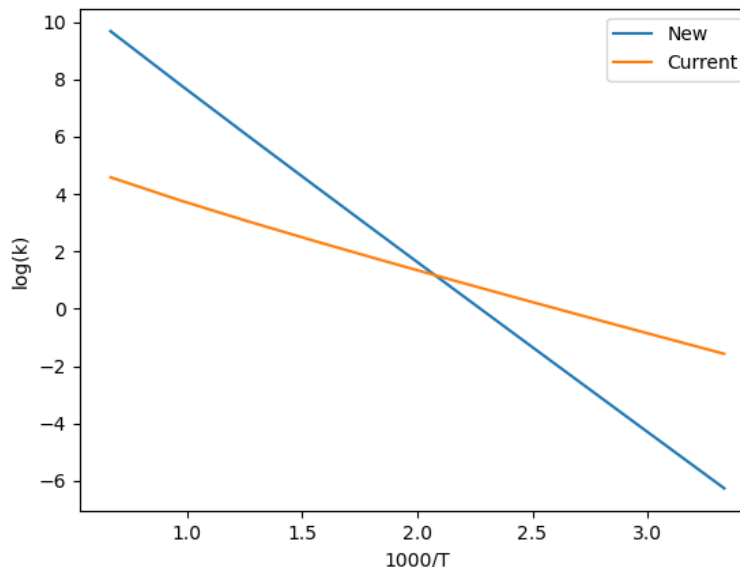


#### New Kinetics:

Arrhenius( $A=(3.03e+11, 's^{-1}')$ ,  $n=0.65$ ,  $E_a=(26570.2, 'cal/mol')$ ,  $T_0=(1, 'K')$ )

#### Current Kinetics

ArrheniusBM( $A=(61.188, 'm^3/(mol*s)')$ ,  $n=1.29312$ ,  $w_0=(297.108, 'kJ/mol')$ ,  $E_0=(37.7031, 'kJ/mol')$ ,  $T_{min}=(300, 'K')$ ,  $T_{max}=(2000, 'K')$ ,  $uncertainty=RateUncertainty(\mu=-0.28976280499384915, var=2.1569028208455543, T_{ref}=1000.0, N=37, data\_mean=0.0, correlation='Root\_N-3R-inRing\_Ext-3R-R\_N-Sp-4R!H=3R\_3R->C\_Ext-3C-R\_2R!H->C')$ ,  $comment=""$ Estimated from node Root\_N-3R-inRing\\_Ext-3R-R\\_N-Sp-4R!H=3R\\_3R->C\\_Ext-3C-R\\_2R!H->C""")



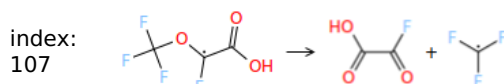
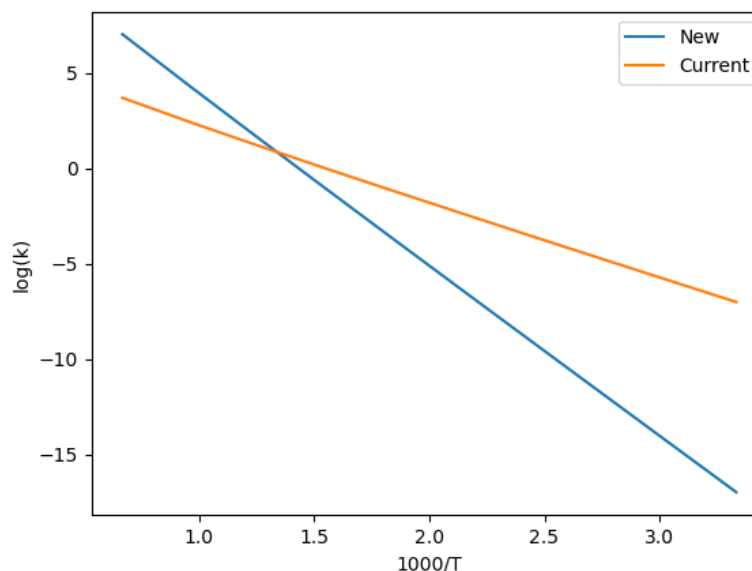
**Note: Training reaction written in opposite direction from reaction family.**

#### New Kinetics:

Arrhenius( $A=(3.93e+09, 's^{-1}')$ ,  $n=1.03$ ,  $E_a=(39998.5, 'cal/mol')$ ,  $T_0=(1, 'K')$ )

#### Current Kinetics

ArrheniusBM( $A=(306.062, 'm^3/(mol*s)')$ ,  $n=1.16366$ ,  $w_0=(301.402, 'kJ/mol')$ ,  $E_0=(71.0975, 'kJ/mol')$ ,  $T_{min}=(300, 'K')$ ,  $T_{max}=(2000, 'K')$ ,  $uncertainty=RateUncertainty(\mu=-0.022037706214473284, var=2.3701416358838845, T_{ref}=1000.0, N=230, data\_mean=0.0, correlation='Root\_N-3R-inRing\_Ext-3R-R\_Sp-4R!H=3R\_Sp-2R!H=1R!H')$ ,  $comment=""$ Estimated from node Root\_N-3R-inRing\\_Ext-3R-R\\_Sp-4R!H=3R\\_Sp-2R!H=1R!H Multiplied by reaction path degeneracy 2.0""")



**Note: Training reaction written in opposite direction from reaction family.**

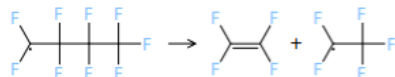
#### New Kinetics:

Arrhenius( $A=(2.03e+09, 's^{-1}')$ ,  $n=1.02$ ,  $E_a=(27425.9, 'cal/mol')$ ,  $T_0=(1, 'K')$ )

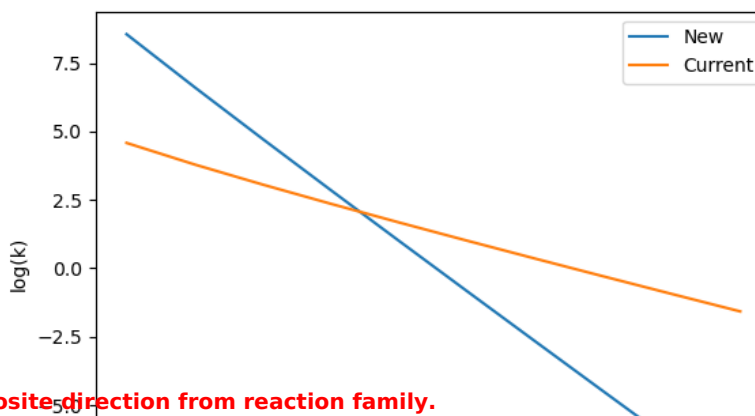
#### Current Kinetics

ArrheniusBM(A=(61.188,'m^3/(mol\*s)'), n=1.29312, w0=(297.108,'kJ/mol'), E0=(37.7031,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=-0.28976280499384915, var=2.1569028208455543, Tref=1000.0, N=37, data\_mean=0.0, correlation='Root\_N-3R-inRing\_Ext-3R-R\_N-Sp-4R!H=3R\_3R->C\_Ext-3C-R\_2R!H->C'), comment=""Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_N-Sp-4R!H=3R\_3R->C\_Ext-3C-R\_2R!H->C""")

index:  
110



**Note: Training reaction written in opposite direction from reaction family.**

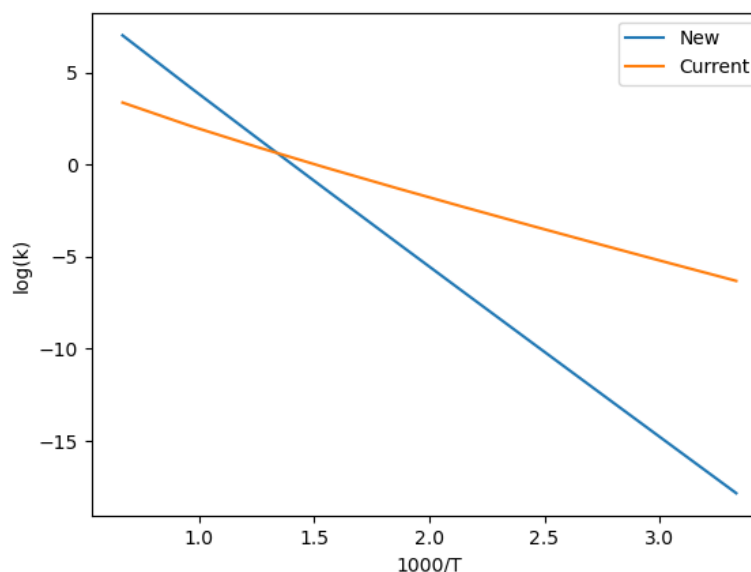


### New Kinetics:

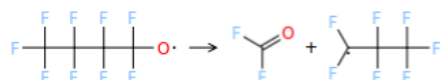
Arrhenius(A=(6.27e+09,'s^-1'), n=1.02, Ea=(41399.2,'cal/mol'), T0=(1,'K'))

### Current Kinetics

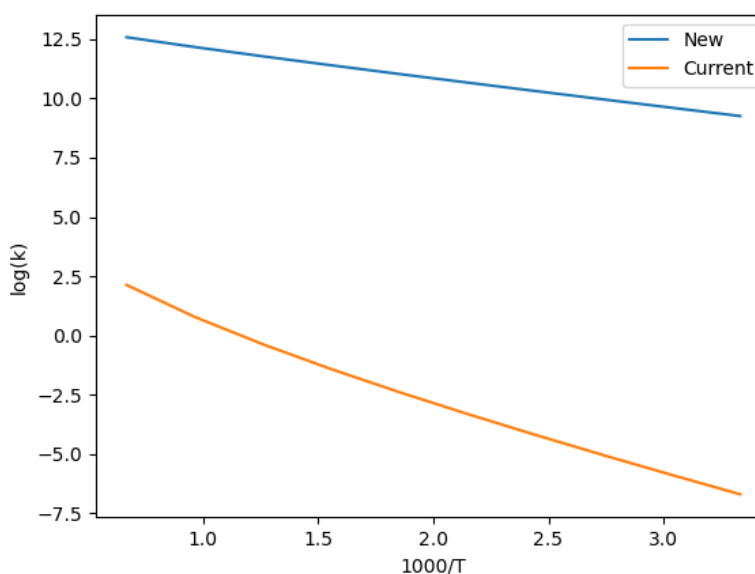
ArrheniusBM(A=(0.00504,'m^3/(mol\*s)'), n=2.41, w0=(301,'kJ/mol'), E0=(57.3723,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=0.0, var=33.13686319048999, Tref=1000.0, N=1, data\_mean=0.0, correlation='Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R\_N-Sp-5R!H=4R!H\_Sp-2R!H=1R!H\_Ext-4R!H-R\_2R!H->C'), comment=""Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R\_N-Sp-5R!H=4R!H\_Sp-2R!H=1R!H\_Ext-4R!H-R\_2R!H->C Multiplied by reaction path degeneracy 2.0""")



index:  
135



**Note: Training reaction written in opposite direction from reaction family.**



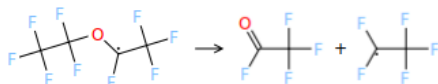
### New Kinetics:

Arrhenius(A=(3.71e+11,'s^-1'), n=0.55, Ea=(5045.12,'cal/mol'), T0=(1,'K'))

### Current Kinetics

ArrheniusBM(A=(2.13223e-11,'m^3/(mol\*s)'), n=4.48095, w0=(299.5,'kJ/mol'), E0=(40.9045,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=-0.6004730311185978, var=1.5705211473983438, Tref=1000.0, N=276, data\_mean=0.0, correlation='Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R\_Ext-3R-R\_Ext-1R!H-R\_N-8R!H-inRing'), comment=""Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R\_Ext-3R-R\_Ext-1R!H-R\_N-8R!H-inRing""")

index:  
136



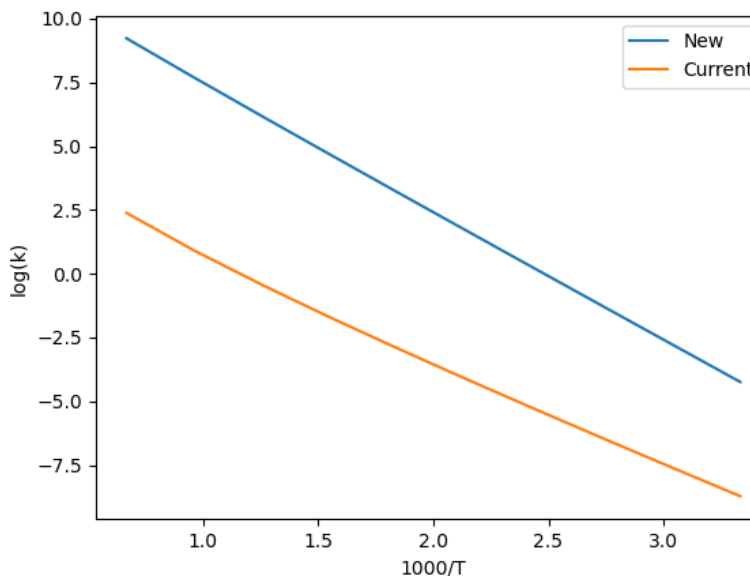
**Note: Training reaction written in opposite direction from reaction family.**

#### New Kinetics:

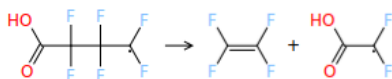
Arrhenius( $A=(2.59 \times 10^{10}, \text{s}^{-1})$ ,  $n=0.65$ ,  $E_a=(22327.4, \text{cal/mol})$ ,  $T_0=(1, \text{K})$ )

#### Current Kinetics

ArrheniusBM( $A=(9.07578 \times 10^{-6}, \text{m}^3/(\text{mol} \cdot \text{s}))$ ,  $n=3.04336$ ,  $w_0=(299.503, \text{kJ/mol})$ ,  $E_0=(64.4187, \text{kJ/mol})$ ,  $T_{\min}=(300, \text{K})$ ,  $T_{\max}=(2000, \text{K})$ ,  $\text{uncertainty}=\text{RateUncertainty}(\mu=-0.3757377757886876$ ,  $\text{var}=2.242054186761003$ ,  $T_{\text{ref}}=1000.0$ ,  $N=1042$ ,  $\text{data\_mean}=0.0$ ,  $\text{correlation}=\text{'Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R'}$ ,),  $\text{comment}=\text{'\"\"\"Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R\"\"\"}'$ )



index:  
156



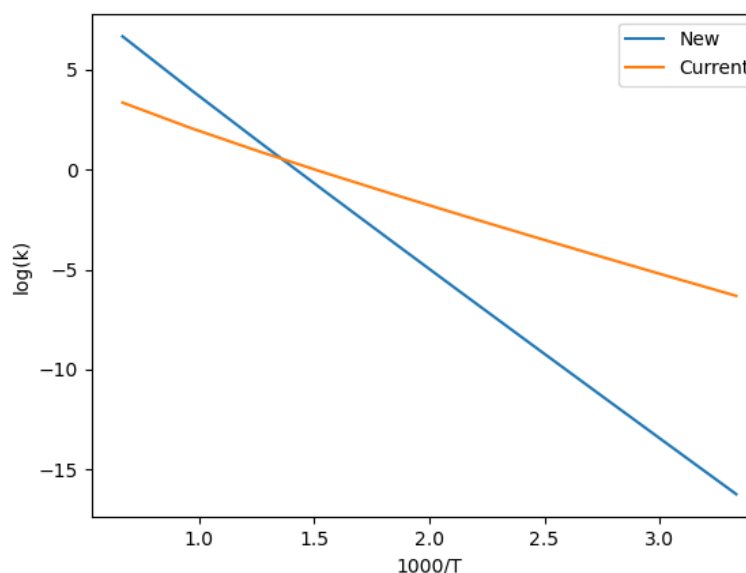
**Note: Training reaction written in opposite direction from reaction family.**

#### New Kinetics:

Arrhenius( $A=(2.78 \times 10^{07}, \text{s}^{-1})$ ,  $n=1.48$ ,  $E_a=(37548.5, \text{cal/mol})$ ,  $T_0=(1, \text{K})$ )

#### Current Kinetics

ArrheniusBM( $A=(0.00504, \text{m}^3/(\text{mol} \cdot \text{s}))$ ,  $n=2.41$ ,  $w_0=(301, \text{kJ/mol})$ ,  $E_0=(57.3723, \text{kJ/mol})$ ,  $T_{\min}=(300, \text{K})$ ,  $T_{\max}=(2000, \text{K})$ ,  $\text{uncertainty}=\text{RateUncertainty}(\mu=0.0$ ,  $\text{var}=33.13686319048999$ ,  $T_{\text{ref}}=1000.0$ ,  $N=1$ ,  $\text{data\_mean}=0.0$ ,  $\text{correlation}=\text{'Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R\_N-Sp-5R!H=4R!H\_Sp-2R!H=1R!H\_Ext-4R!H-R\_2R!H->C'}$ ,),  $\text{comment}=\text{'\"\"\"Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R\_N-Sp-5R!H=4R!H\_Sp-2R!H=1R!H\_Ext-4R!H-R\_2R!H->C Multiplied by reaction path degeneracy 2.0\"\"\"}'$ )



index:  
169



**Note: Training reaction written in opposite direction from reaction family.**

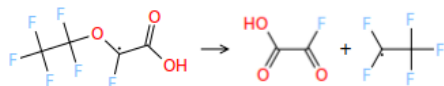
#### New Kinetics:

Arrhenius( $A=(1.59 \times 10^{07}, \text{s}^{-1})$ ,  $n=1.64$ ,  $E_a=(23421.2, \text{cal/mol})$ ,  $T_0=(1, \text{K})$ )

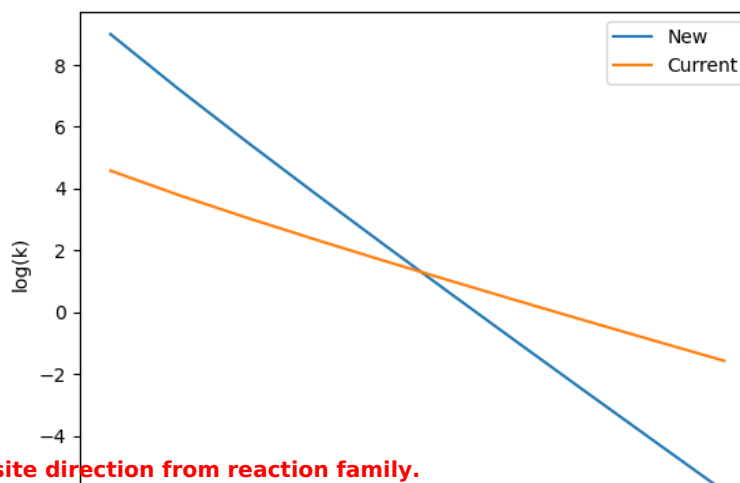
### Current Kinetics

ArrheniusBM(A=(61.188,'m<sup>3</sup>/(mol\*s)'), n=1.29312, w0=(297.108,'kJ/mol'), E0=(37.7031,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=-0.28976280499384915, var=2.1569028208455543, Tref=1000.0, N=37, data\_mean=0.0, correlation='Root\_N-3R-inRing\_Ext-3R-R\_N-Sp-4R!H=3R\_3R->C\_Ext-3C-R\_2R!H->C'), comment=""Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_N-Sp-4R!H=3R\_3R->C\_Ext-3C-R\_2R!H->C""")

index:  
173



Note: Training reaction written in opposite direction from reaction family.



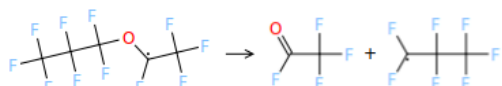
### New Kinetics:

Arrhenius(A=(6.21e+08,'s<sup>-1</sup>'), n=0.88, Ea=(23310.1,'cal/mol'), T0=(1,'K'))

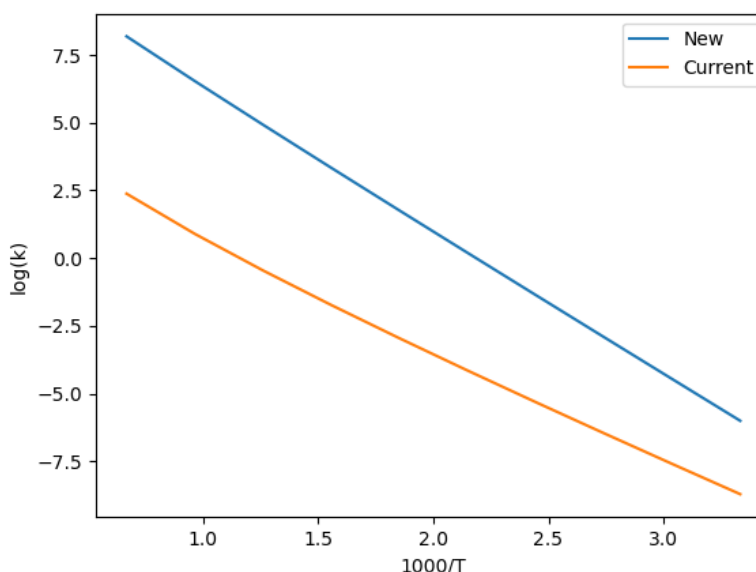
### Current Kinetics

ArrheniusBM(A=(9.07578e-06,'m<sup>3</sup>/(mol\*s)'), n=3.04336, w0=(299.503,'kJ/mol'), E0=(64.4187,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=-0.3757377757886876, var=2.242054186761003, Tref=1000.0, N=1042, data\_mean=0.0, correlation='Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R'), comment=""Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R""")

index:  
191



Note: Training reaction written in opposite direction from reaction family.

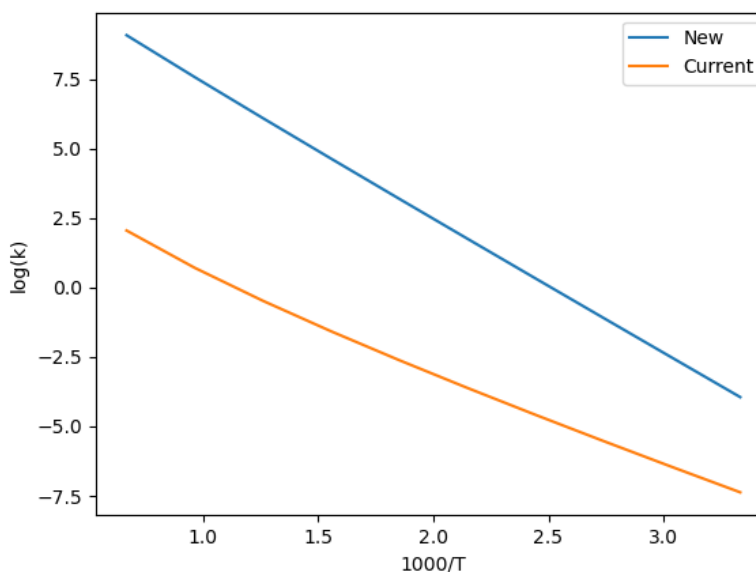


### New Kinetics:

Arrhenius(A=(6.62e+09,'s<sup>-1</sup>'), n=0.75, Ea=(21448.5,'cal/mol'), T0=(1,'K'))

### Current Kinetics

ArrheniusBM(A=(2.06973e-08,'m<sup>3</sup>/(mol\*s)'), n=3.60774, w0=(299.574,'kJ/mol'), E0=(49.539,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=-0.5239778944948545, var=2.087050032983542, Tref=1000.0, N=387, data\_mean=0.0, correlation='Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R\_Ext-3R-R'), comment=""Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R\_Ext-3R-R""")



index:  
213



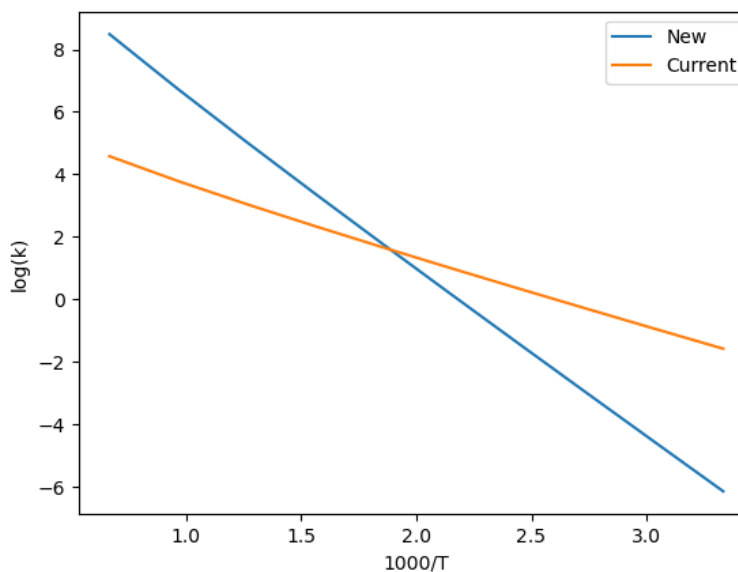
Note: Training reaction written in opposite direction from reaction family.

#### New Kinetics:

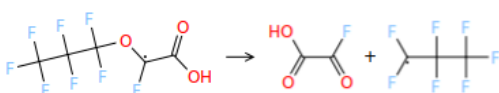
Arrhenius( $A=(1.2\text{e}+07, \text{s}^{-1})$ ,  $n=1.51$ ,  $E_a=(23274.4, \text{cal/mol})$ ,  $T_0=(1, \text{K})$ )

#### Current Kinetics

ArrheniusBM( $A=(61.188, \text{m}^3/(\text{mol}\cdot\text{s}))$ ,  $n=1.29312$ ,  $w_0=(297.108, \text{kJ/mol})$ ,  $E_0=(37.7031, \text{kJ/mol})$ ,  $T_{\min}=(300, \text{K})$ ,  $T_{\max}=(2000, \text{K})$ ,  $\text{uncertainty}=\text{RateUncertainty}(\mu=-0.28976280499384915, \text{var}=2.1569028208455543, T_{\text{ref}}=1000.0, N=37, \text{data\_mean}=0.0, \text{correlation}=\text{'Root\_N-3R-inRing\_Ext-3R-R\_N-Sp-4R!H=3R\_3R->C\_Ext-3C-R\_2R!H->C'})$ ,  $\text{comment}=\text{'\"\"\"Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_N-Sp-4R!H=3R\_3R->C\_Ext-3C-R\_2R!H->C\"\"\"}'$ )



index:  
217



Note: Training reaction written in opposite direction from reaction family.

#### New Kinetics:

Arrhenius( $A=(6.96\text{e}+09, \text{s}^{-1})$ ,  $n=0.66$ ,  $E_a=(22657.3, \text{cal/mol})$ ,  $T_0=(1, \text{K})$ )

#### Current Kinetics

ArrheniusBM( $A=(2.06973\text{e}-08, \text{m}^3/(\text{mol}\cdot\text{s}))$ ,  $n=3.60774$ ,  $w_0=(299.574, \text{kJ/mol})$ ,  $E_0=(49.539, \text{kJ/mol})$ ,  $T_{\min}=(300, \text{K})$ ,  $T_{\max}=(2000, \text{K})$ ,  $\text{uncertainty}=\text{RateUncertainty}(\mu=-0.5239778944948545, \text{var}=2.087050032983542, T_{\text{ref}}=1000.0, N=387, \text{data\_mean}=0.0, \text{correlation}=\text{'Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R\_Ext-3R-R'})$ ,  $\text{comment}=\text{'\"\"\"Estimated from node Root\_N-3R-inRing\_Ext-3R-R\_Ext-4R!H-R\_Ext-3R-R\_Ext-3R-R\"\"\"}'$ )

