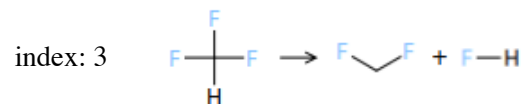


## 3 reactions matched to 1,2\_Insertion\_carbene



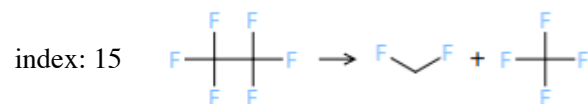
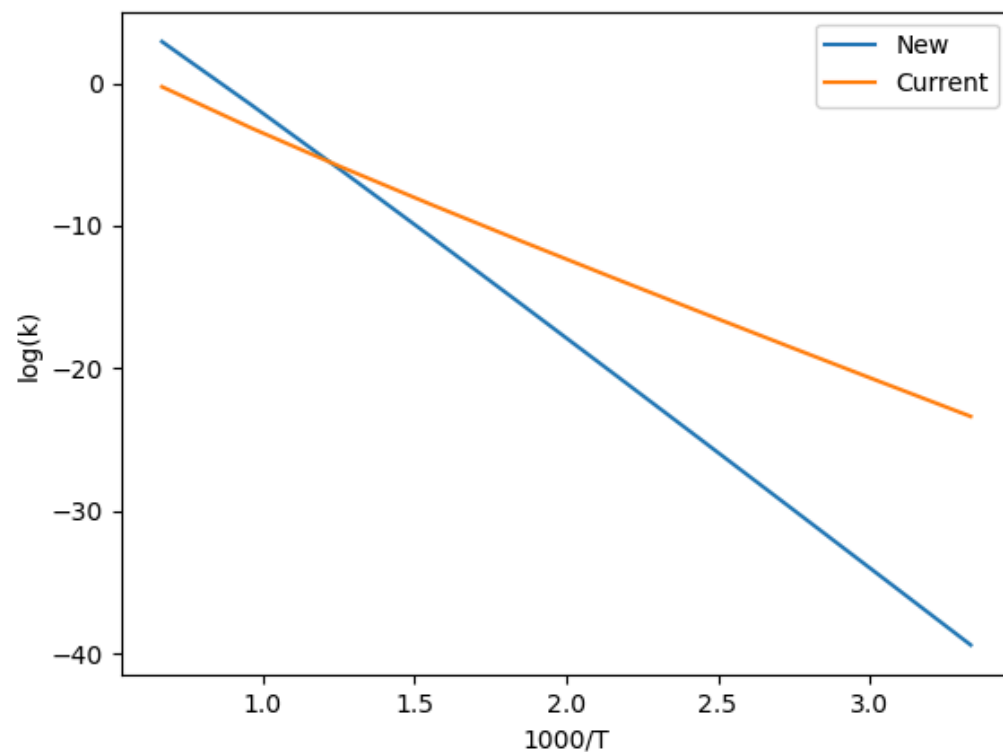
**Note: Training reaction written in opposite direction from reaction family.**

**New Kinetics:**

Arrhenius( $A=(2.15 \times 10^{23}, \text{s}^{-1})$ ,  $n=-2.93$ ,  $E_a=(76170, \text{cal/mol})$ ,  $T_0=(1, \text{K})$ )

**Current Kinetics**

ArrheniusBM( $A=(3.98081 \times 10^{-9}, \text{m}^3/(\text{mol} \cdot \text{s}))$ ,  $n=4.16158$ ,  $w_0=(730.5, \text{kJ/mol})$ ,  $E_0=(145.218, \text{kJ/mol})$ ,  $T_{\min}=(300, \text{K})$ ,  $T_{\max}=(2000, \text{K})$ ,  $\text{uncertainty}=\text{RateUncertainty}(\mu=0.0, \text{var}=33.13686319048999, T_{\text{ref}}=1000.0, N=1, \text{data\_mean}=0.0, \text{correlation}=\text{'HY\_3Br1sCC11sF1sHI1s->F1s\_2Br1sCl1sF1sHI1s->F1s\_4Br1sCl1sF1sI1s->F1s'})$ ,  $\text{comment}=\text{'\"\"\"Estimated from node HY\_3Br1sCC11sF1sHI1s->F1s\_2Br1sCl1sF1sHI1s->F1s\_4Br1sCl1sF1sI1s->F1s\"\"\"}'$ )



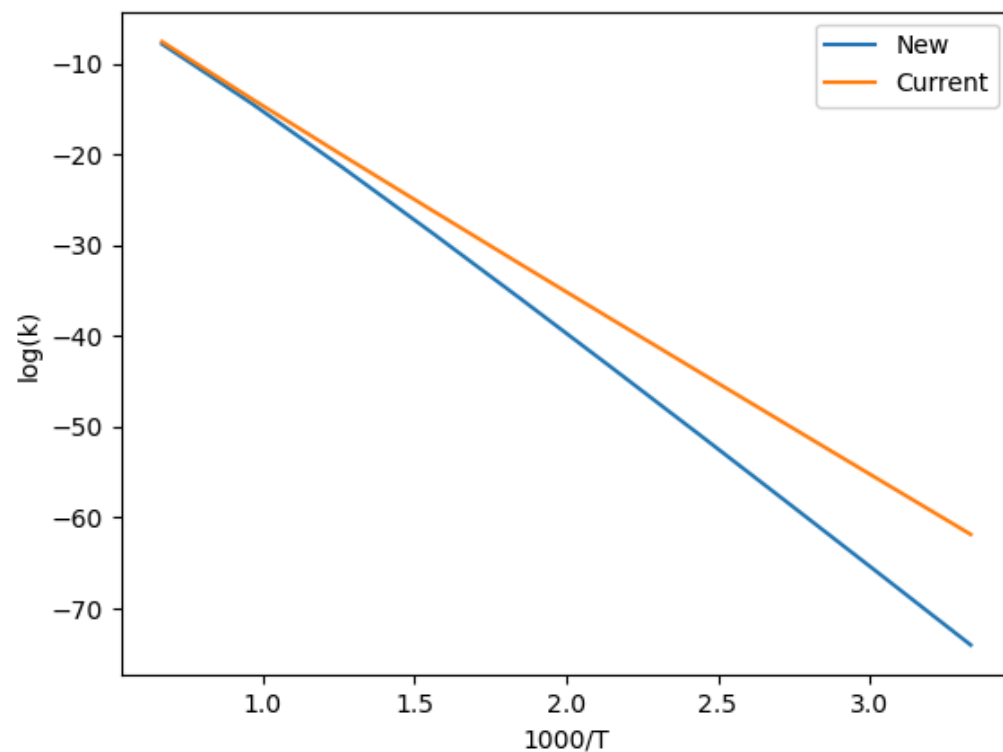
**Note: Training reaction written in opposite direction from reaction family.**

**New Kinetics:**

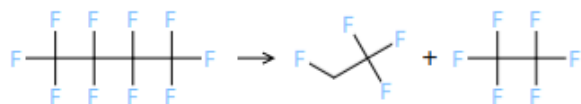
Arrhenius( $A=(1.82\text{e}+41, \text{'s}^{-1}\text{'})$ ,  $n=-9.72$ ,  $E_a=(125200, \text{'cal/mol}\text{'})$ ,  $T_0=(1, \text{'K}\text{'})$ )

**Current Kinetics**

ArrheniusBM( $A=(5.34328\text{e}-06, \text{'m}^3/(\text{mol}\cdot\text{s})\text{'})$ ,  $n=3.3552$ ,  $w_0=(658, \text{'kJ/mol}\text{'})$ ,  $E_0=(372.673, \text{'kJ/mol}\text{'})$ ,  $T_{\min}=(300, \text{'K}\text{'})$ ,  $T_{\max}=(2000, \text{'K}\text{'})$ ,  $\text{uncertainty}=\text{RateUncertainty}(\mu=0.0, \text{var}=33.13686319048999, T_{\text{ref}}=1000.0, N=1, \text{data\_mean}=0.0, \text{correlation}=\text{'CY\_N-2Br1sCl1sF1sHI1s->H\_Ext-4Cs-R'\text{'}})$ ,  $\text{comment}=\text{'\"\"\"Estimated from node CY\_N-2Br1sCl1sF1sHI1s->H\_Ext-4Cs-R Multiplied by reaction path degeneracy 4.0\"\"\"'}$ )



index: 87



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

**New Kinetics:**

Arrhenius( $A=(3.99 \times 10^{42}, \text{s}^{-1})$ ,  $n=-9.51$ ,  $E_a=(128100, \text{cal/mol})$ ,  $T_0=(1, \text{K})$ )

**Current Kinetics**

ArrheniusBM( $A=(2.10281 \times 10^{54}, \text{m}^3/(\text{mol} \cdot \text{s}))$ ,  $n=-13.541$ ,  $w_0=(581.04, \text{kJ/mol})$ ,  $E_0=(336.403, \text{kJ/mol})$ ,  $T_{\min}=(300, \text{K})$ ,  $T_{\max}=(2000, \text{K})$ ,  $\text{uncertainty}=\text{RateUncertainty}(\mu=1.513119107657762$ ,  $\text{var}=99.27123869380007$ ,  $T_{\text{ref}}=1000.0$ ,  $N=63$ ,  $\text{data\_mean}=0.0$ ,  $\text{correlation}=\text{'Root'}$ ),  $\text{comment}=""$ Estimated from node Root Multiplied by reaction path degeneracy 6.0""")

