### 8 reactions matched to 1,2 Insertion CO

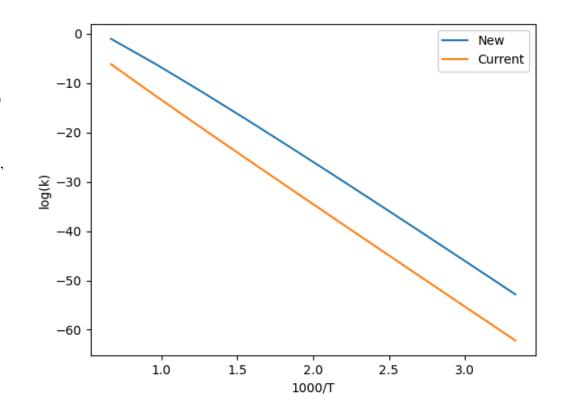
Note: Training reaction written in opposite direction from reaction family.

## **New Kinetics:**

Arrhenius(A=(8.99e+36,'s^-1'), n=-7.46, Ea=(97870,'cal/mol'), T0=(1,'K'))

### **Current Kinetics**

ArrheniusBM(A=(0.0107824,'m^3/(mol\*s)'), n=2.93313, w0= (794.5,'kJ/mol'), E0=(387.509,'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\_1COCbCdCsCtHNOSSidSis->Cs\_N-2Br1sCbCdCl1sCsCtF1sHI1sNSSidSis->Cs\_Ext-1Cs-R\_2Br1sCl1sF1sH->F1s',), comment="""Estimated from node Root\_1COCbCdCsCtHNOSSidSis->Cs\_N-2Br1sCbCdCl1sCsCtF1sHI1sNSSidSis->Cs\_Ext-1Cs-R\_2Br1sCl1sF1sH->F1s Multiplied by reaction path degeneracy 4.0""")



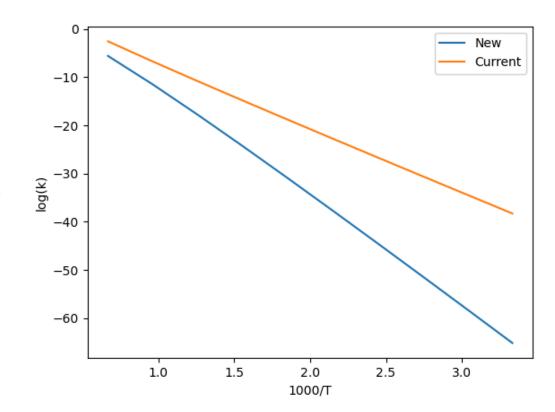
index: 26

$$F \rightarrow CO + F \rightarrow CH$$

Arrhenius(A=(2.83e+37,'s^-1'), n=-8.4, Ea=(112300,'cal/mol'), T0=(1,'K'))

### **Current Kinetics**

ArrheniusBM(A=(0.000742267,'m^3/(mol\*s)'), n=2.83796, w0= (753.2,'kJ/mol'), E0=(242.307,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=1.2632766423807829, var=145.9379134136138, Tref=1000.0, N=5, data\_mean=0.0, correlation='Root\_N-1COCbCdCsCtHNOSSidSis->Cs', comment=""Estimated from node Root\_N-1COCbCdCsCtHNOSSidSis->Cs""")

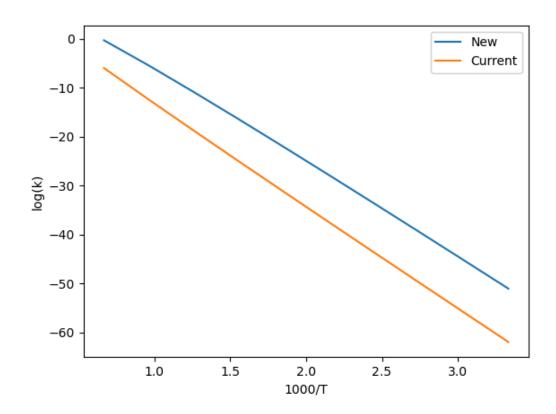


index: 44 
$$\rightarrow$$
 F  $\rightarrow$  CO + F

Arrhenius(A=(6.86e+31,'s^-1'), n=-5.8, Ea=(94100,'cal/mol'), T0=(1,'K'))

### **Current Kinetics**

ArrheniusBM(A=(0.0161736,'m^3/(mol\*s)'), n=2.93313, w0= (794.5,'kJ/mol'), E0=(387.509,'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\_1COCbCdCsCtHNOSSidSis->Cs\_N-2Br1sCbCdCl1sCsCtF1sHI1sNSSidSis->Cs\_Ext-1Cs-R\_2Br1sCl1sF1sH->F1s',), comment="""Estimated from node Root\_1COCbCdCsCtHNOSSidSis->Cs\_N-2Br1sCbCdCl1sCsCtF1sHI1sNSSidSis->Cs\_Ext-1Cs-R\_2Br1sCl1sF1sH->F1s Multiplied by reaction path degeneracy 6.0""")

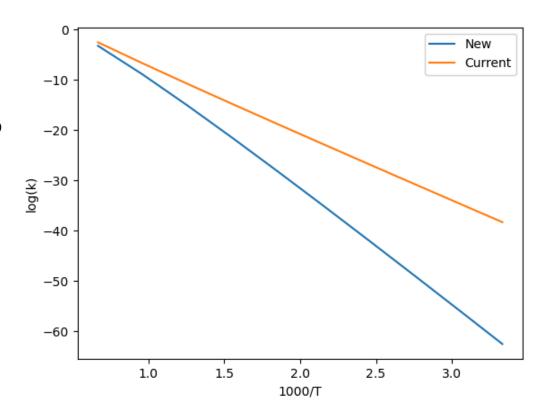


index: 69 
$$\stackrel{\text{HO}}{\triangleright}$$
  $\stackrel{\text{F}}{\models}$   $\stackrel{\text{F}}{\models}$   $\stackrel{\text{F}}{\models}$   $\stackrel{\text{CO}}{\models}$   $\stackrel{\text{HO}}{\models}$   $\stackrel{\text{F}}{\models}$ 

Arrhenius(A=(1.91e+46,'s^-1'), n=-10.36, Ea=(114100,'cal/mol'), T0=(1,'K'))

### **Current Kinetics**

ArrheniusBM(A=(0.000742267,'m^3/(mol\*s)'), n=2.83796, w0= (753.2,'kJ/mol'), E0=(242.307,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=1.2632766423807829, var=145.9379134136138, Tref=1000.0, N=5, data\_mean=0.0, correlation='Root\_N-1COCbCdCsCtHNOSSidSis->Cs', comment=""Estimated from node Root\_N-1COCbCdCsCtHNOSSidSis->Cs""")

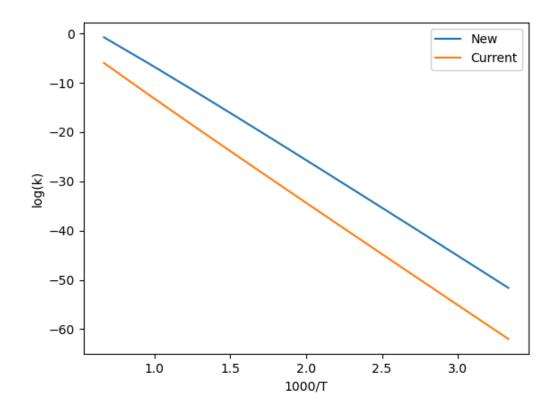


index: 91

Arrhenius(A=(1.55e+25,'s^-1'), n=-3.95, Ea=(92010,'cal/mol'), T0=(1,'K'))

### **Current Kinetics**

ArrheniusBM(A=(0.0161736,'m^3/(mol\*s)'), n=2.93313, w0= (794.5,'kJ/mol'), E0=(387.509,'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\_1COCbCdCsCtHNOSSidSis->Cs\_N-2Br1sCbCdCl1sCsCtF1sHI1sNSSidSis->Cs\_Ext-1Cs-R\_2Br1sCl1sF1sH->F1s',), comment=""Estimated from node Root\_1COCbCdCsCtHNOSSidSis->Cs\_N-2Br1sCbCdCl1sCsCtF1sHI1sNSSidSis->Cs\_Ext-1Cs-R\_2Br1sCl1sF1sH->F1s Multiplied by reaction path degeneracy 6.0""")

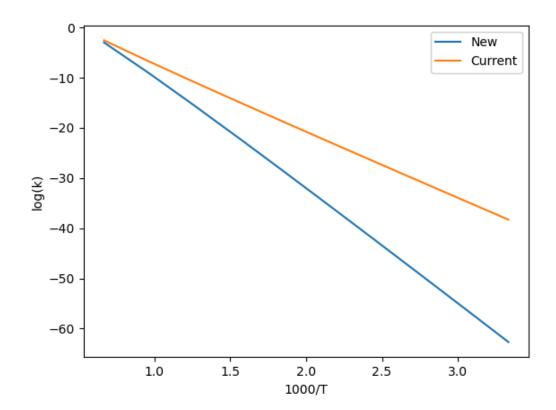


index: 120 
$$\stackrel{\text{HO}}{\triangleright}$$
  $\stackrel{\text{F}}{\models}$   $\stackrel{\text{F}}{\models}$   $\stackrel{\text{F}}{\models}$   $\stackrel{\text{F}}{\models}$   $\stackrel{\text{F}}{\models}$   $\stackrel{\text{F}}{\models}$   $\stackrel{\text{F}}{\models}$   $\stackrel{\text{OH}}{\models}$ 

Arrhenius(A=(1.14e+33,'s^-1'), n=-6.3, Ea=(110000,'cal/mol'), T0=(1,'K'))

### **Current Kinetics**

ArrheniusBM(A=(0.000742267,'m^3/(mol\*s)'), n=2.83796, w0= (753.2,'kJ/mol'), E0=(242.307,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=1.2632766423807829, var=145.9379134136138, Tref=1000.0, N=5, data\_mean=0.0, correlation='Root\_N-1COCbCdCsCtHNOSSidSis->Cs',), comment="""Estimated from node Root\_N-1COCbCdCsCtHNOSSidSis->Cs""")

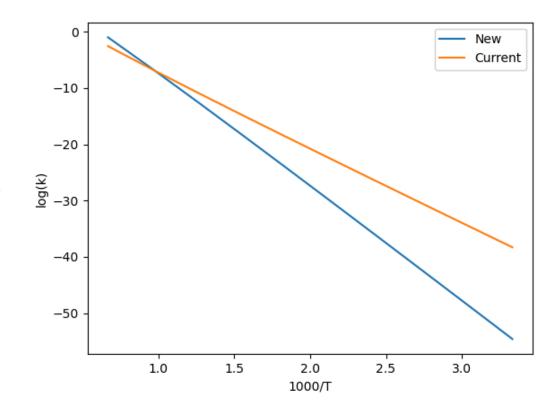


index: 127 
$$F \leftarrow F \rightarrow CO + F \rightarrow F \rightarrow F$$

Arrhenius(A=(4e+23,'s^-1'), n=-3.34, Ea=(95970,'cal/mol'), T0=(1,'K'))

### **Current Kinetics**

ArrheniusBM(A=(0.000742267,'m^3/(mol\*s)'), n=2.83796, w0= (753.2,'kJ/mol'), E0=(242.307,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=1.2632766423807829, var=145.9379134136138, Tref=1000.0, N=5, data\_mean=0.0, correlation='Root\_N-1COCbCdCsCtHNOSSidSis->Cs',), comment="""Estimated from node Root\_N-1COCbCdCsCtHNOSSidSis->Cs""")



Arrhenius(A=(2.29e+30,'s^-1'), n=-5.75, Ea=(98980,'cal/mol'), T0=(1,'K'))

# **Current Kinetics**

 $\label{eq:arrheniusBM} ArrheniusBM(A=(0.000742267,'m^3/(mol*s)'), n=2.83796, w0=(753.2,'kJ/mol'), E0=(242.307,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=1.2632766423807829, var=145.9379134136138, Tref=1000.0, N=5, data_mean=0.0, correlation='Root_N-1COCbCdCsCtHNOSSidSis->Cs', comment=""Estimated from node Root_N-1COCbCdCsCtHNOSSidSis->Cs""")$ 

