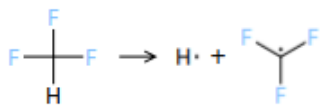**87 reactions matched to R_Recombination**

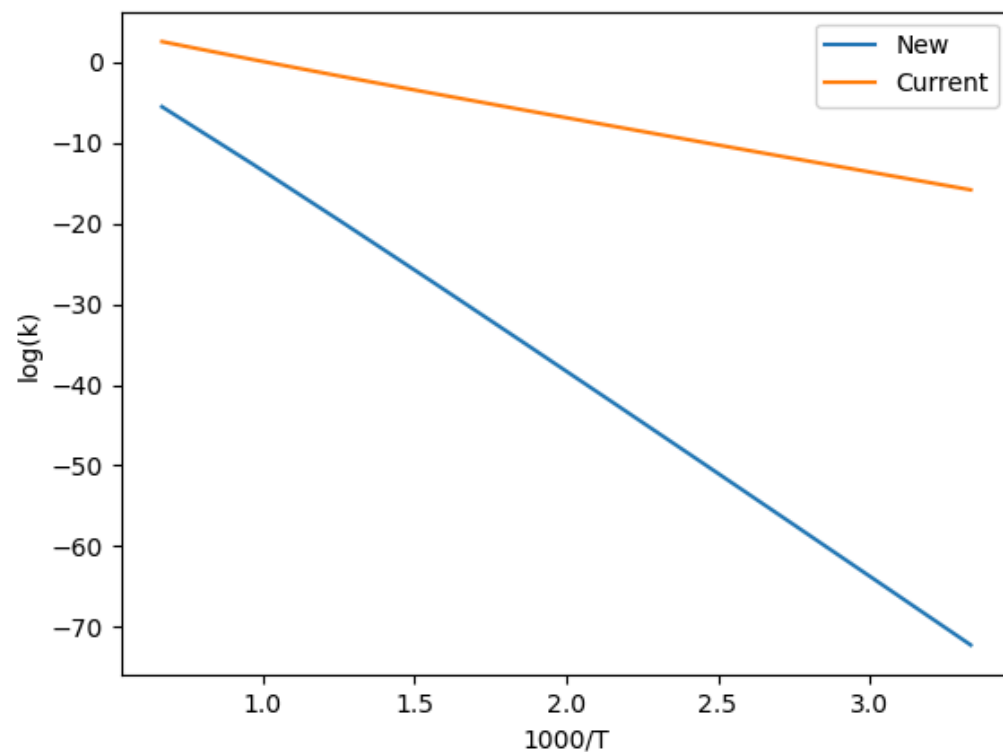index: 1

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

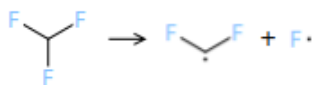
New Kinetics:
Arrhenius(A=(1.96e+26,'s^-1'), n=-4.52, Ea=(119900,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(4.1766,'m^3/(mol*s)'), n=1.94174, w0=(205.5,'kJ/mol'),
E0=(122.15,'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_1R->H_N-2R->S_N-
2BrCClFHNO-inRing_N-2BrCClFHNO->O_N-2CHN->N_2CH->C_Ext-
2C-R_3R!H->F_Ext-2C-R_N-4R!H->C_Ext-2C-R',),
comment="""Estimated from node Root_1R->H_N-2R->S_N-
2BrCClFHNO-inRing_N-2BrCClFHNO->O_N-2CHN->N_2CH->C_Ext-
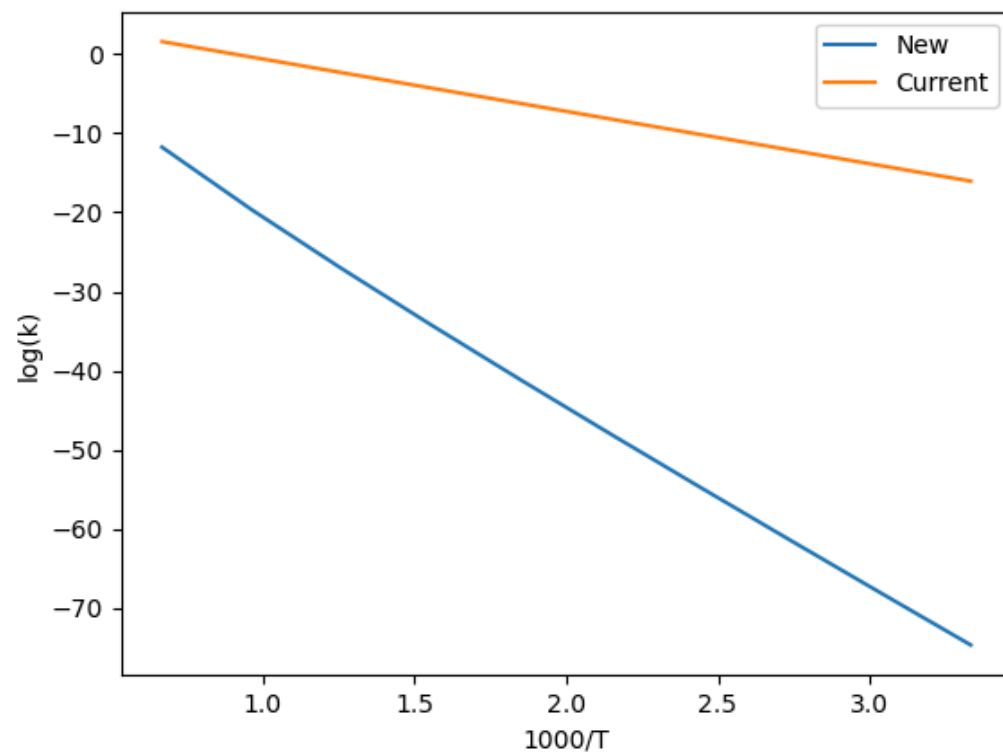2C-R_3R!H->F_Ext-2C-R_N-4R!H->C_Ext-2C-R""")

index: 2

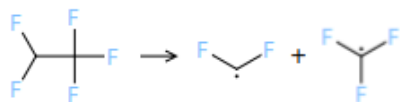**Note: Training reaction written in opposite direction from reaction family.**

New Kinetics:
Arrhenius(A=(1.23e-34,'s^-1'), n=11.31, Ea=(94450,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(1e+06,'m^3/(mol*s)'), n=0, w0=(242.5,'kJ/mol'), E0=
(126.651,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF-
>C',), comment="""Estimated from node Root_N-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
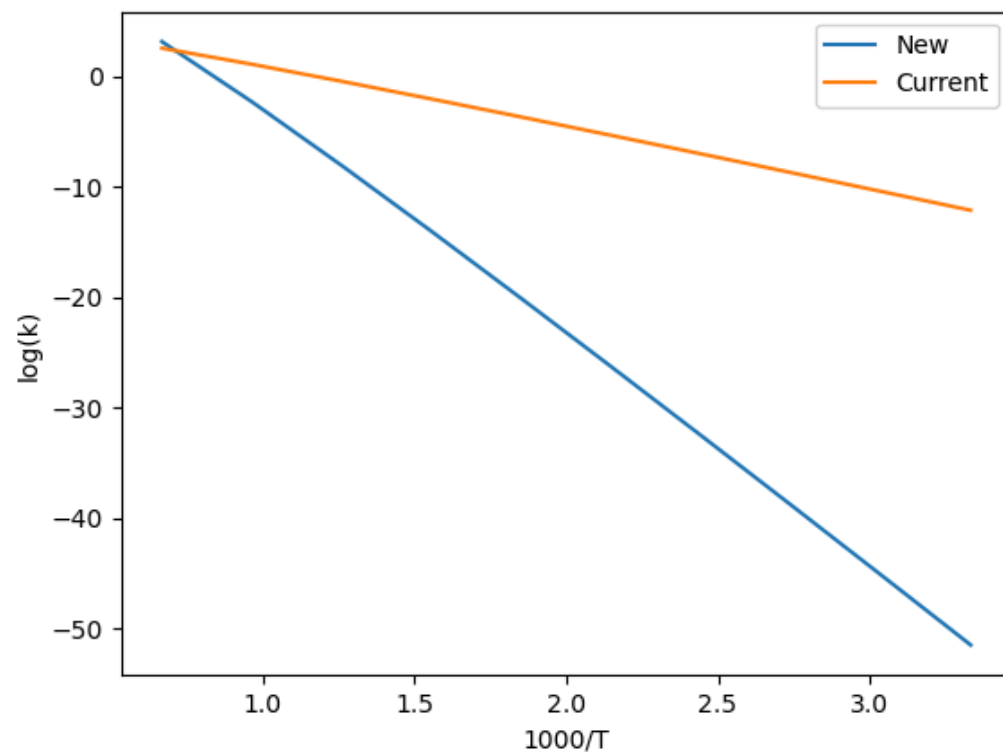inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF-
>C""")

index: 9

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

New Kinetics:
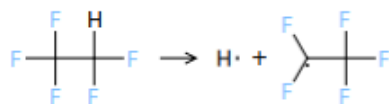Arrhenius(A=(2.2e+42,'s^-1'), n=-7.63, Ea=(102800,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.83587e+13,'m^3/(mol*s)'), n=-2.16473, w0=
(173,'kJ/mol'), E0=(116.106,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_N-4R!H->O_4BrCClF->F_Ext-1C-R_N-5R!H->Cl_Ext-2CF-R_N-
5BrCFINOPSSi->Br_Ext-1C-R',), comment="""Estimated from node
Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-
1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF-
>Br_Ext-1C-R_3R!H->F_Ext-2CF-R_N-4R!H->O_4BrCClF->F_Ext-1C-
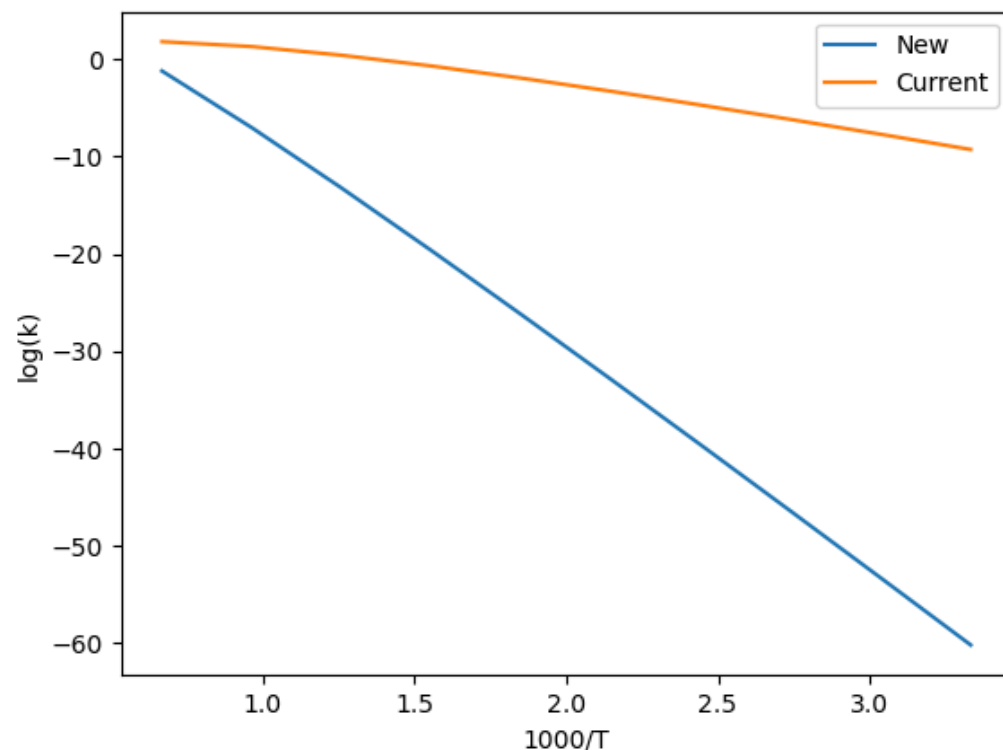R_N-5R!H->Cl_Ext-2CF-R_N-5BrCFINOPSSi->Br_Ext-1C-R""")

index: 11

Note: Training reaction written in opposite direction from reaction family.
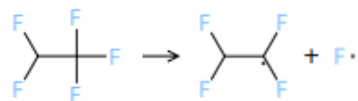
New Kinetics:
Arrhenius(A=(1.57e+43,'s^-1'), n=-8.85, Ea=(111800,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(1.21692e+34,'m^3/(mol*s)'), n=-8.80473, w0=
(205.5,'kJ/mol'), E0=(123.739,'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_1R->H_N-2R->S_N-
2BrCClFHNO-inRing_N-2BrCClFHNO->O_N-2CHN->N_2CH->C_Ext-
2C-R_3R!H->F_Ext-2C-R_4R!H->C_Ext-4C-R_N-5R!H->Cl_N-
5BrCFINOPSSi->Br_N-5CF->C_Sp-4C-2C_Ext-4C-R_Ext-2C-R_Ext-4C-
R',), comment="""Estimated from node Root_1R->H_N-2R->S_N-
2BrCClFHNO-inRing_N-2BrCClFHNO->O_N-2CHN->N_2CH->C_Ext-
2C-R_3R!H->F_Ext-2C-R_4R!H->C_Ext-4C-R_N-5R!H->Cl_N-
5BrCFINOPSSi->Br_N-5CF->C_Sp-4C-2C_Ext-4C-R_Ext-2C-R_Ext-4C-
R""")

index: 12

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

New Kinetics:
Arrhenius(A=(3.97e+39,'s^-1'), n=-8.78, Ea=(130500,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(1e+06,'m^3/(mol*s)'), n=0, w0=(242.5,'kJ/mol'), E0=
(126.651,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF-
>C',), comment="""Estimated from node Root_N-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
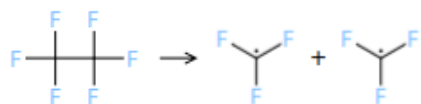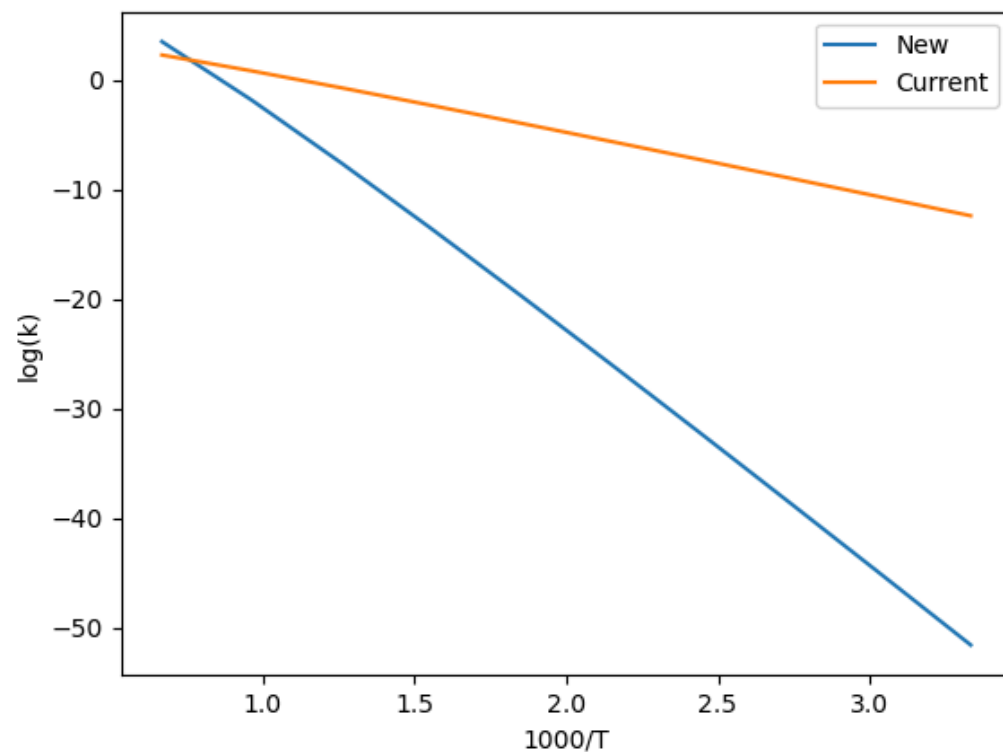inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF-
>C""")

index: 13

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

New Kinetics:
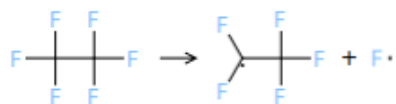Arrhenius(A=(5.53e+48,'s^-1'), n=-9.41, Ea=(105700,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(1.41794e+13,'m^3/(mol*s)'), n=-2.16473, w0=
(173,'kJ/mol'), E0=(116.106,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_N-4R!H->O_4BrCClF->F_Ext-1C-R_N-5R!H->Cl_Ext-2CF-R_N-
5BrCFINOPSSi->Br_Ext-1C-R',), comment="""Estimated from node
Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-
1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF-
->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_N-4R!H->O_4BrCClF->F_Ext-1C-
R_N-5R!H->Cl_Ext-2CF-R_N-5BrCFINOPSSi->Br_Ext-1C-R""")
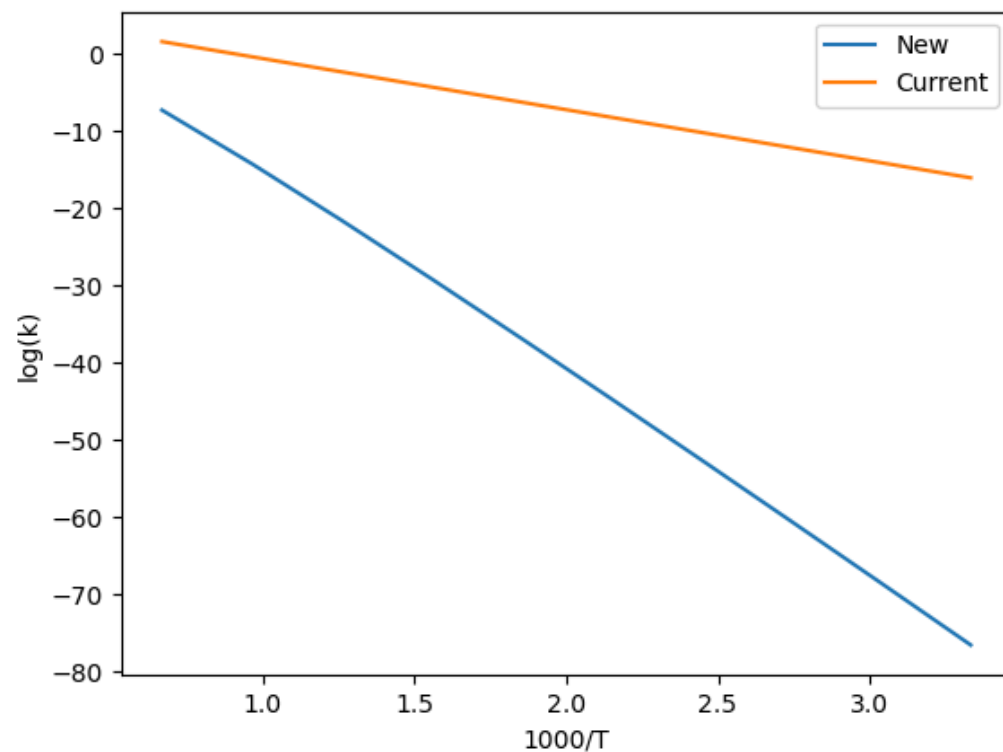

index: 14

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

New Kinetics:
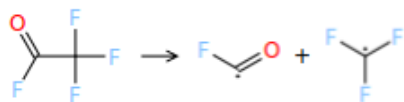Arrhenius(A=(6.35e+40,'s^-1'), n=-9.18, Ea=(129900,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(1e+06,'m^3/(mol*s)'), n=0, w0=(242.5,'kJ/mol'), E0=
(126.651,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF-
>C',), comment="""Estimated from node Root_N-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
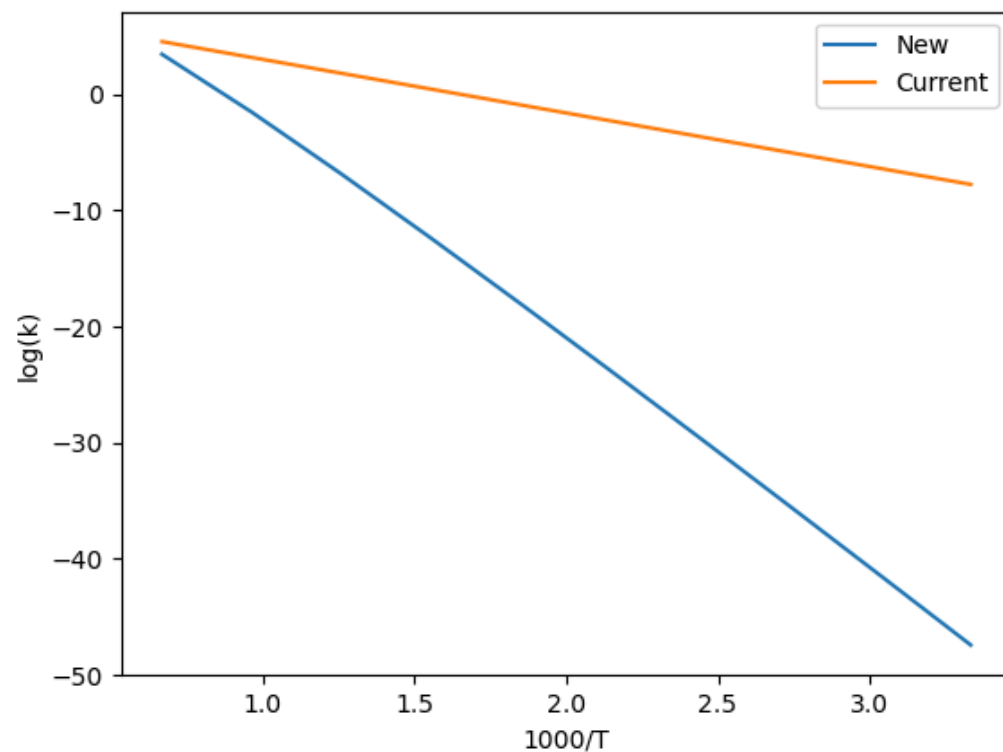inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF-
>C""")

index: 17

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

New Kinetics:
Arrhenius(A=(1.36e+43,'s^-1'), n=-8.05, Ea=(96940,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(4e+07,'m^3/(mol*s)'), n=0, w0=(173,'kJ/mol'), E0=
(88.2769,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_4R!H->O',), comment="""Estimated from node Root_N-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_4R!H->O""")

index: 20

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

New Kinetics:
Arrhenius(A=(1.96e+49,'s^-1'), n=-10.51, Ea=(104000,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(4e+07,'m^3/(mol*s)'), n=0, w0=(173,'kJ/mol'), E0=(88.2769,'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-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O',), comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O""")

index: 25

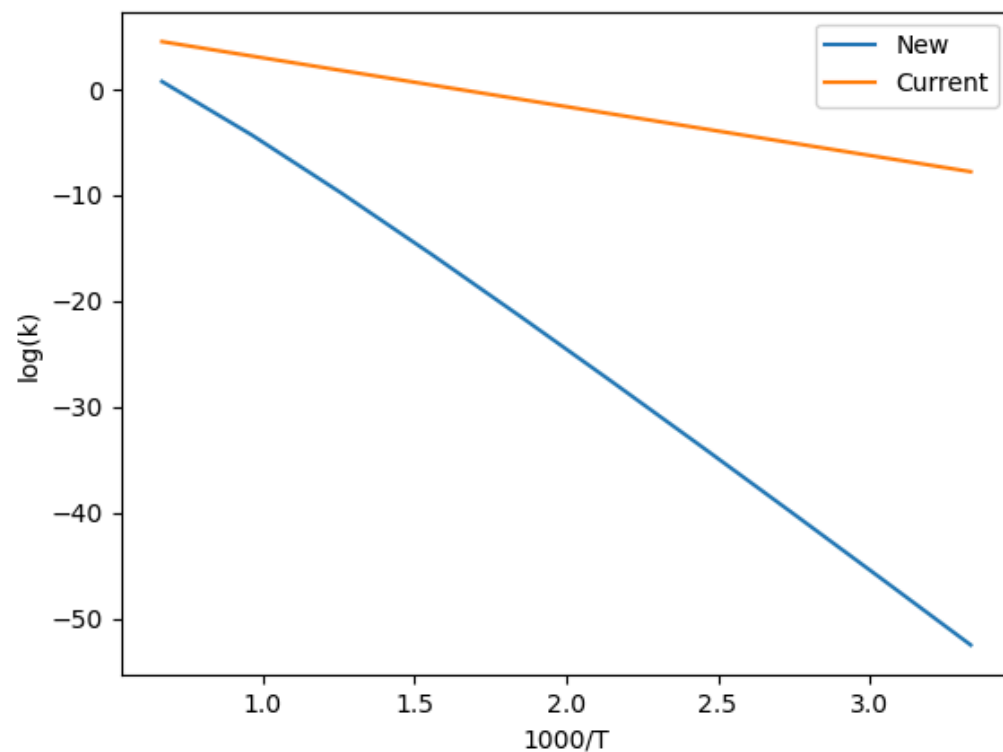**Note: Training reaction written in opposite direction from reaction family.**

New Kinetics:
Arrhenius(A=(1.16e+44,'s^-1'), n=-8.51, Ea=(96540,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(4e+07,'m^3/(mol*s)'), n=0, w0=(173,'kJ/mol'), E0=
(88.2769,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_4R!H->O',), comment="""Estimated from node Root_N-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
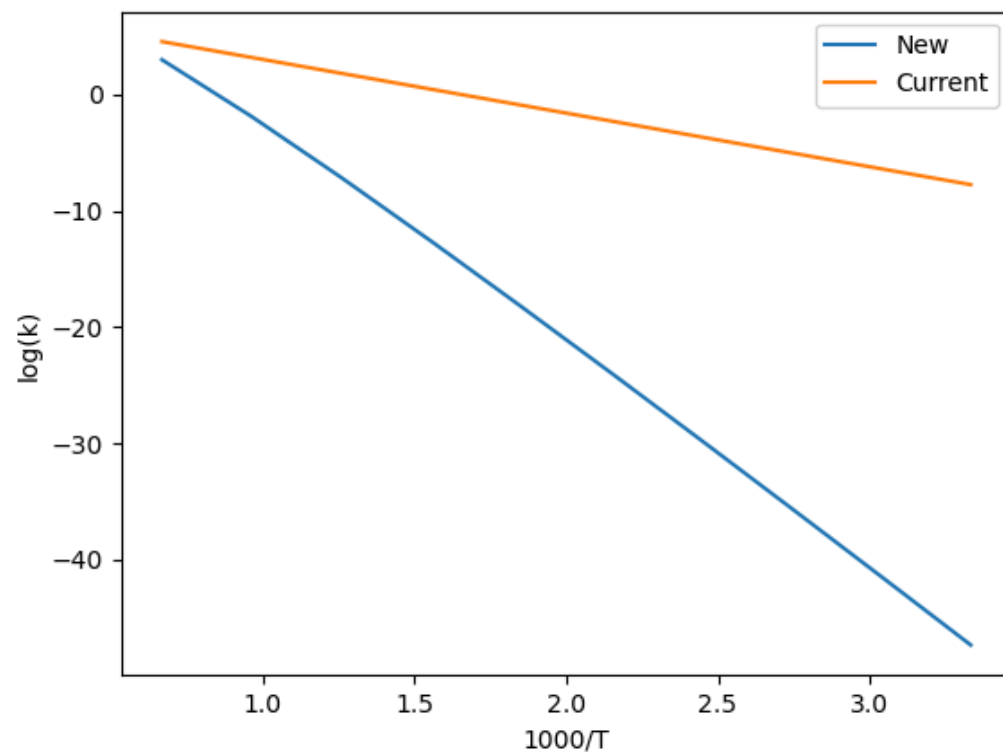2CF-R_4R!H->O""")

index: 33

Note: Training reaction written in opposite direction from reaction family.
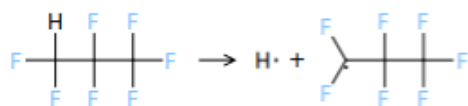
New Kinetics:
Arrhenius(A=(1.97e+38,'s^-1'), n=-7.3, Ea=(110600,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(1e+07,'m^3/(mol*s)'), n=0, w0=(205.5,'kJ/mol'), E0=
(117.474,'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_1R->H_N-2R->S_N-
2BrCClFHNO-inRing_N-2BrCClFHNO->O_N-2CHN->N_2CH->C_Ext-
2C-R_3R!H->F_Ext-2C-R_4R!H->C_Ext-4C-R_N-5R!H->Cl_N-
5BrCFINOPSSi->Br_5CF->C',), comment="""Estimated from node
Root_1R->H_N-2R->S_N-2BrCClFHNO-inRing_N-2BrCClFHNO->O_N-
2CHN->N_2CH->C_Ext-2C-R_3R!H->F_Ext-2C-R_4R!H->C_Ext-4C-
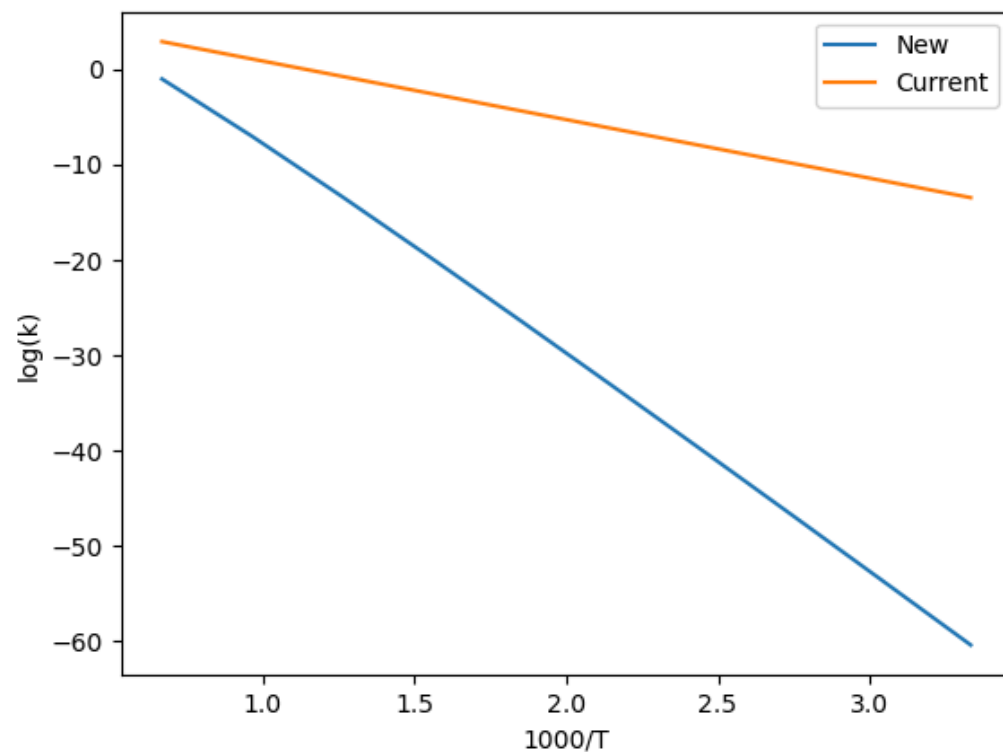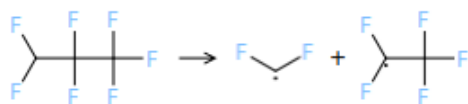R_N-5R!H->Cl_N-5BrCFINOPSSi->Br_5CF->C""")

index: 34

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

New Kinetics:
Arrhenius(A=(1.67e+37,'s^-1'), n=-6.09, Ea=(97630,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
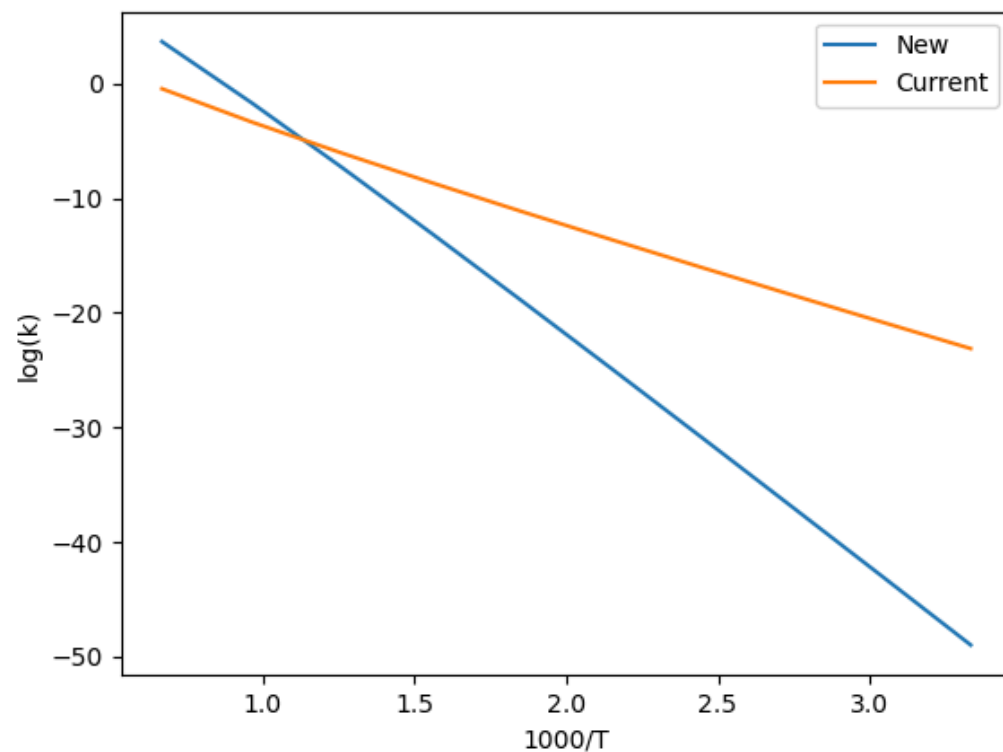1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

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

New Kinetics:
Arrhenius(A=(6.57e+38,'s^-1'), n=-6.57, Ea=(100000,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
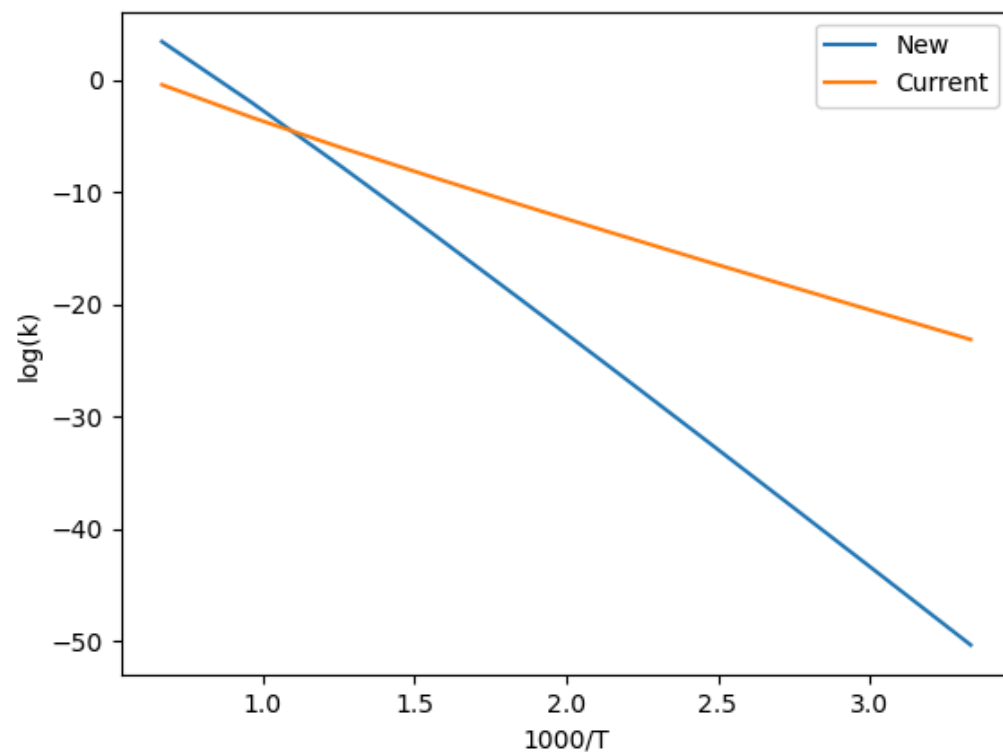>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
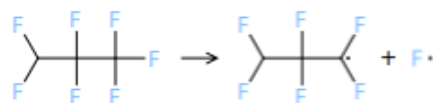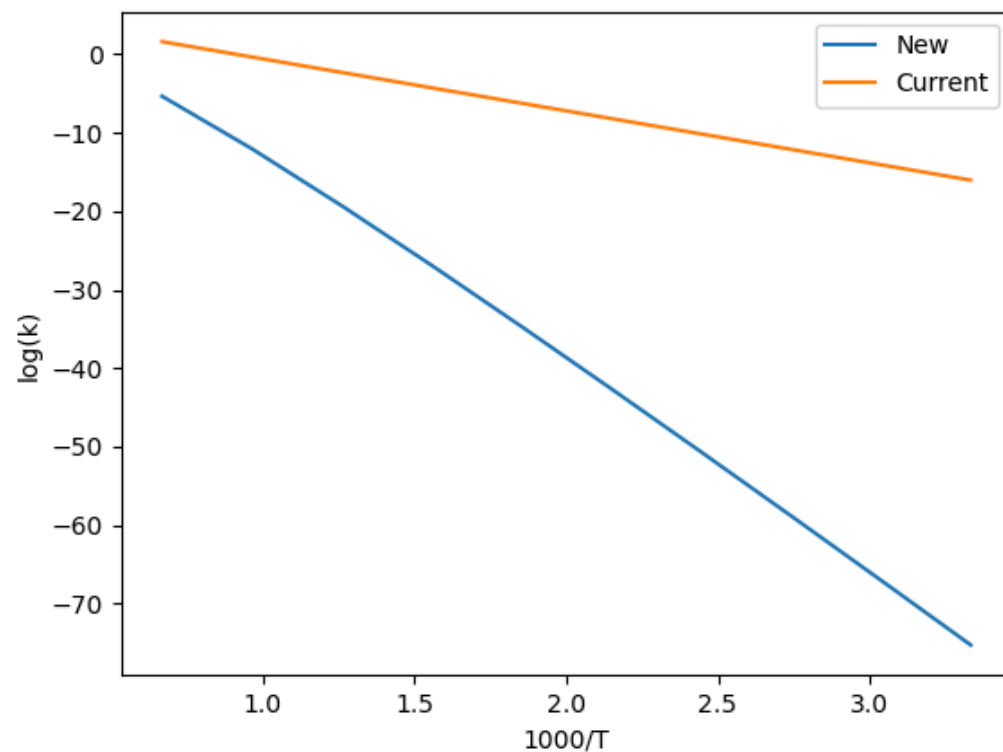
New Kinetics:
Arrhenius(A=(7.6e+55,'s^-1'), n=-13.06, Ea=(135600,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(1e+06,'m^3/(mol*s)'), n=0, w0=(242.5,'kJ/mol'), E0=
(126.651,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF-
>C',), comment="""Estimated from node Root_N-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF-
>C""")

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

New Kinetics:
Arrhenius(A=(7.05e+41,'s^-1'), n=-7.29, Ea=(99830,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

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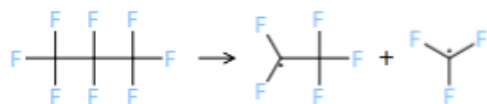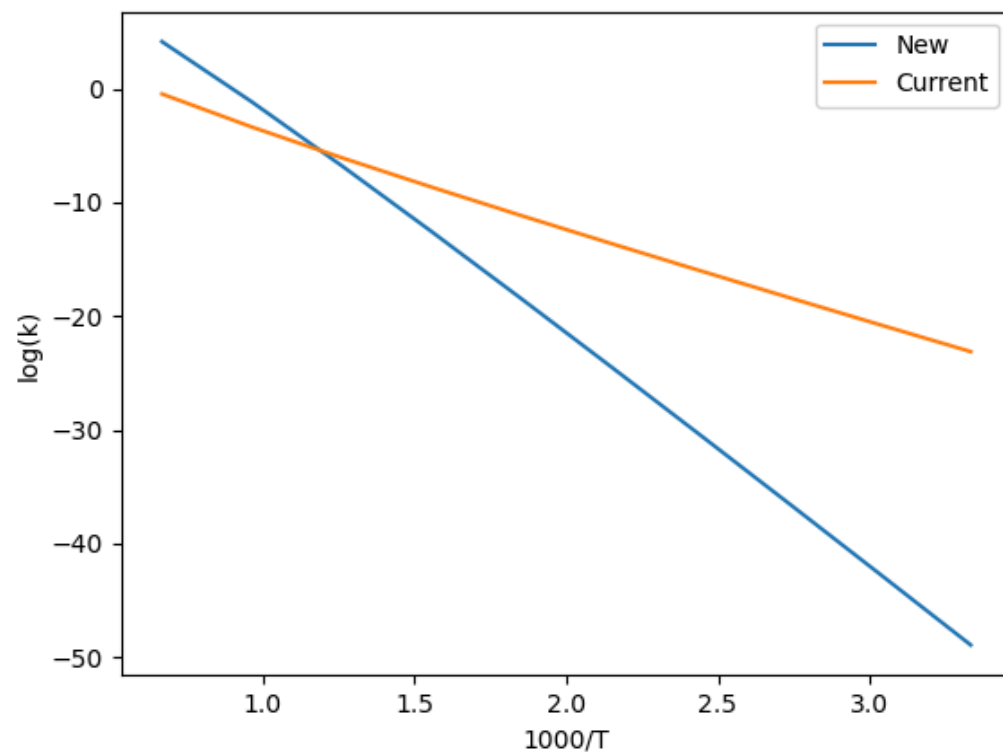**Note: Training reaction written in opposite direction from reaction family.**
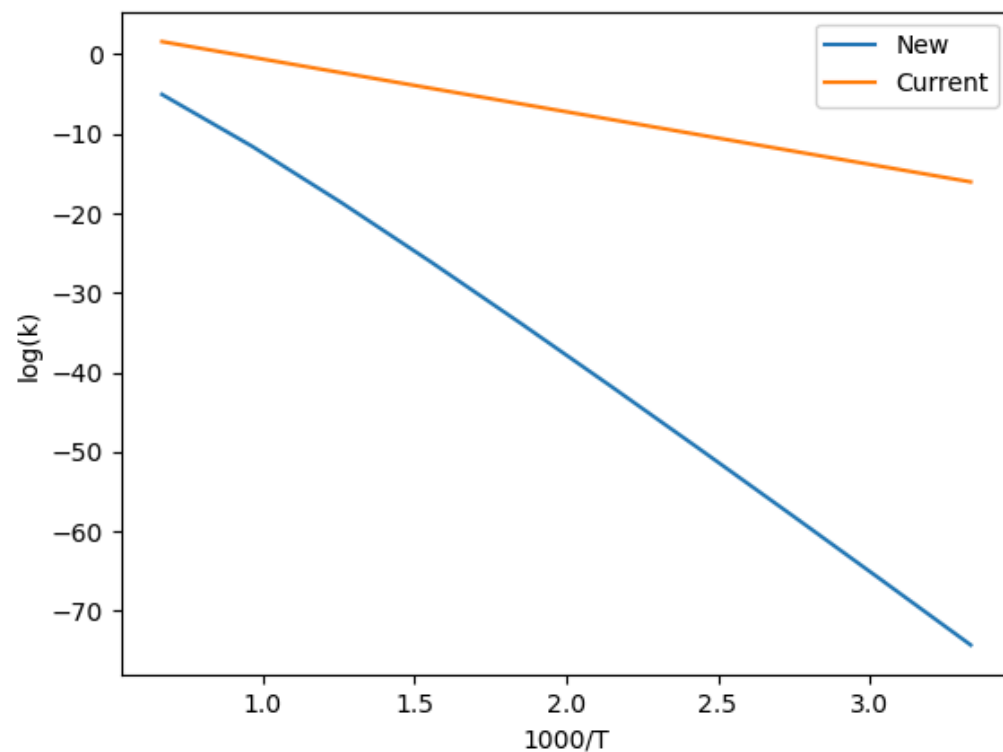
New Kinetics:
Arrhenius(A=(7.61e+60,'s^-1'), n=-14.51, Ea=(136200,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(1e+06,'m^3/(mol*s)'), n=0, w0=(242.5,'kJ/mol'), E0=(126.651,'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-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C',), comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C""")

index: 42

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

New Kinetics:
Arrhenius(A=(6.76e+39,'s^-1'), n=-7.05, Ea=(93490,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

index: 43

Note: Training reaction written in opposite direction from reaction family.
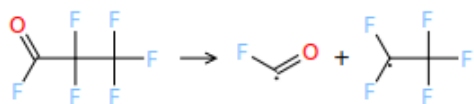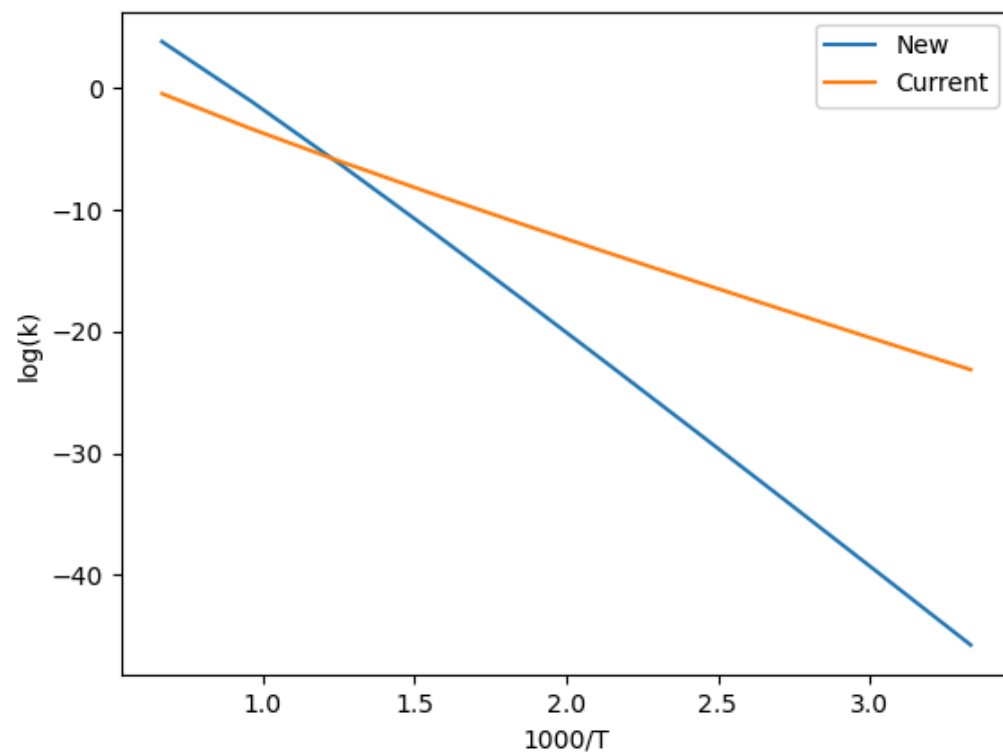
New Kinetics:
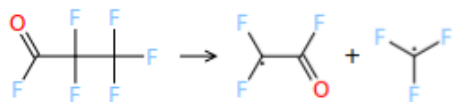Arrhenius(A=(2.54e+40,'s^-1'), n=-7.09, Ea=(93410,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
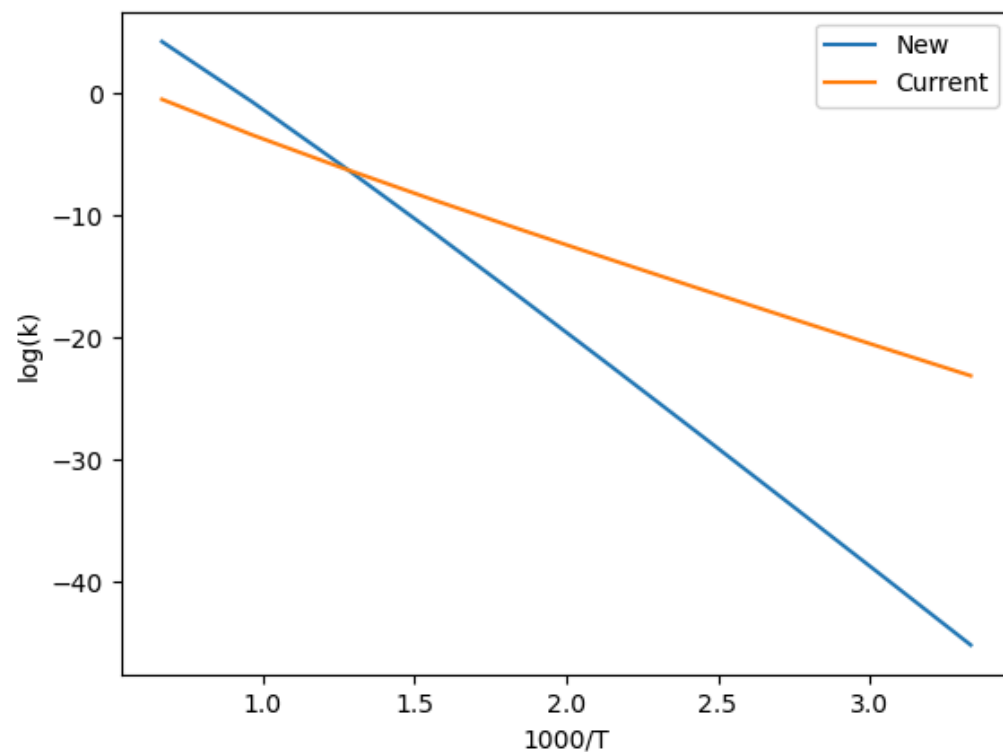>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
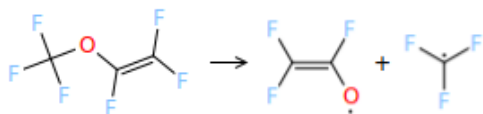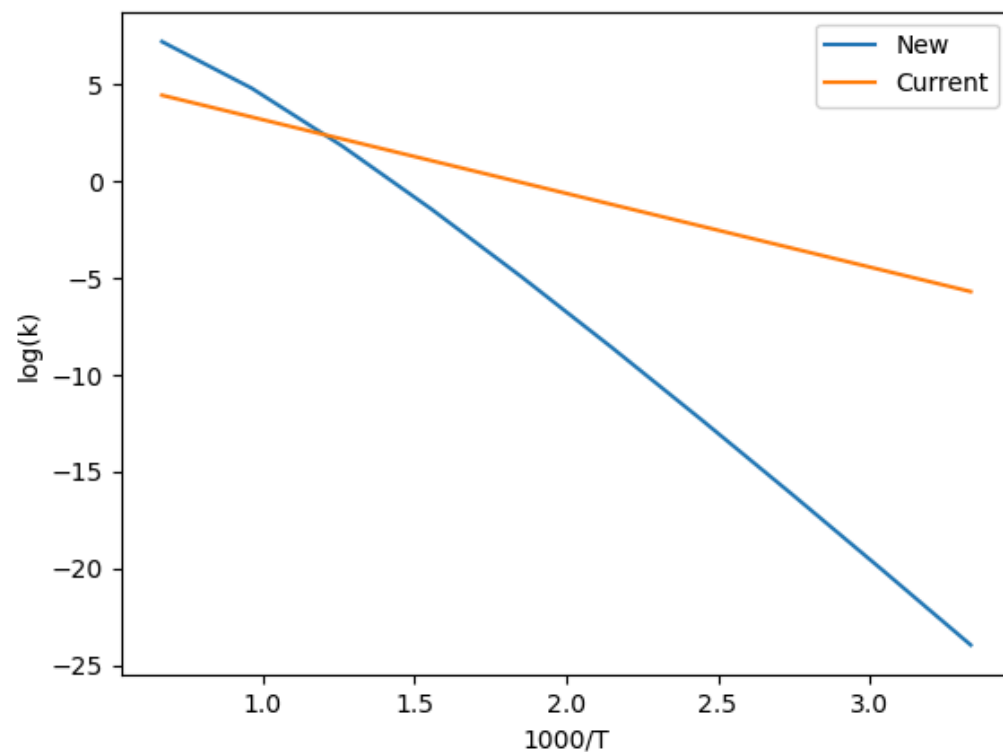
New Kinetics:
Arrhenius(A=(7.82e+57,'s^-1'), n=-12.81, Ea=(68760,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(9.04e+06,'m^3/(mol*s)'), n=2.17087e-08, w0=
(179,'kJ/mol'), E0=(72.7054,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-
3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
R_2R->C_Ext-2C-R_Ext-2C-R""")

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

New Kinetics:
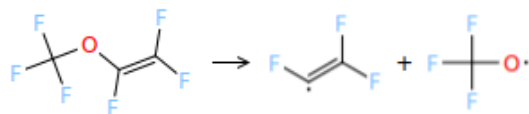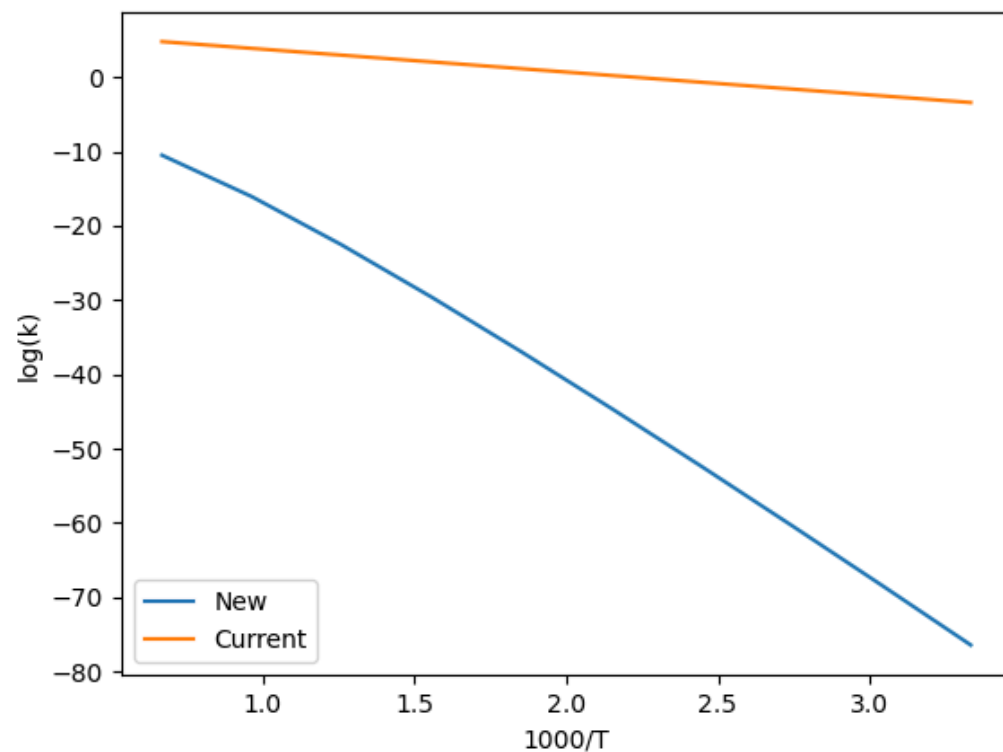Arrhenius(A=(3.3e+77,'s^-1'), n=-21.34, Ea=(138800,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(7.38316e+06,'m^3/(mol*s)'), n=1.31229e-07, w0=
(179,'kJ/mol'), E0=(58.9141,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'),
uncertainty=RateUncertainty(mu=-0.016021952005170214,
var=0.3543710496450803, Tref=1000.0, N=2, data_mean=0.0,
correlation='Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS-
>Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
R_2R->C""")

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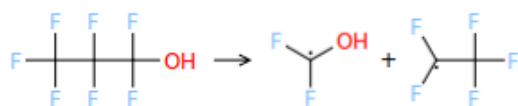**Note: Training reaction written in opposite direction from reaction family.**

New Kinetics:

Arrhenius(A=(1.36e+53,'s^-1'), n=-11.34, Ea=(102100,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

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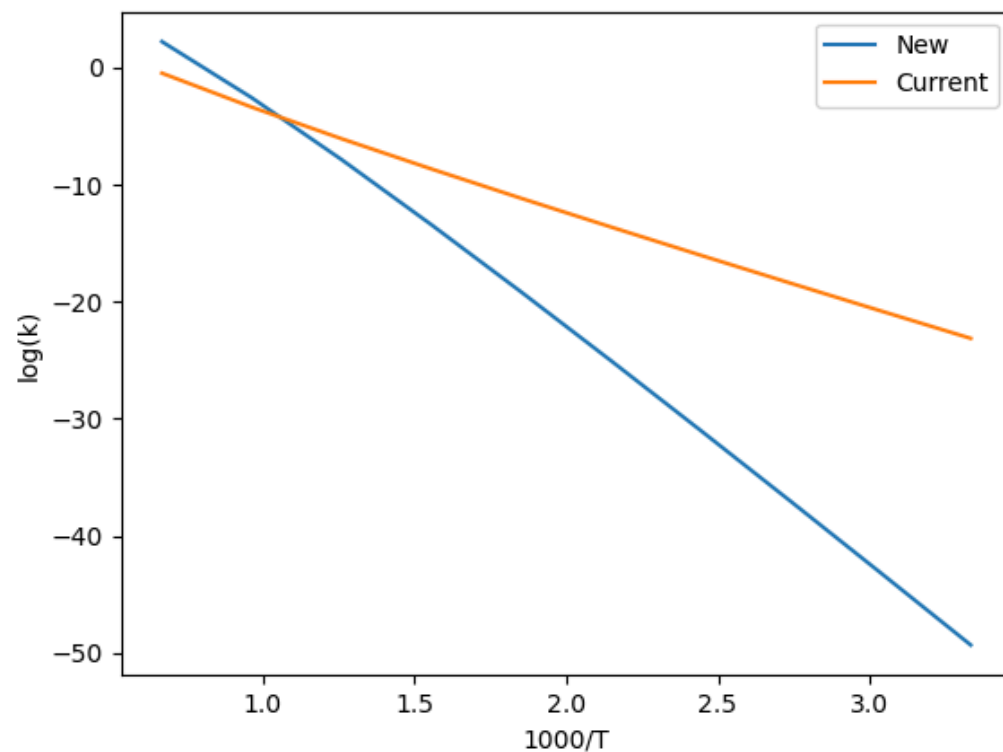**Note: Training reaction written in opposite direction from reaction family.**

New Kinetics:
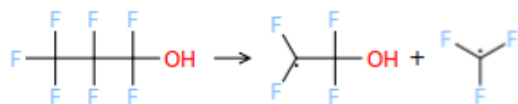Arrhenius(A=(2.92e+53,'s^-1'), n=-11.46, Ea=(103100,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
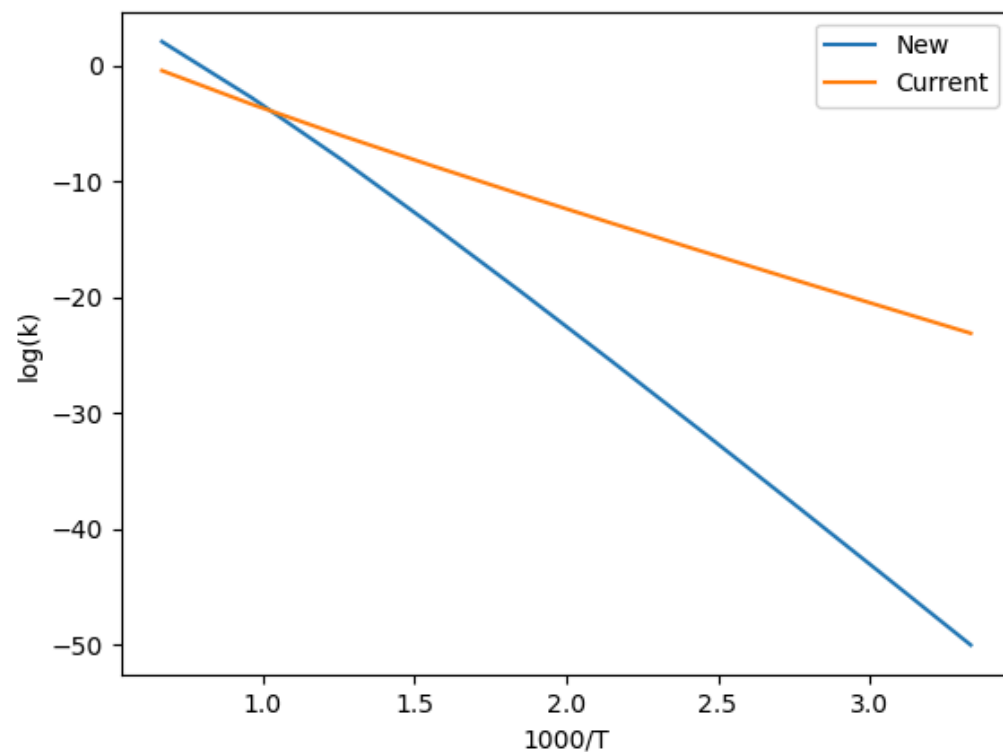>F_Ext-2CF-R_Ext-4R!H-R""")

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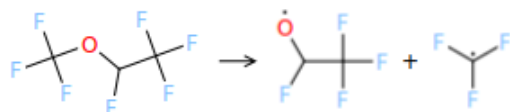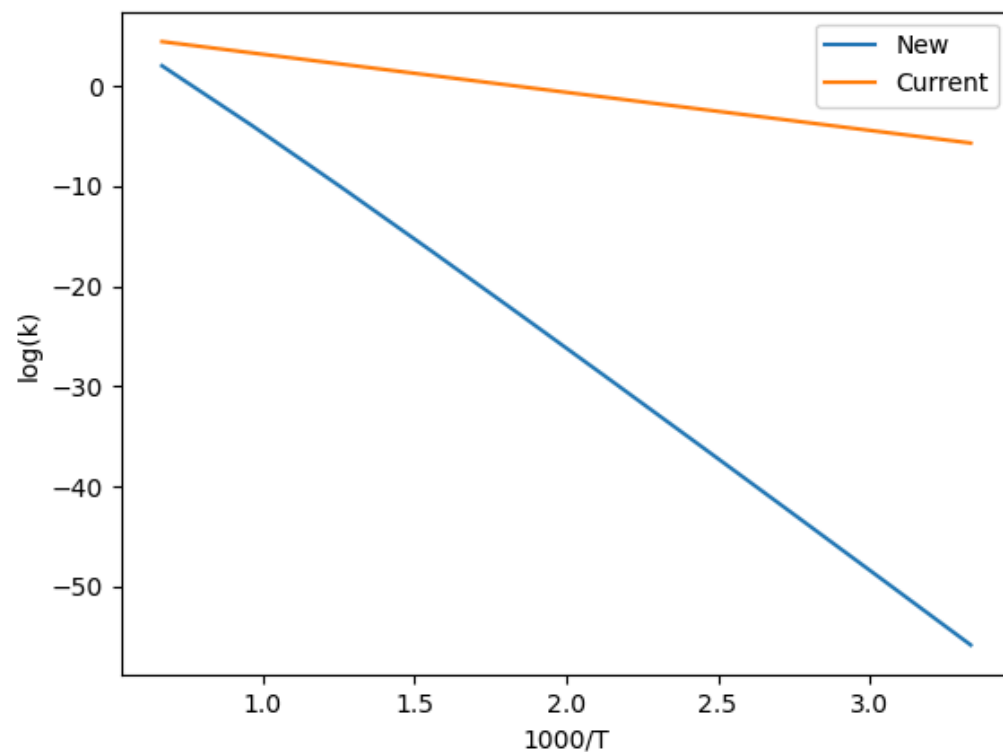**Note: Training reaction written in opposite direction from reaction family.**
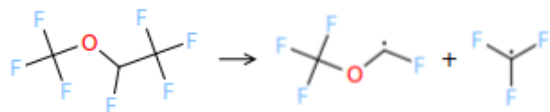
New Kinetics:

Arrhenius(A=(4.71e+35,'s^-1'), n=-5.73, Ea=(106100,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(9.04e+06,'m^3/(mol*s)'), n=2.17087e-08, w0=(179,'kJ/mol'), E0=(72.7054,'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-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R""")
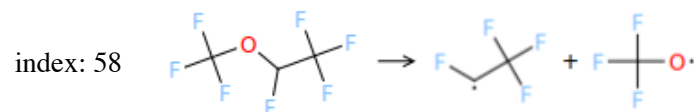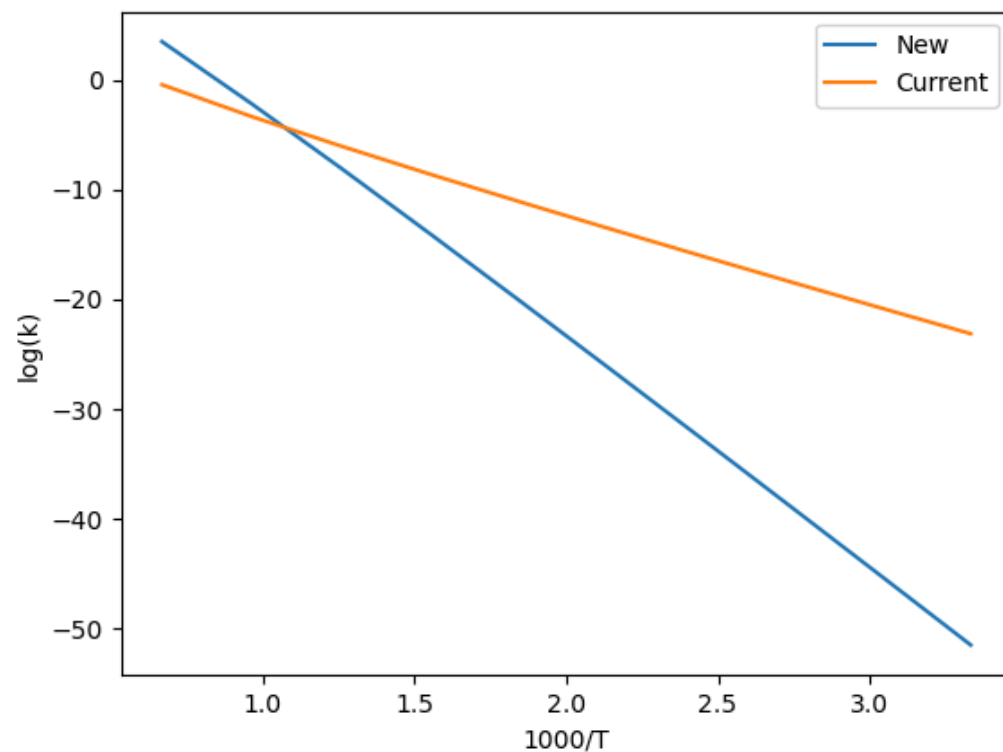
index: 57

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

New Kinetics:
Arrhenius(A=(9.01e+34,'s^-1'), n=-5.3, Ea=(100600,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
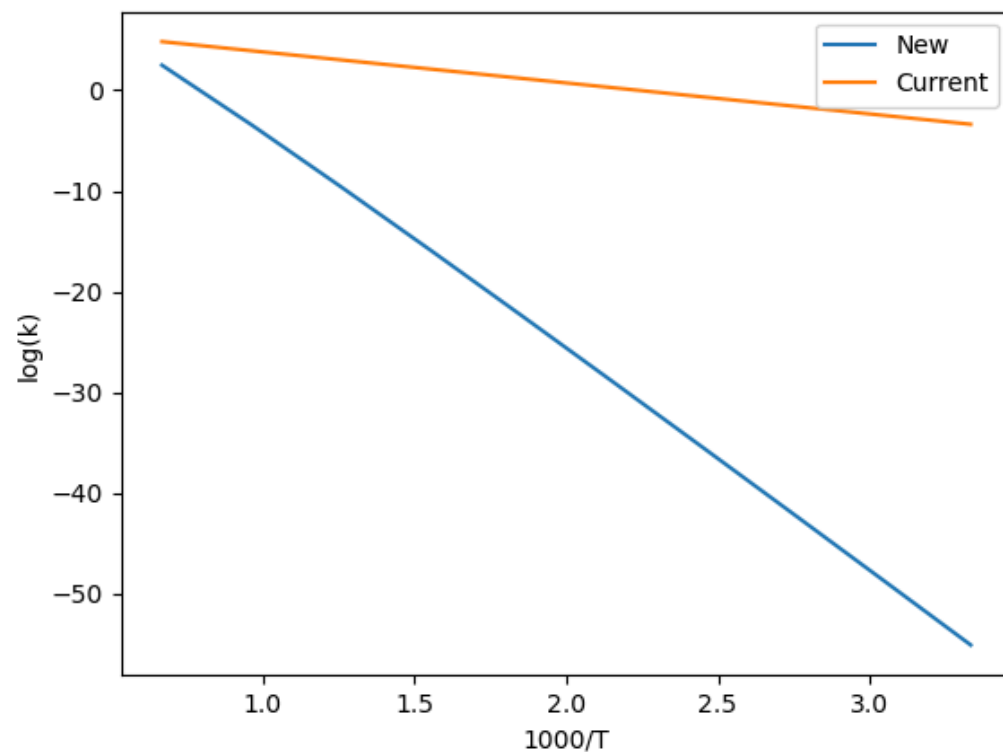1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

index: 58

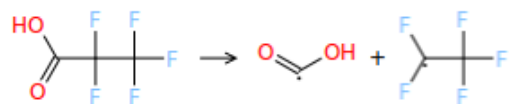**Note: Training reaction written in opposite direction from reaction family.**

New Kinetics:
Arrhenius(A=(2.51e+35,'s^-1'), n=-5.53, Ea=(105400,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(7.38316e+06,'m^3/(mol*s)'), n=1.31229e-07, w0=
(179,'kJ/mol'), E0=(58.9141,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'),
uncertainty=RateUncertainty(mu=-0.016021952005170214,
var=0.3543710496450803, Tref=1000.0, N=2, data_mean=0.0,
correlation='Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS-
>Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
R_2R->C""")

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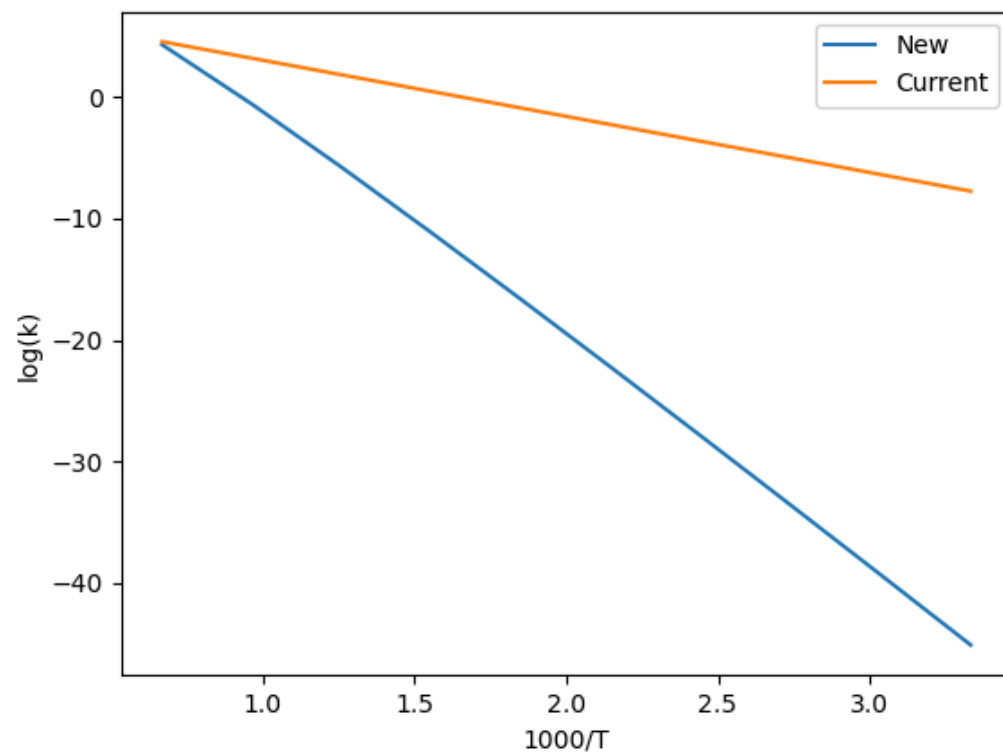**Note: Training reaction written in opposite direction from reaction family.**
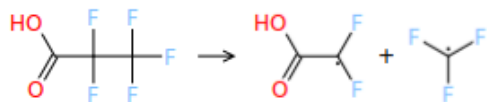
New Kinetics:
Arrhenius(A=(9.69e+40,'s^-1'), n=-7.27, Ea=(93430,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(4e+07,'m^3/(mol*s)'), n=0, w0=(173,'kJ/mol'), E0=
(88.2769,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_4R!H->O',), comment="""Estimated from node Root_N-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_4R!H->O""")

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

New Kinetics:
Arrhenius(A=(1.39e+43,'s^-1'), n=-7.84, Ea=(96330,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
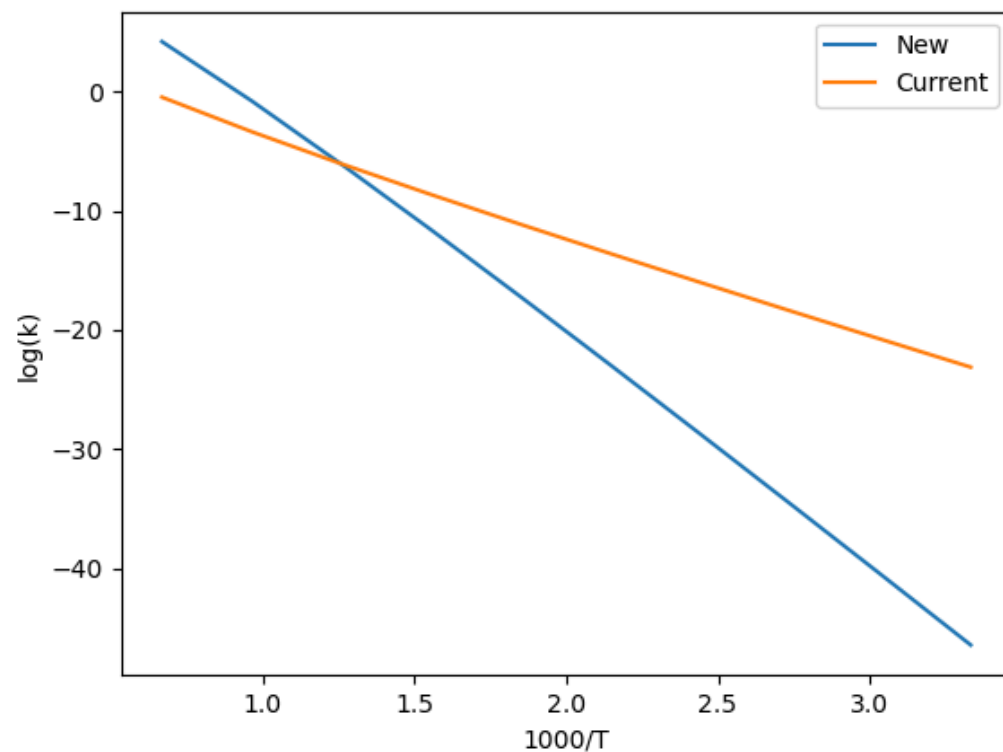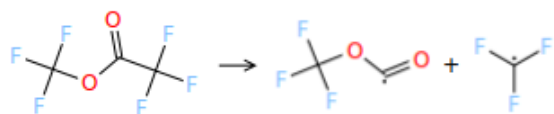>F_Ext-2CF-R_Ext-4R!H-R""")

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

New Kinetics:
Arrhenius(A=(4.22e+39,'s^-1'), n=-6.91, Ea=(94000,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
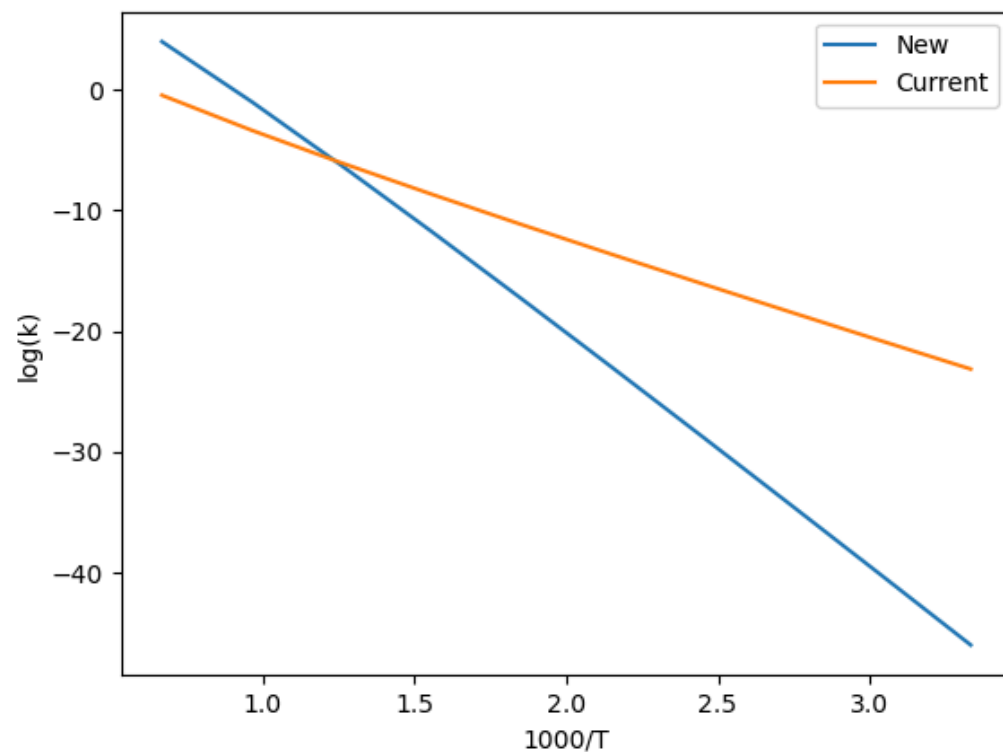>F_Ext-2CF-R_Ext-4R!H-R""")

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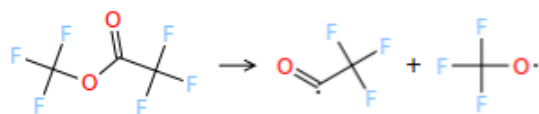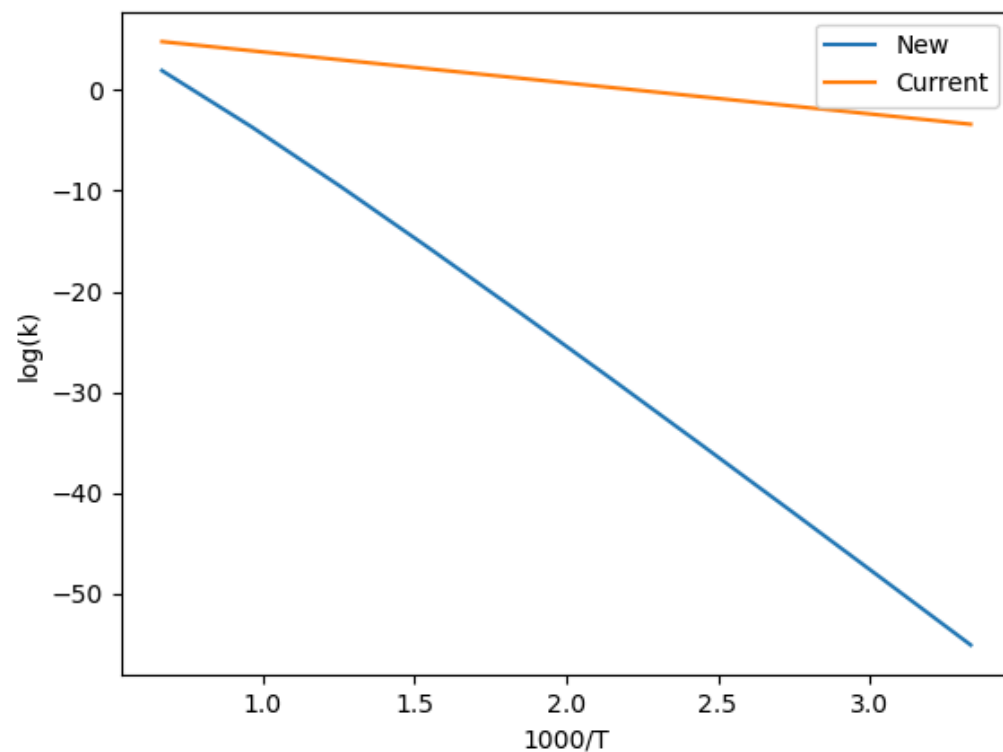**Note: Training reaction written in opposite direction from reaction family.**
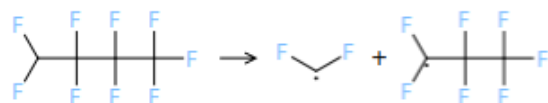
New Kinetics:
Arrhenius(A=(2.66e+46,'s^-1'), n=-9.02, Ea=(108700,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(7.38316e+06,'m^3/(mol*s)'), n=1.31229e-07, w0=
(179,'kJ/mol'), E0=(58.9141,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'),
uncertainty=RateUncertainty(mu=-0.016021952005170214,
var=0.3543710496450803, Tref=1000.0, N=2, data_mean=0.0,
correlation='Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS-
>Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
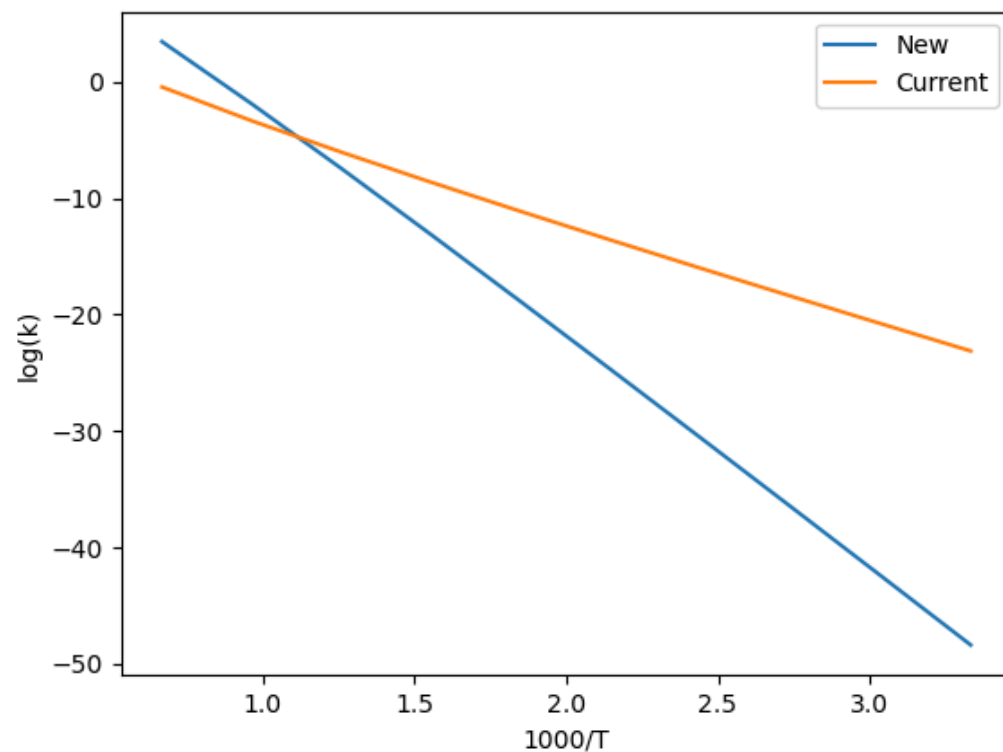>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
R_2R->C""")

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Note: Training reaction written in opposite direction from reaction family.
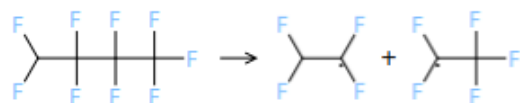
New Kinetics:
Arrhenius(A=(9.53e+32,'s^-1'), n=-4.95, Ea=(94840,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

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

New Kinetics:
Arrhenius(A=(2.11e+33,'s^-1'), n=-4.96, Ea=(93600,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
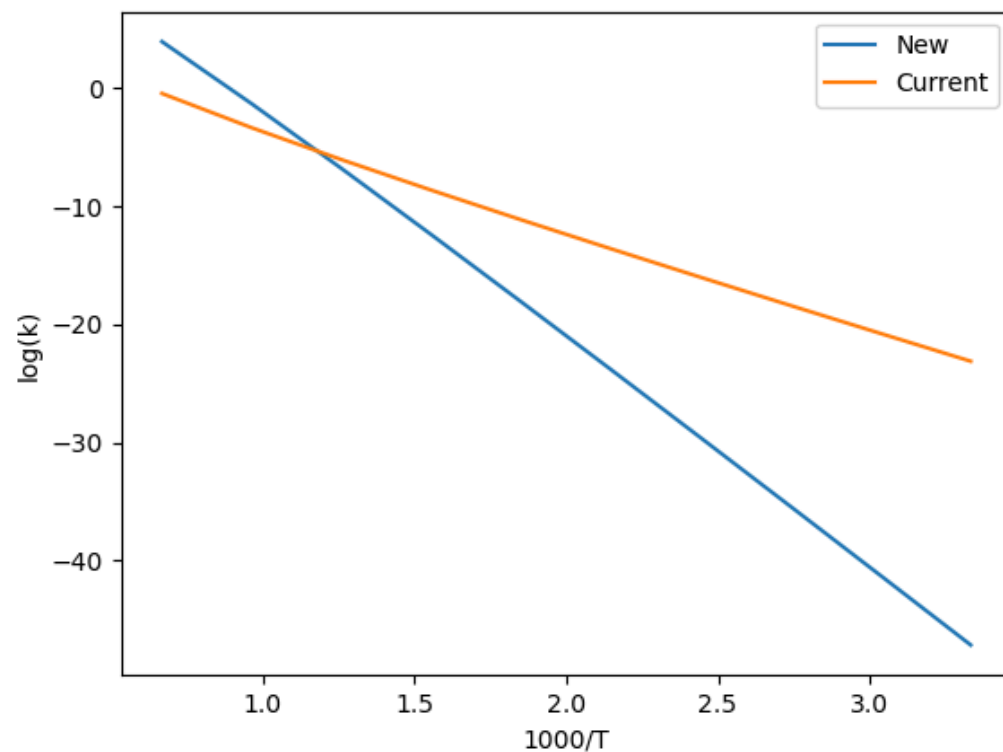>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
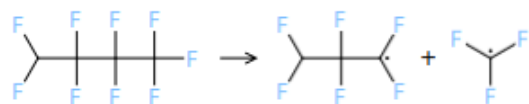
New Kinetics:
Arrhenius(A=(1.15e+34,'s^-1'), n=-5.25, Ea=(96420,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
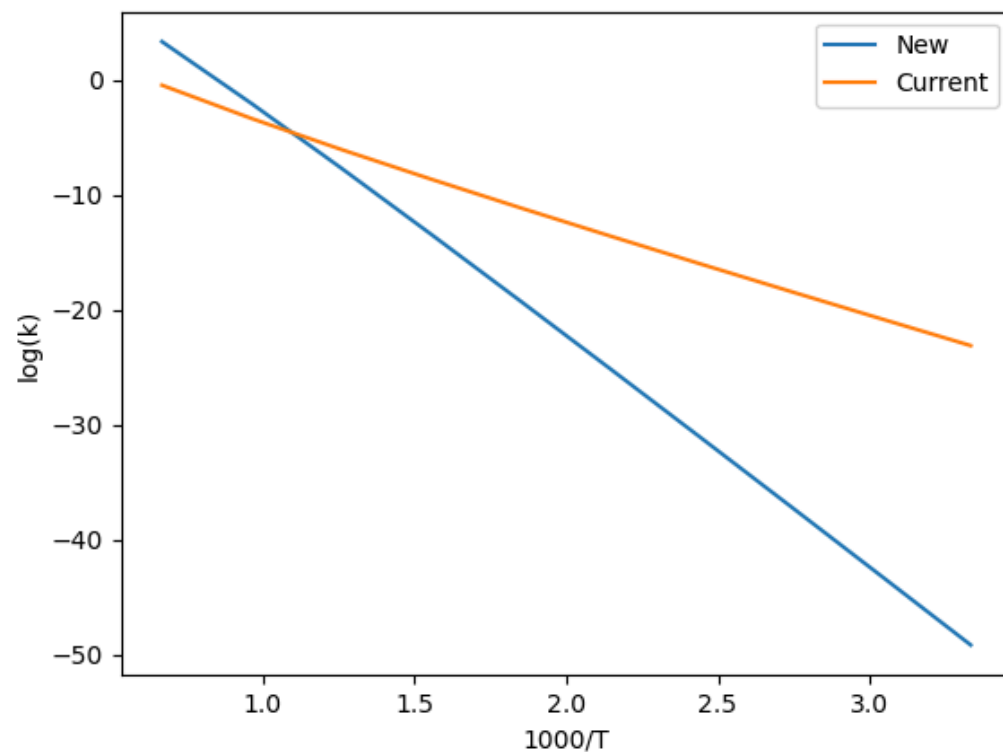>F_Ext-2CF-R_Ext-4R!H-R""")

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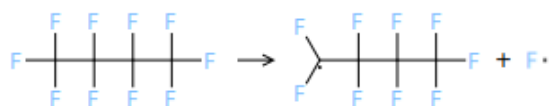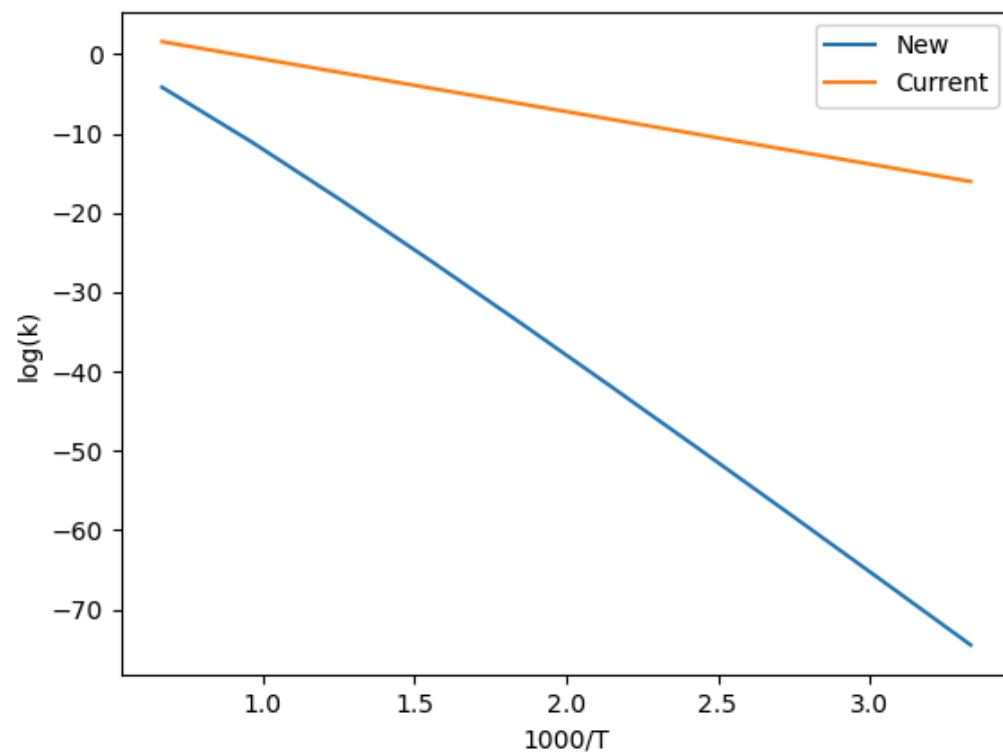**Note: Training reaction written in opposite direction from reaction family.**
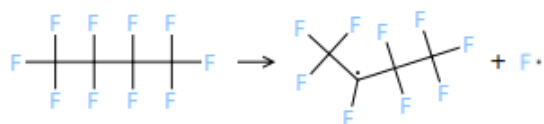
New Kinetics:
Arrhenius(A=(1.41e+50,'s^-1'), n=-10.96, Ea=(133800,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(1e+06,'m^3/(mol*s)'), n=0, w0=(242.5,'kJ/mol'), E0=(126.651,'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-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C',), comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF->C""")

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

New Kinetics:
Arrhenius(A=(1.93e+46,'s^-1'), n=-9.77, Ea=(124500,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(1e+06,'m^3/(mol*s)'), n=0, w0=(242.5,'kJ/mol'), E0=
(126.651,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF-
>C',), comment="""Estimated from node Root_N-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_N-2CF-
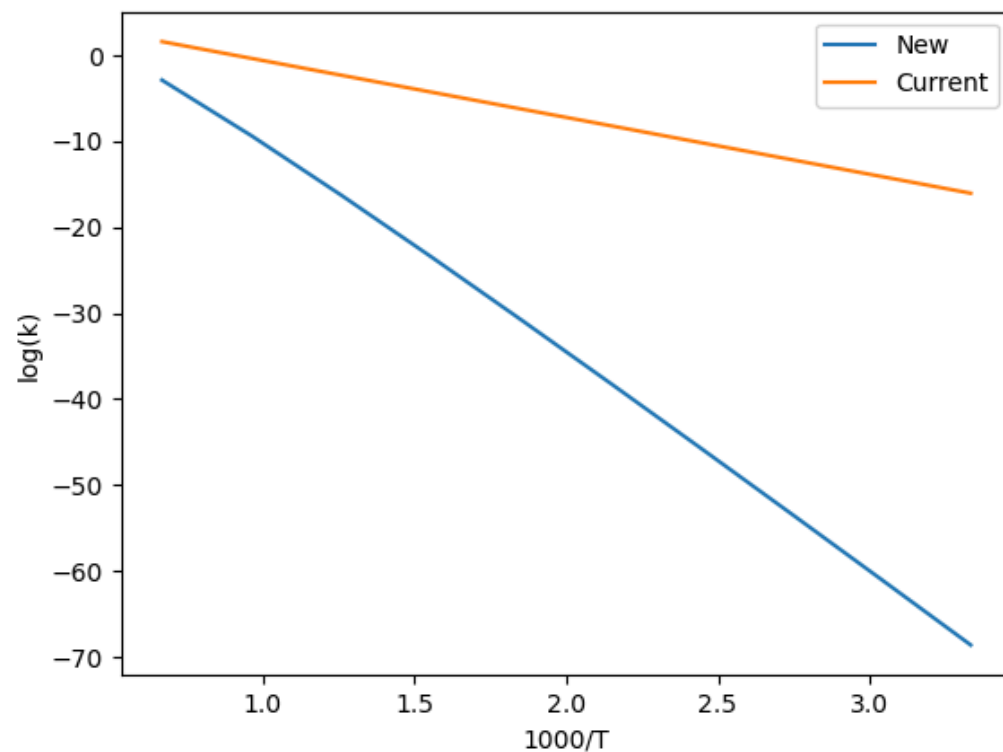>C""")

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Note: Training reaction written in opposite direction from reaction family.
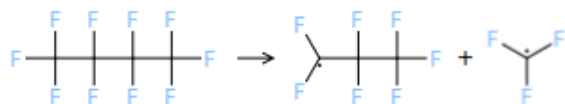
New Kinetics:
Arrhenius(A=(2.74e+37,'s^-1'), n=-6.16, Ea=(97340,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

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

New Kinetics:
Arrhenius(A=(1.57e+36,'s^-1'), n=-5.7, Ea=(93720,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(1.31566e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
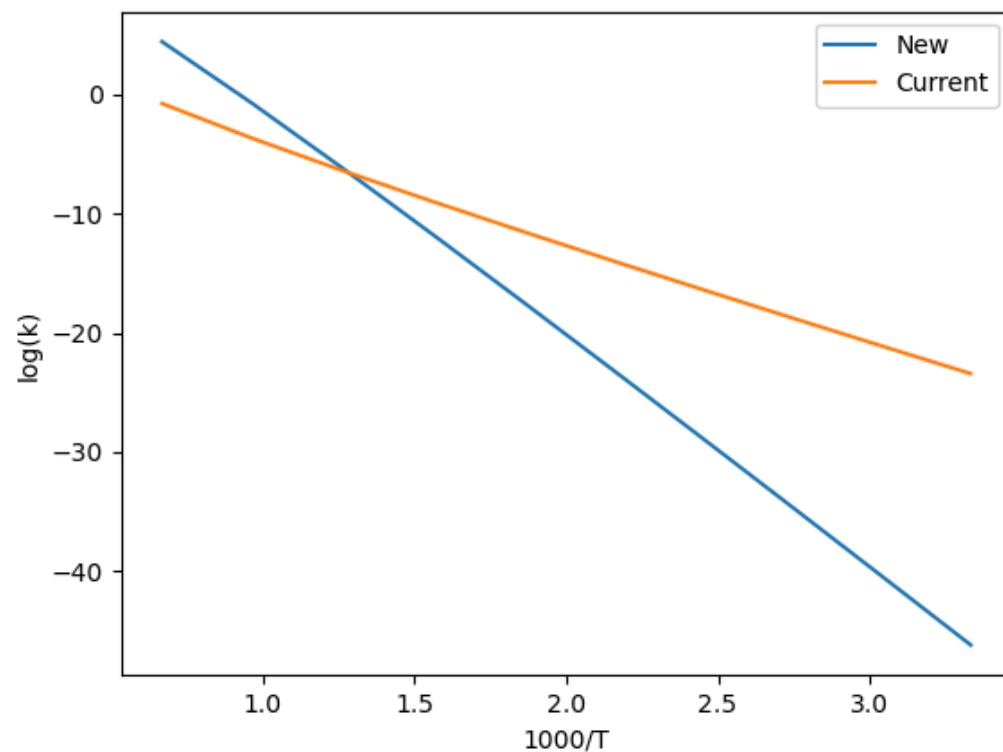>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
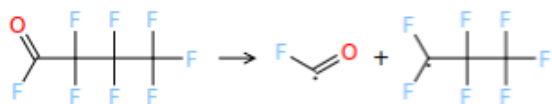
New Kinetics:
Arrhenius(A=(6.45e+34,'s^-1'), n=-5.69, Ea=(90800,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
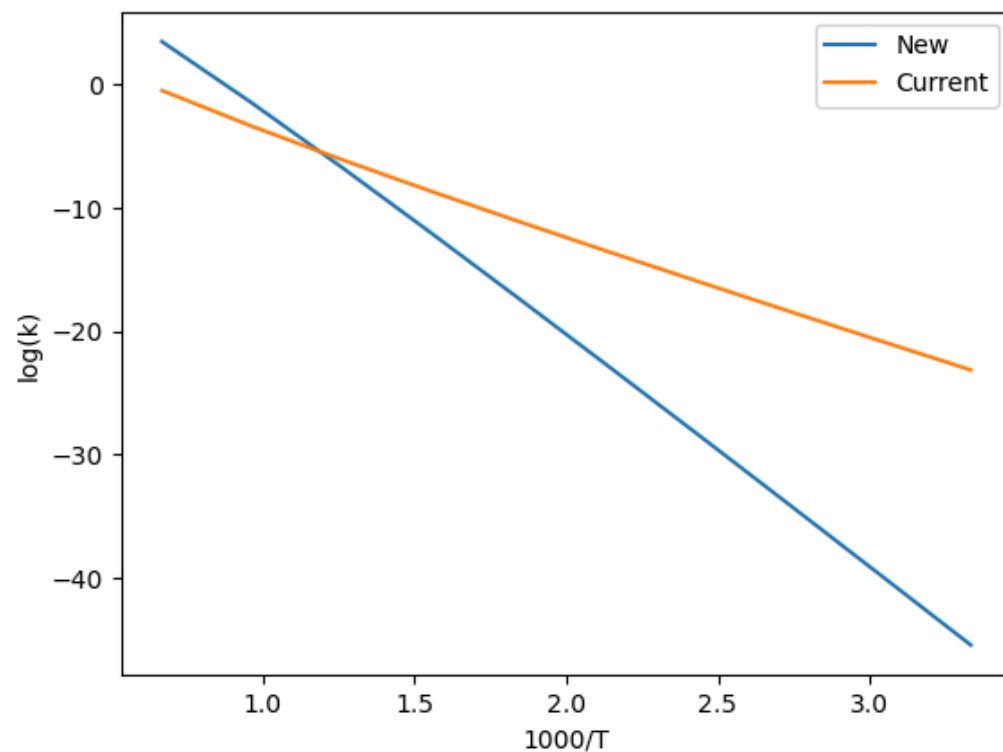>F_Ext-2CF-R_Ext-4R!H-R""")

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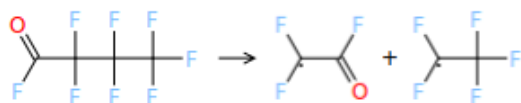**Note: Training reaction written in opposite direction from reaction family.**

New Kinetics:
Arrhenius(A=(4.26e+34,'s^-1'), n=-5.41, Ea=(87330,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

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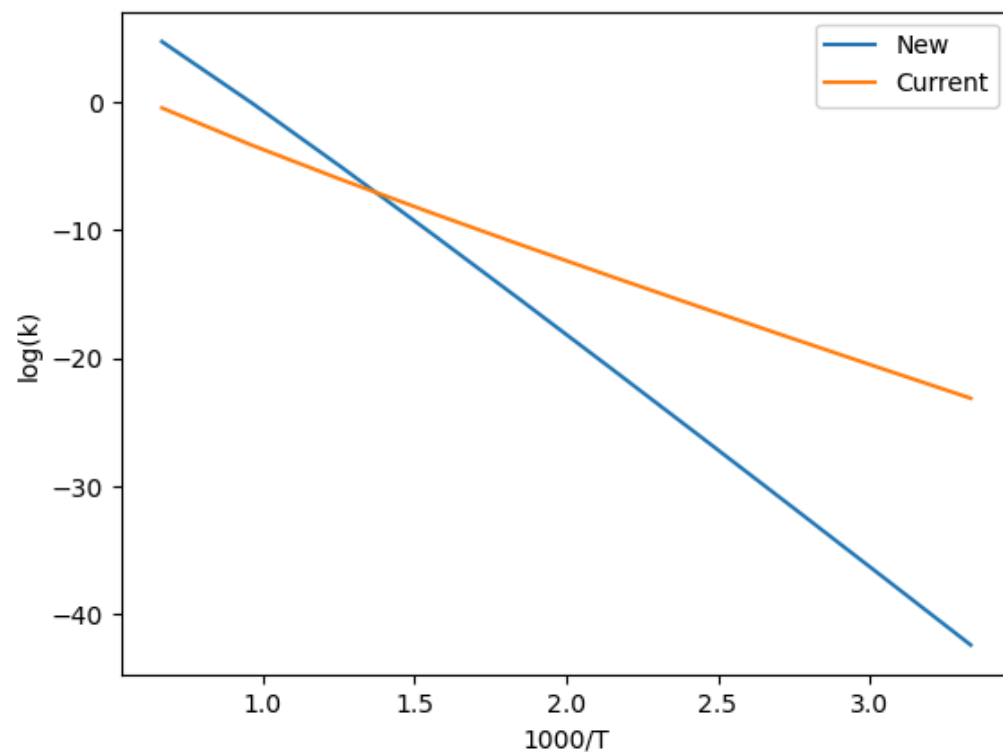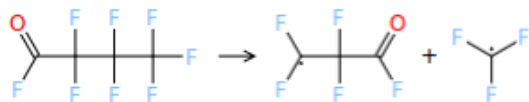**Note: Training reaction written in opposite direction from reaction family.**

New Kinetics:
Arrhenius(A=(1.25e+37,'s^-1'), n=-6.29, Ea=(97650,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
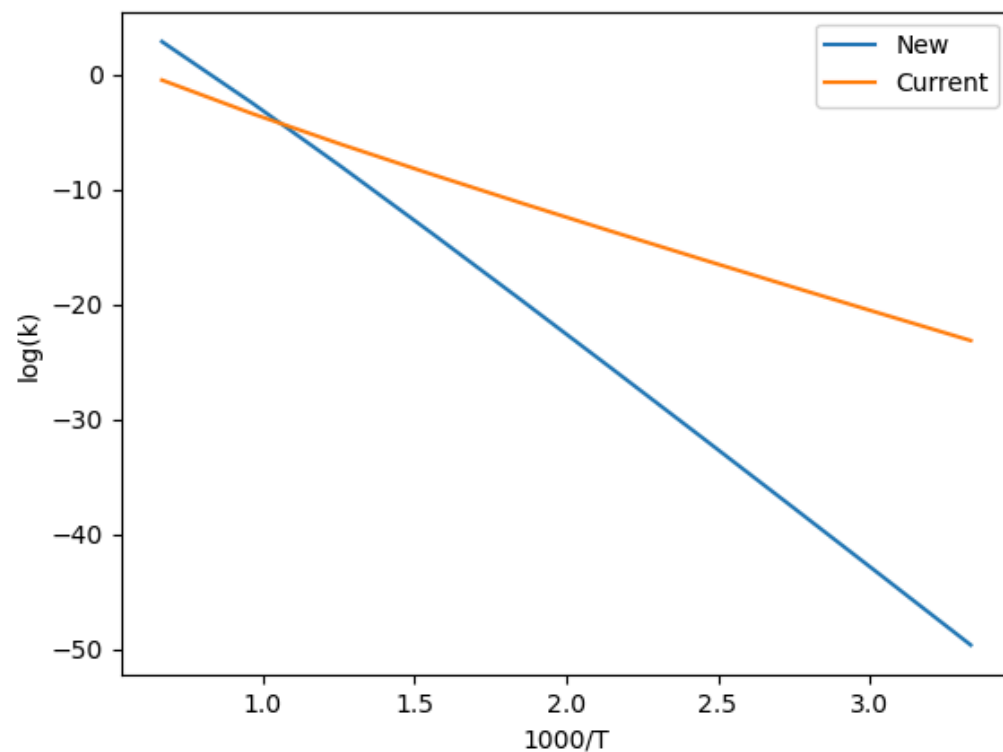>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
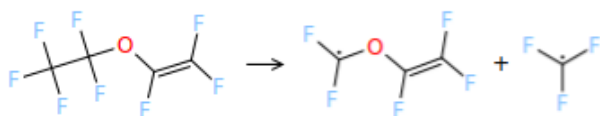
New Kinetics:
Arrhenius(A=(1.84e+65,'s^-1'), n=-17.04, Ea=(104800,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")

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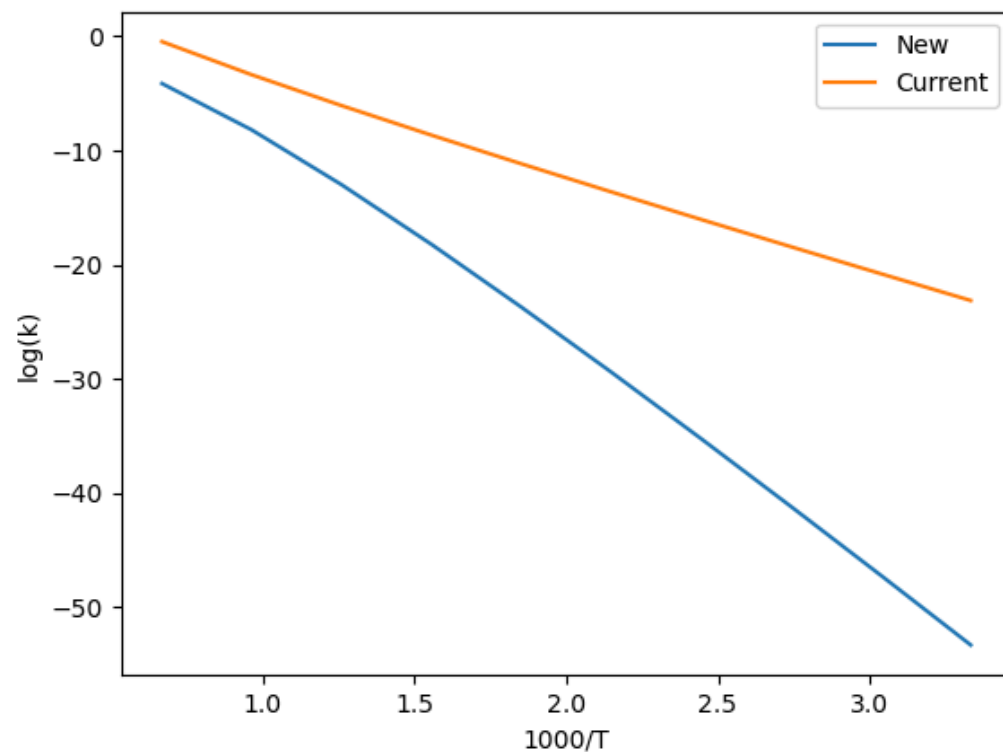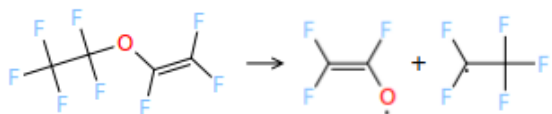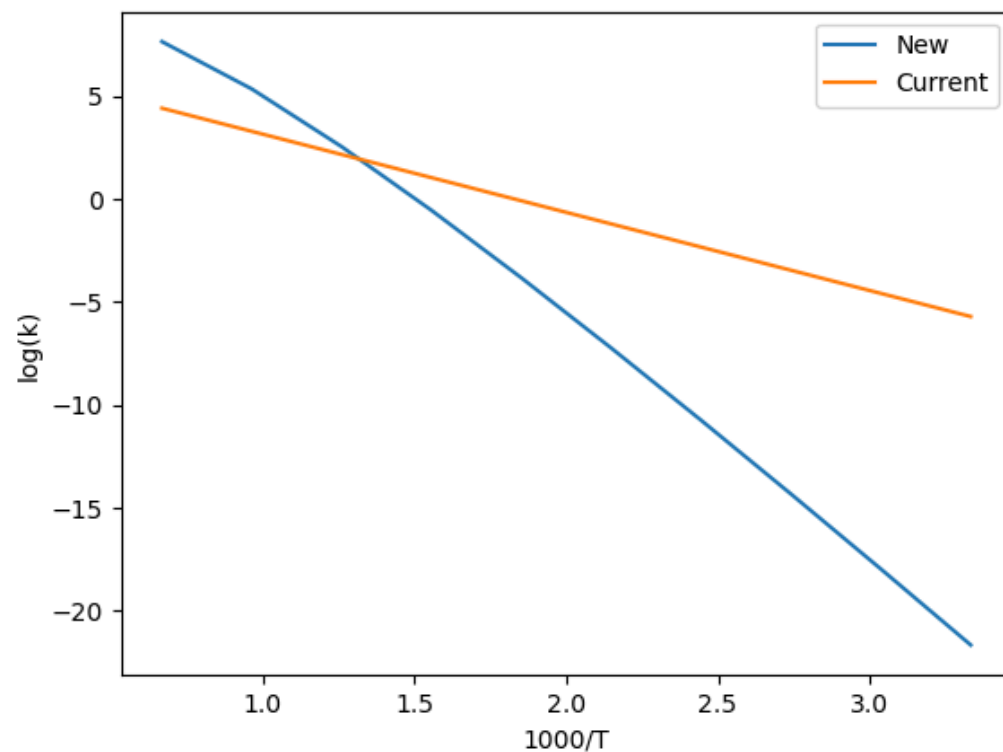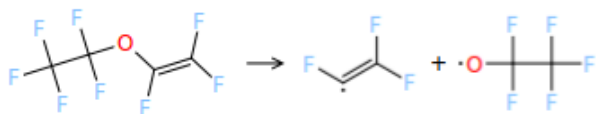**Note: Training reaction written in opposite direction from reaction family.**

New Kinetics:
Arrhenius(A=(1.16e+54,'s^-1'), n=-11.66, Ea=(64310,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(9.04e+06,'m^3/(mol*s)'), n=2.17087e-08, w0=
(179,'kJ/mol'), E0=(72.7054,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-
3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
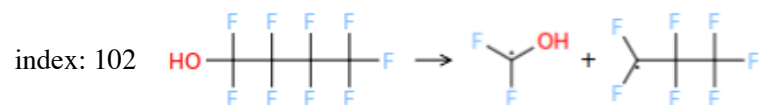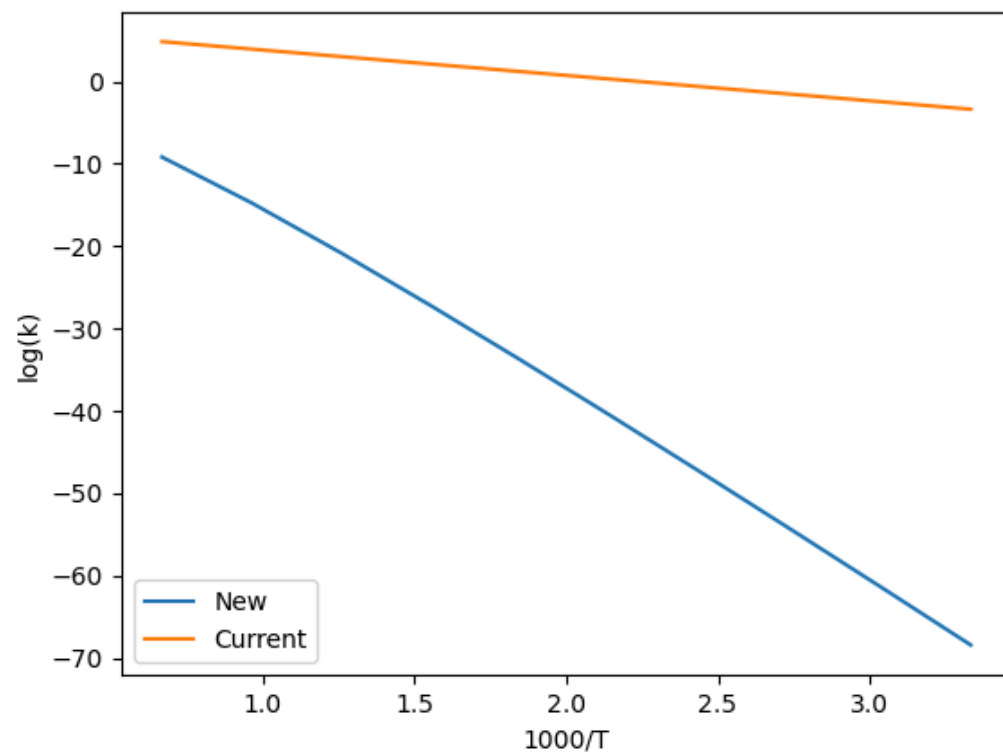R_2R->C_Ext-2C-R_Ext-2C-R""")

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

New Kinetics:
Arrhenius(A=(4.27e+46,'s^-1'), n=-12.24, Ea=(116300,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(7.38316e+06,'m^3/(mol*s)'), n=1.31229e-07, w0=
(179,'kJ/mol'), E0=(58.9141,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'),
uncertainty=RateUncertainty(mu=-0.016021952005170214,
var=0.3543710496450803, Tref=1000.0, N=2, data_mean=0.0,
correlation='Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS-
>Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
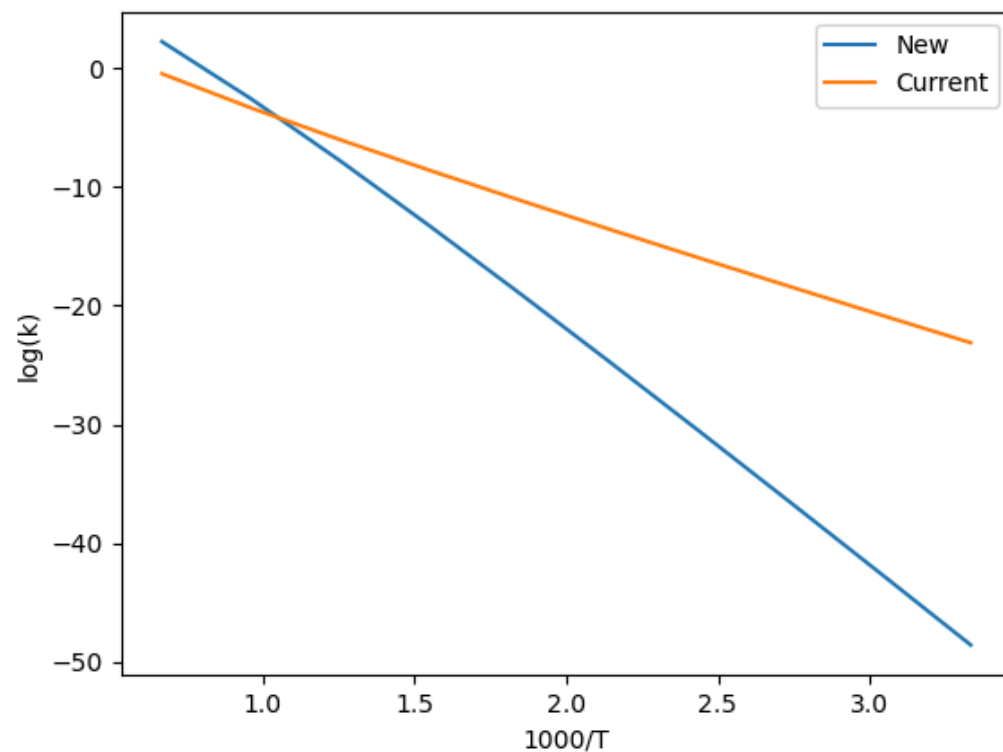>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
R_2R->C""")

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

New Kinetics:
Arrhenius(A=(1.57e+47,'s^-1'), n=-9.62, Ea=(98780,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

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

New Kinetics:
Arrhenius(A=(1.92e+47,'s^-1'), n=-9.54, Ea=(96620,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
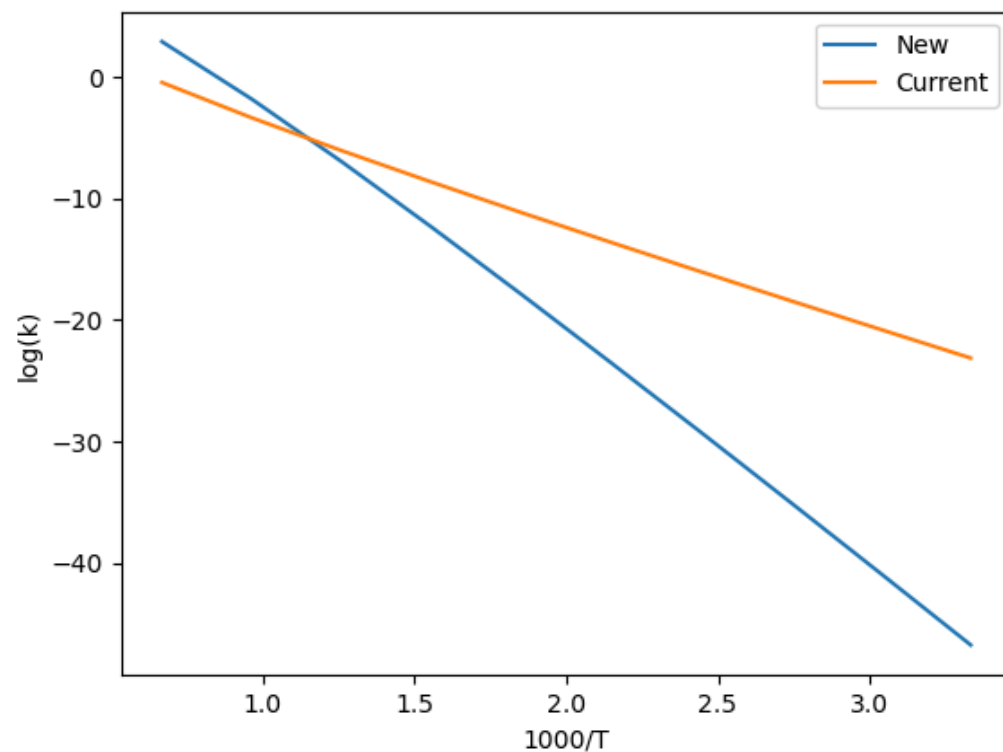1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

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

New Kinetics:
Arrhenius(A=(1.34e+47,'s^-1'), n=-9.62, Ea=(99230,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
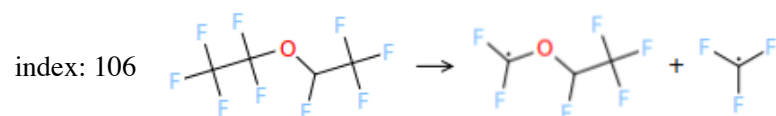inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
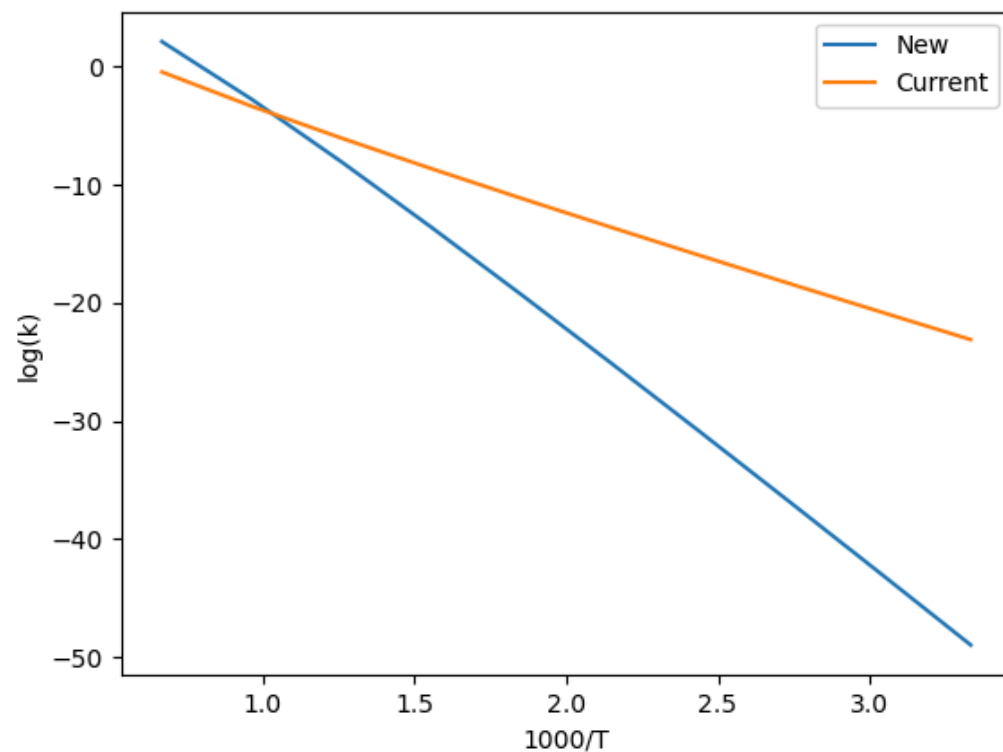1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

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

New Kinetics:
Arrhenius(A=(3.37e+35,'s^-1'), n=-5.79, Ea=(100100,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
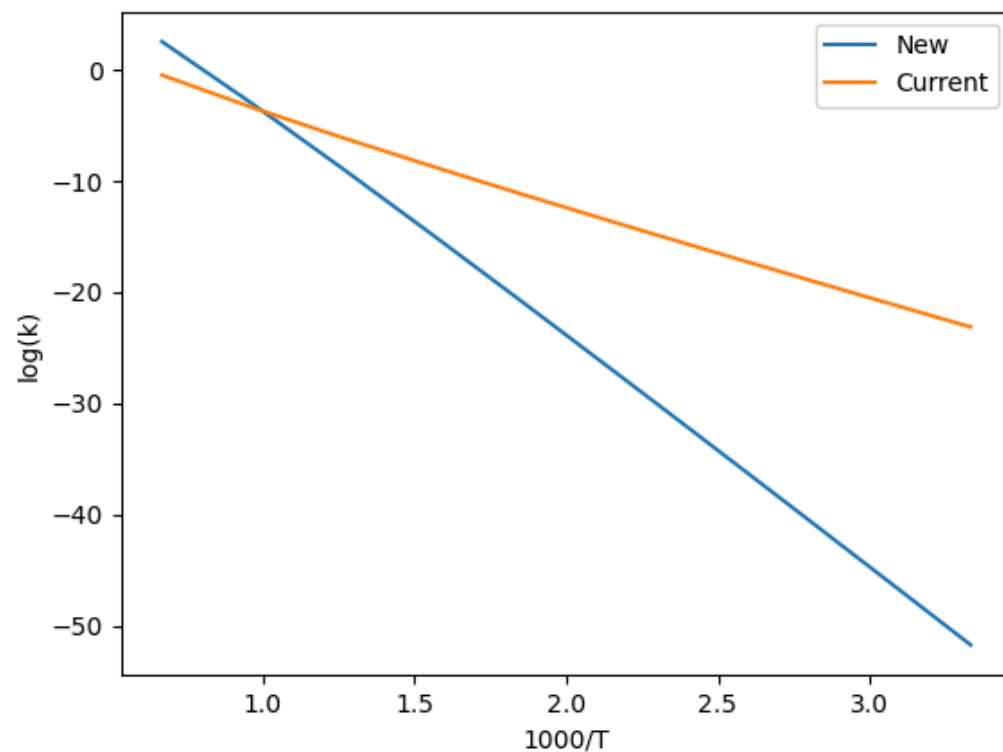inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

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

New Kinetics:
Arrhenius(A=(9.17e+34,'s^-1'), n=-5.59, Ea=(99970,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
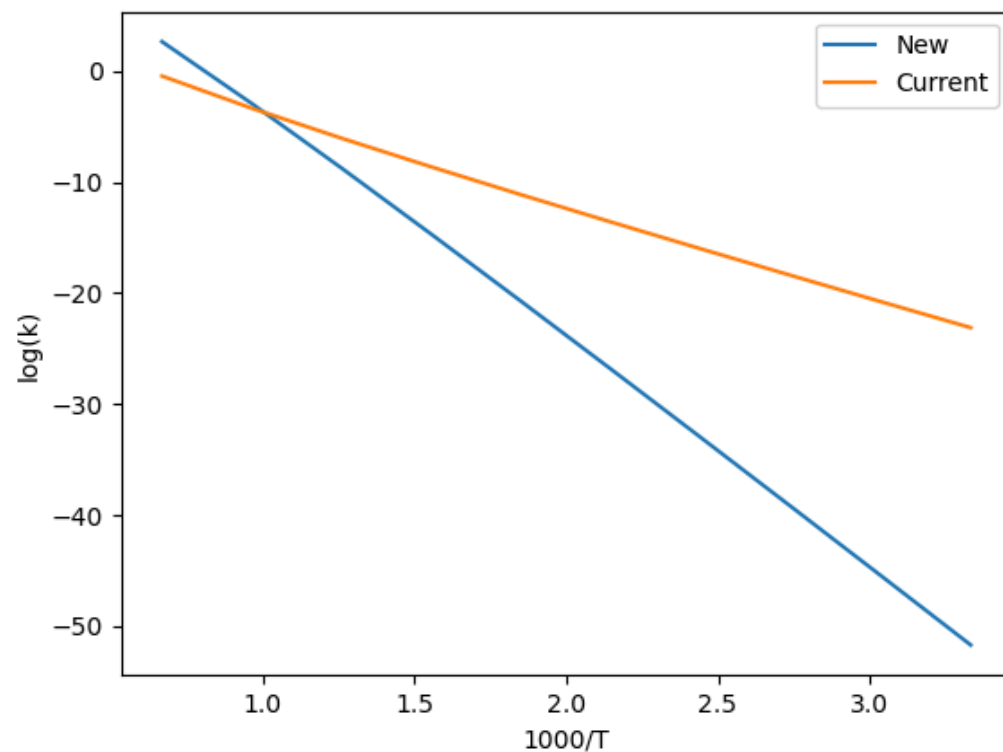inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
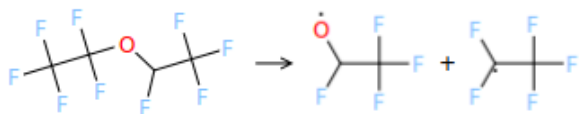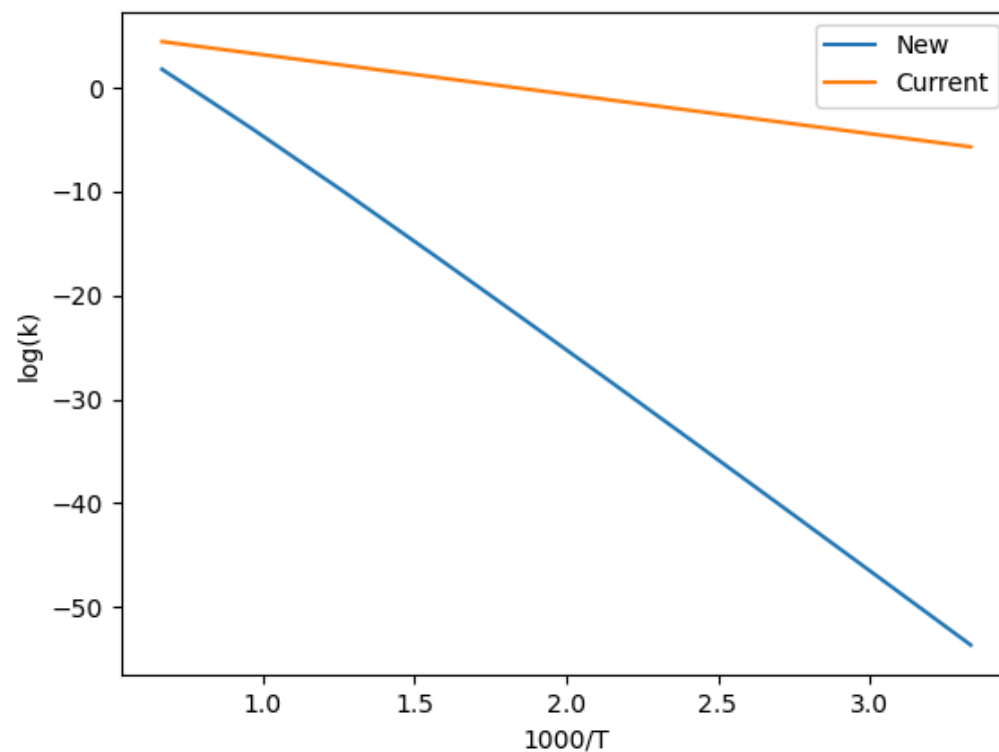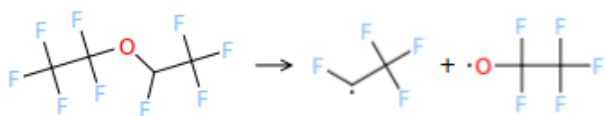
New Kinetics:
Arrhenius(A=(1.41e+34,'s^-1'), n=-5.53, Ea=(101700,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(9.04e+06,'m^3/(mol*s)'), n=2.17087e-08, w0=
(179,'kJ/mol'), E0=(72.7054,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-
3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
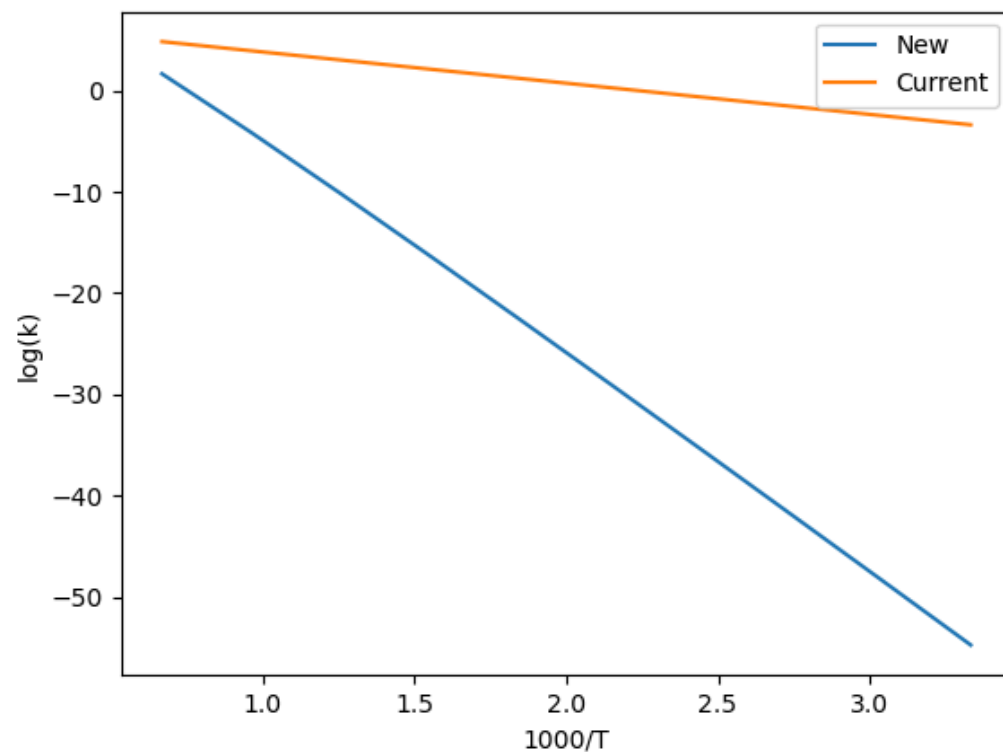R_2R->C_Ext-2C-R_Ext-2C-R""")

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Note: Training reaction written in opposite direction from reaction family.
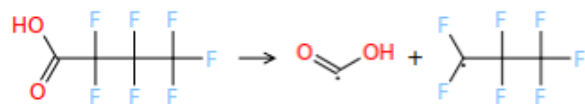
New Kinetics:
Arrhenius(A=(2.27e+33,'s^-1'), n=-5.26, Ea=(103000,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(7.38316e+06,'m^3/(mol*s)'), n=1.31229e-07, w0=
(179,'kJ/mol'), E0=(58.9141,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'),
uncertainty=RateUncertainty(mu=-0.016021952005170214,
var=0.3543710496450803, Tref=1000.0, N=2, data_mean=0.0,
correlation='Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS-
>Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
R_2R->C""")

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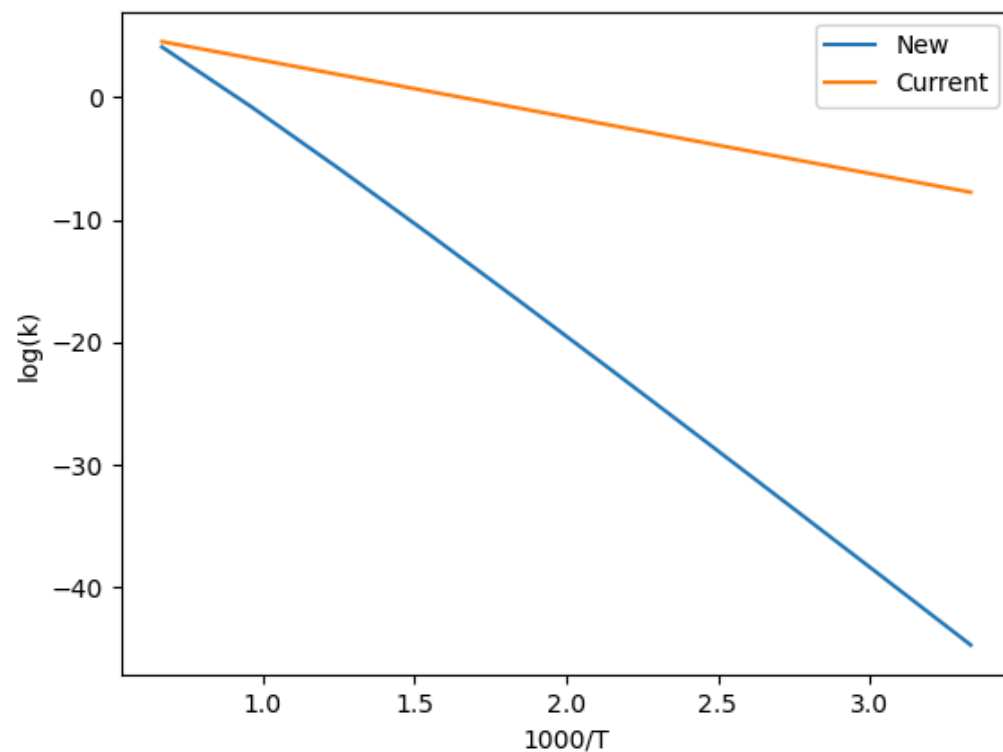**Note: Training reaction written in opposite direction from reaction family.**
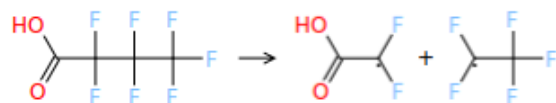
New Kinetics:
Arrhenius(A=(2.16e+37,'s^-1'), n=-6.28, Ea=(91270,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(4e+07,'m^3/(mol*s)'), n=0, w0=(173,'kJ/mol'), E0=(88.2769,'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-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O',), comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_4R!H->O""")
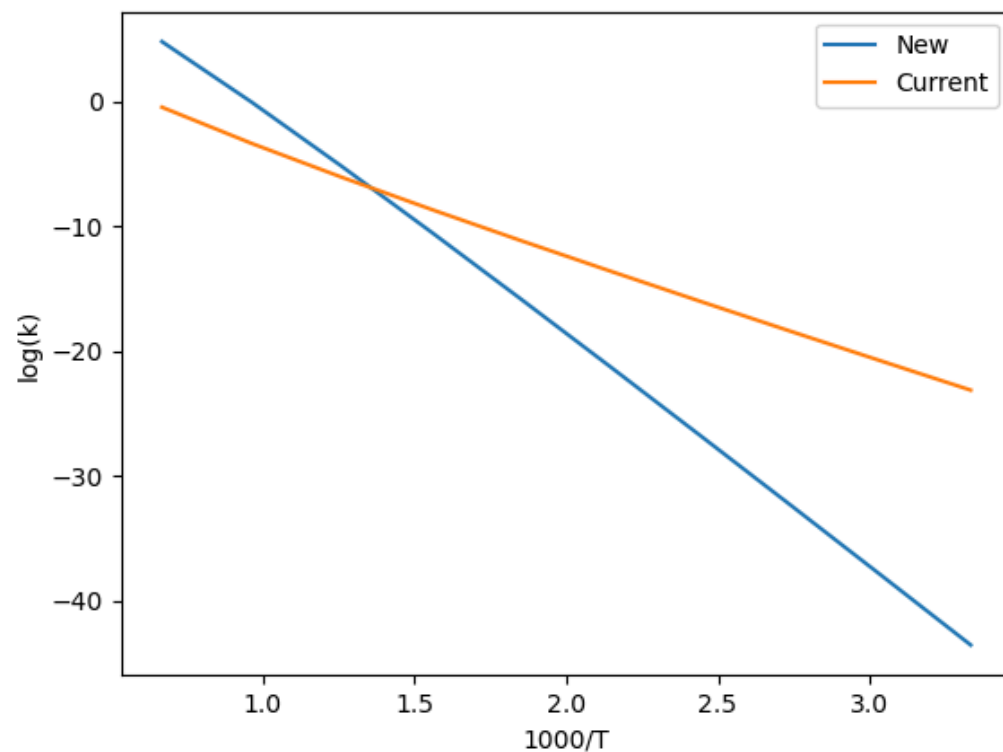
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Note: Training reaction written in opposite direction from reaction family.

New Kinetics:
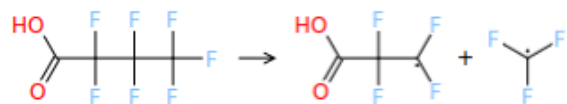Arrhenius(A=(6.25e+37,'s^-1'), n=-6.24, Ea=(90440,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

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

New Kinetics:
Arrhenius(A=(4.88e+41,'s^-1'), n=-7.47, Ea=(99630,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
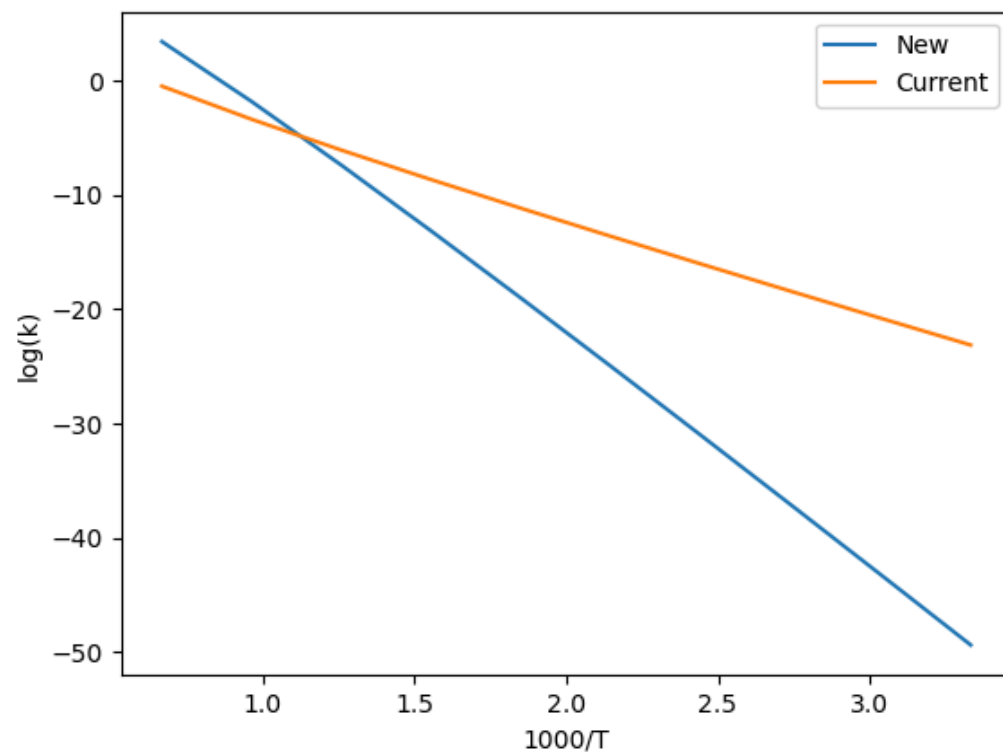>F_Ext-2CF-R_Ext-4R!H-R""")

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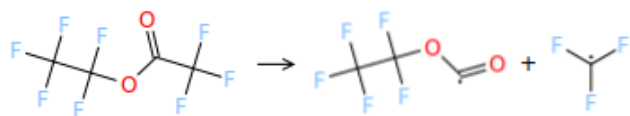**Note: Training reaction written in opposite direction from reaction family.**

New Kinetics:
Arrhenius(A=(2.92e+33,'s^-1'), n=-5.17, Ea=(91520,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
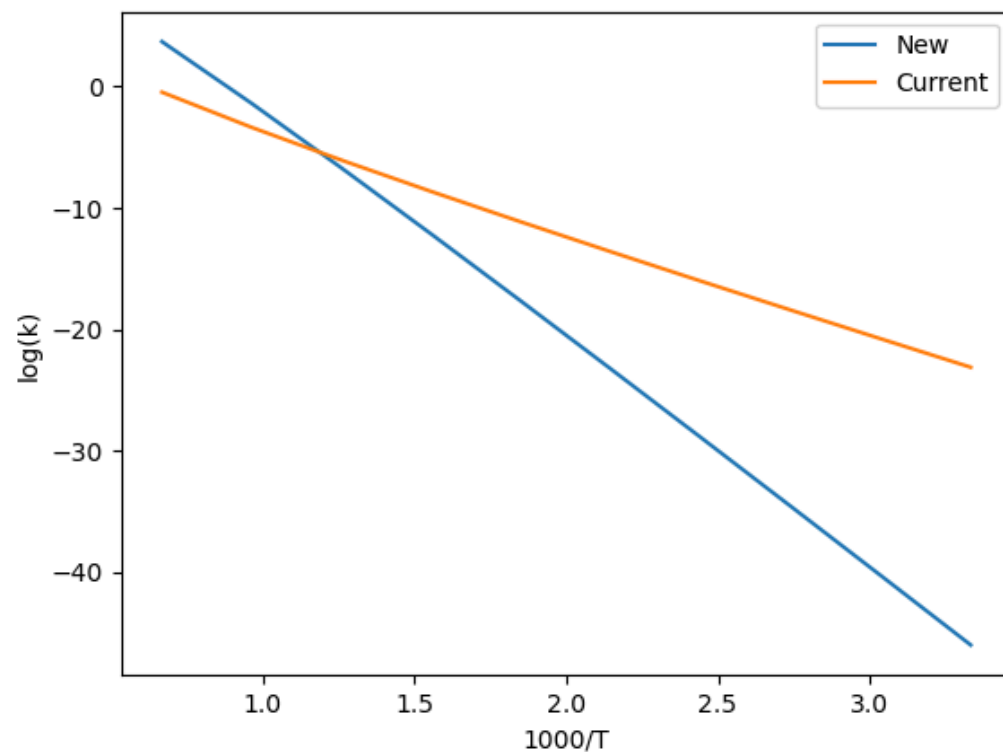>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
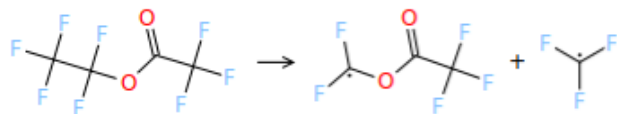
New Kinetics:
Arrhenius(A=(6.11e+35,'s^-1'), n=-5.78, Ea=(99500,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
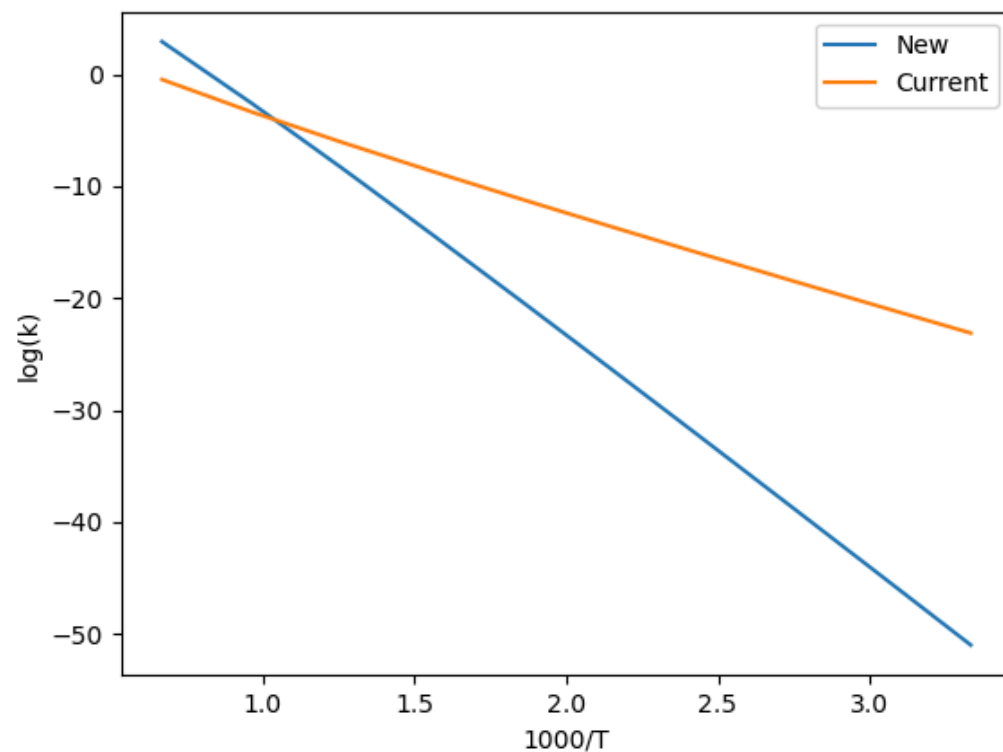inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
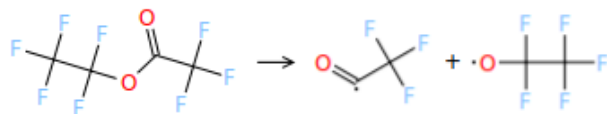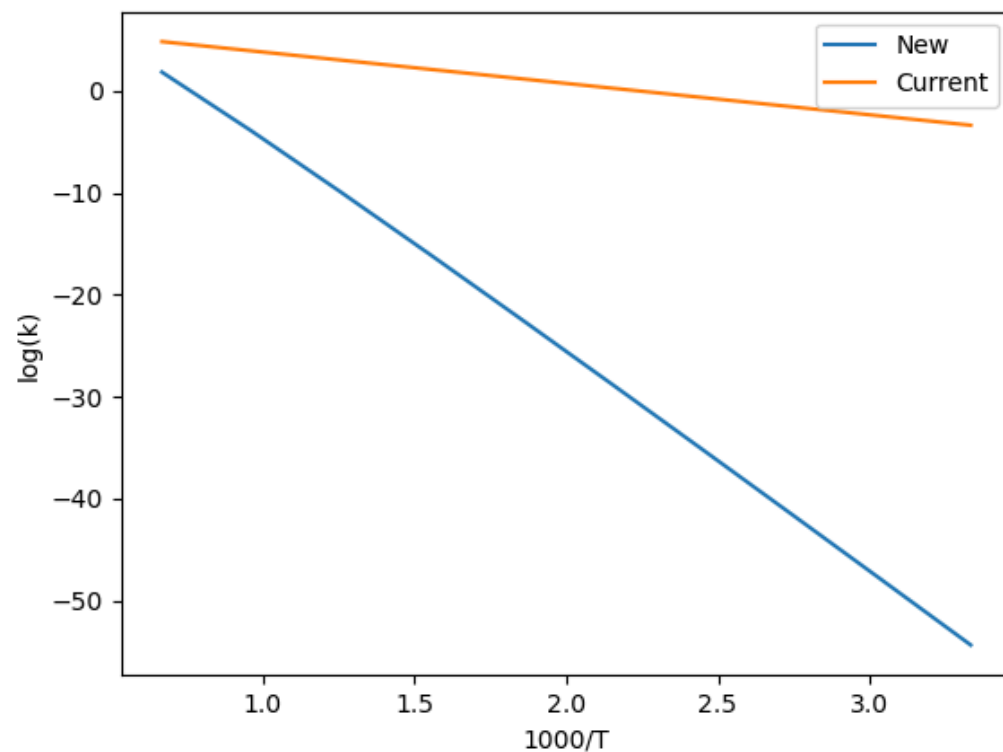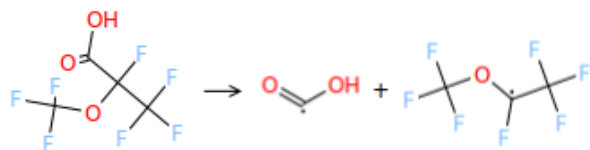
New Kinetics:
Arrhenius(A=(1.6e+34,'s^-1'), n=-5.47, Ea=(103000,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(7.38316e+06,'m^3/(mol*s)'), n=1.31229e-07, w0=
(179,'kJ/mol'), E0=(58.9141,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'),
uncertainty=RateUncertainty(mu=-0.016021952005170214,
var=0.3543710496450803, Tref=1000.0, N=2, data_mean=0.0,
correlation='Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS-
>Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
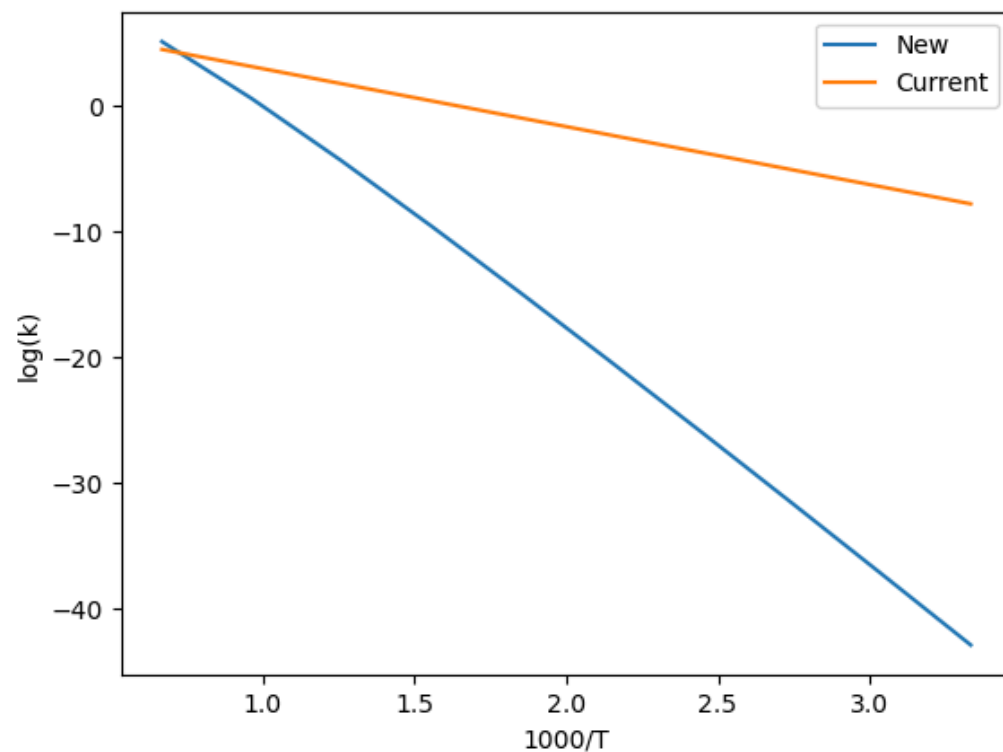>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
R_2R->C""")

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Note: Training reaction written in opposite direction from reaction family.
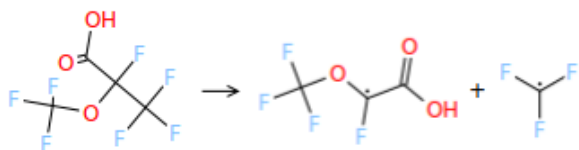
New Kinetics:
Arrhenius(A=(6.32e+49,'s^-1'), n=-9.74, Ea=(94130,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(4e+07,'m^3/(mol*s)'), n=0, w0=(173,'kJ/mol'), E0=
(88.2769,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_4R!H->O',), comment="""Estimated from node Root_N-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_4R!H->O""")

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

New Kinetics:
Arrhenius(A=(1.96e+51,'s^-1'), n=-10.15, Ea=(96240,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
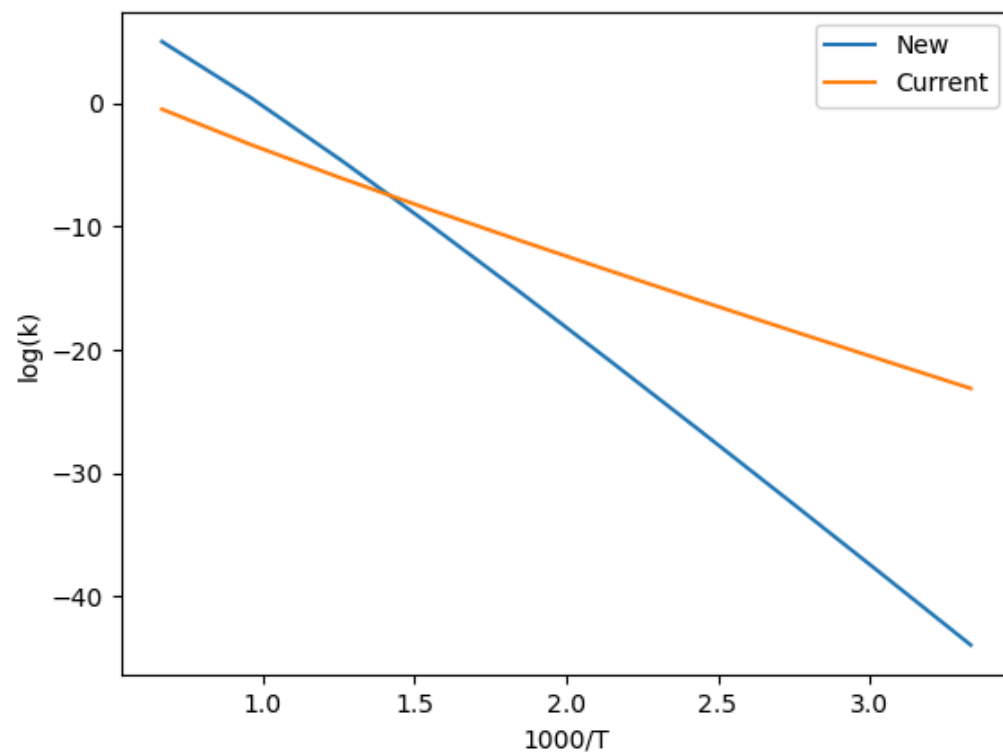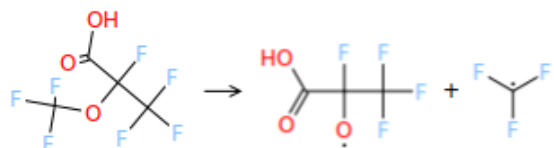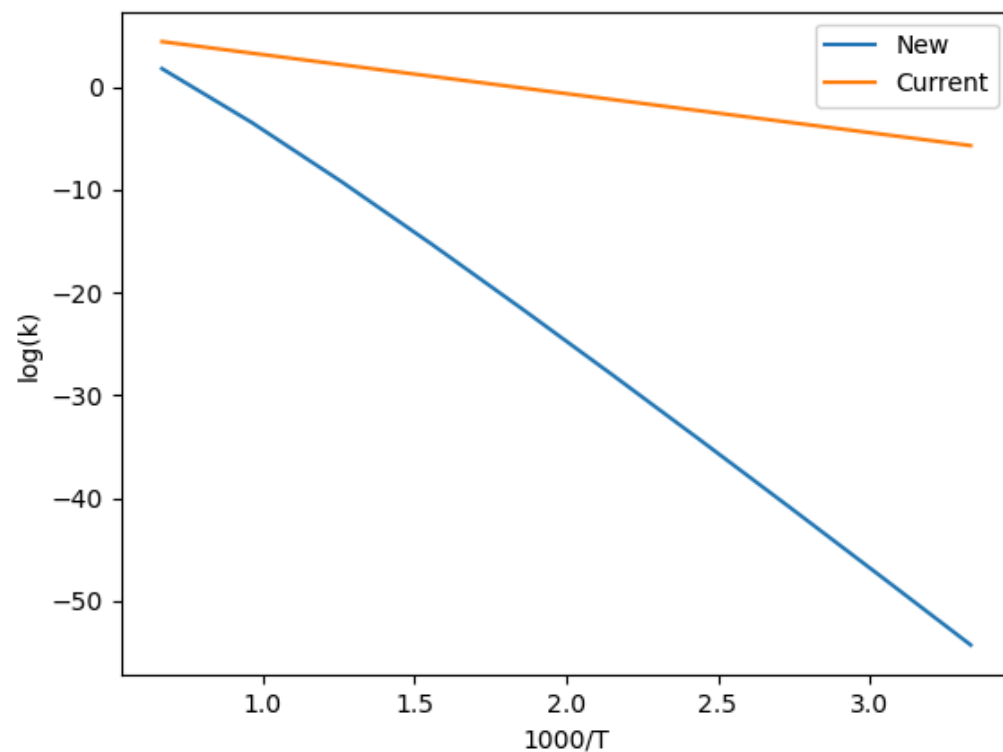>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
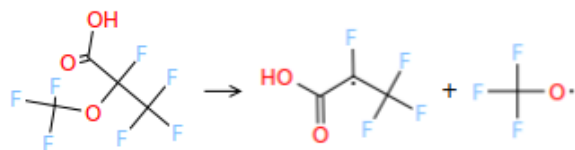
New Kinetics:
Arrhenius(A=(1.26e+56,'s^-1'), n=-12.02, Ea=(110700,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(9.04e+06,'m^3/(mol*s)'), n=2.17087e-08, w0=
(179,'kJ/mol'), E0=(72.7054,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-
3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
R_2R->C_Ext-2C-R_Ext-2C-R""")

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

New Kinetics:
Arrhenius(A=(2.56e+53,'s^-1'), n=-10.93, Ea=(101500,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(9.04e+06,'m^3/(mol*s)'), n=2.17087e-08, w0=(179,'kJ/mol'), E0=(72.7054,'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-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R""")
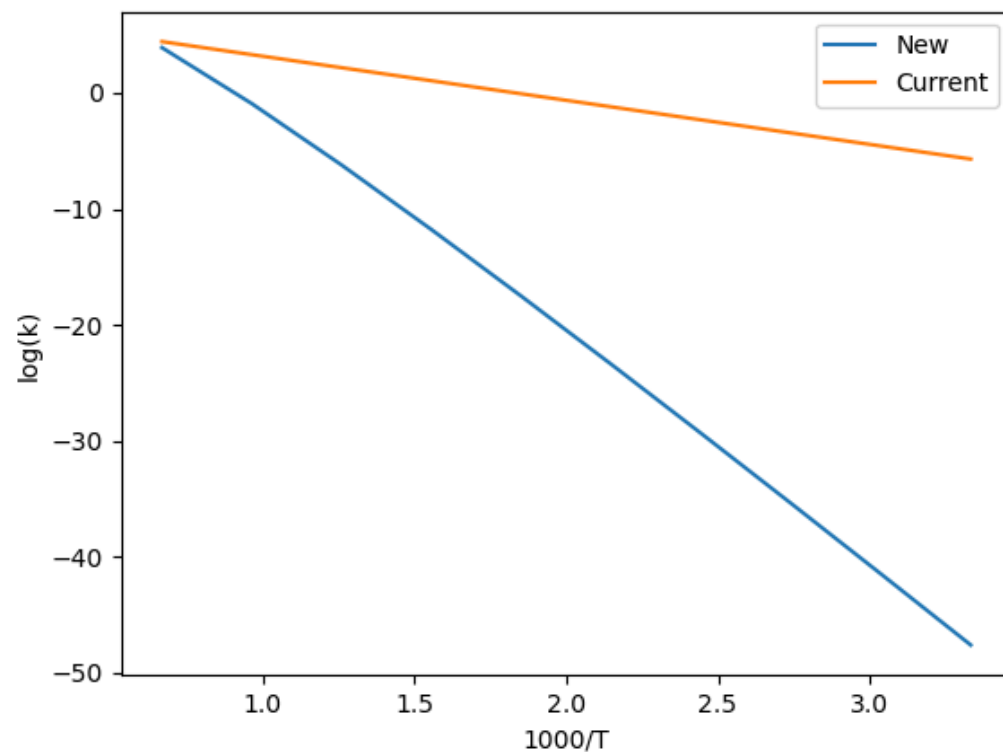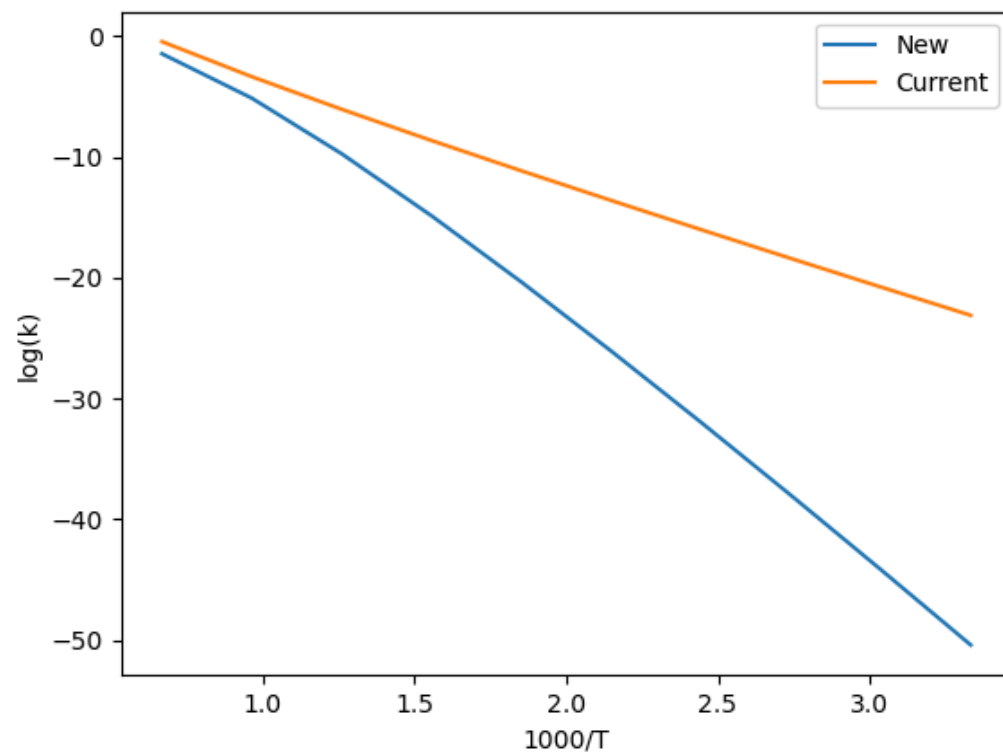
index: 140

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

New Kinetics:
Arrhenius(A=(6.18e+82,'s^-1'), n=-21.49, Ea=(109800,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-2CF-R_Ext-4R!H-R""")

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

New Kinetics:
Arrhenius(A=(2.76e+82,'s^-1'), n=-21.29, Ea=(108800,'cal/mol'), T0=
(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
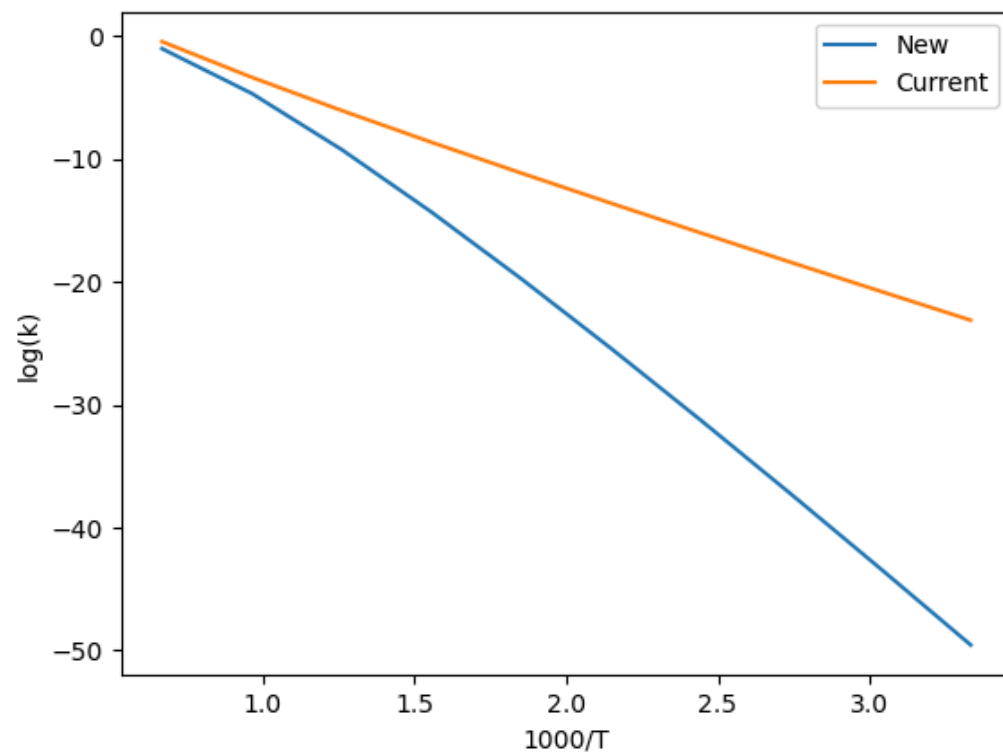inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
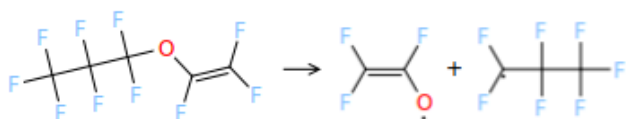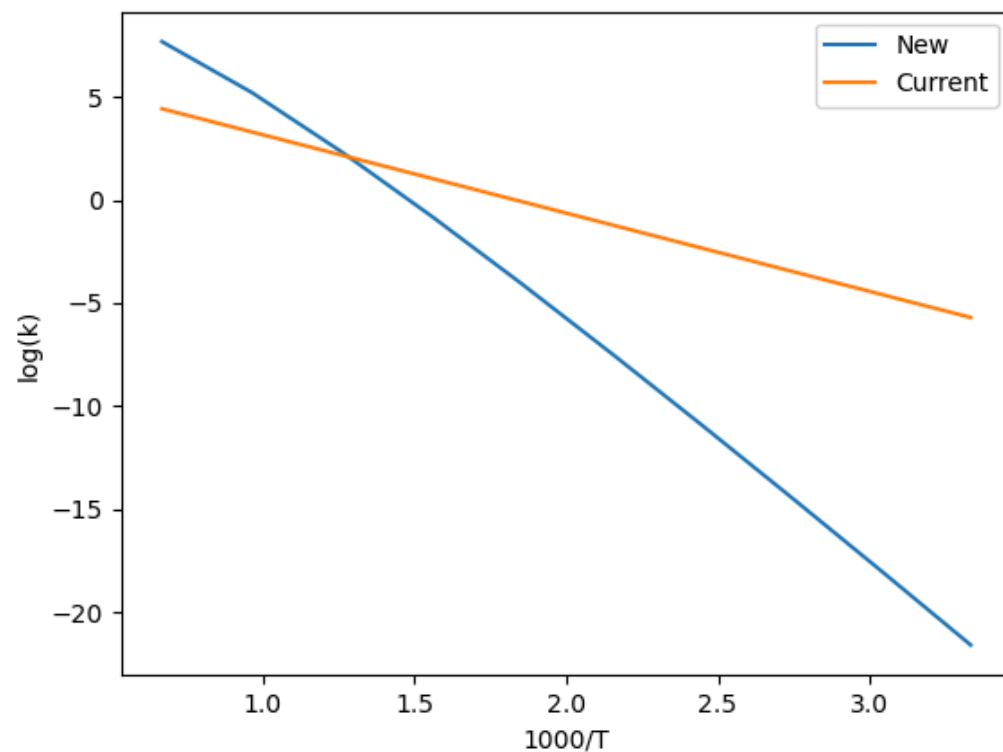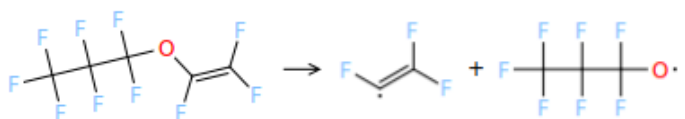
New Kinetics:
Arrhenius(A=(1.08e+47,'s^-1'), n=-9.56, Ea=(61700,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(9.04e+06,'m^3/(mol*s)'), n=2.17087e-08, w0=
(179,'kJ/mol'), E0=(72.7054,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-
3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
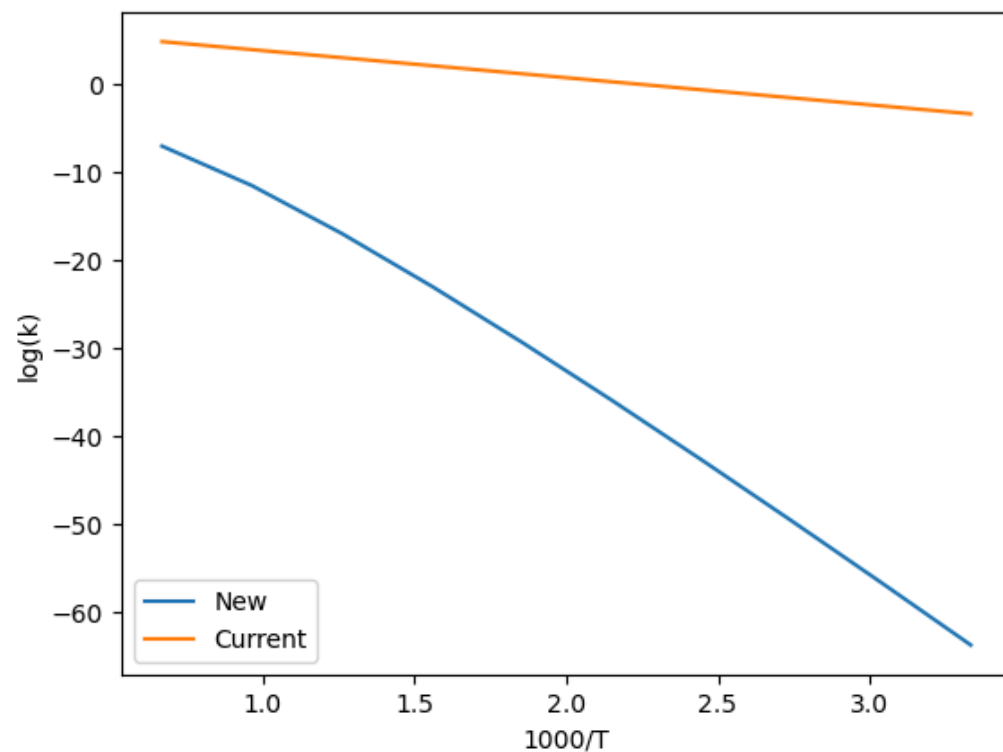R_2R->C_Ext-2C-R_Ext-2C-R""")

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Note: Training reaction written in opposite direction from reaction family.
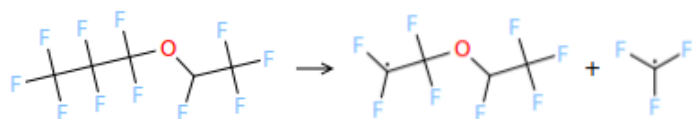
New Kinetics:
Arrhenius(A=(1.87e+81,'s^-1'), n=-22.13, Ea=(123800,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(7.38316e+06,'m^3/(mol*s)'), n=1.31229e-07, w0=(179,'kJ/mol'), E0=(58.9141,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'), uncertainty=RateUncertainty(mu=-0.016021952005170214, var=0.3543710496450803, Tref=1000.0, N=2, data_mean=0.0, correlation='Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C',), comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C""")

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

New Kinetics:
Arrhenius(A=(1.27e+43,'s^-1'), n=-8.5, Ea=(99240,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
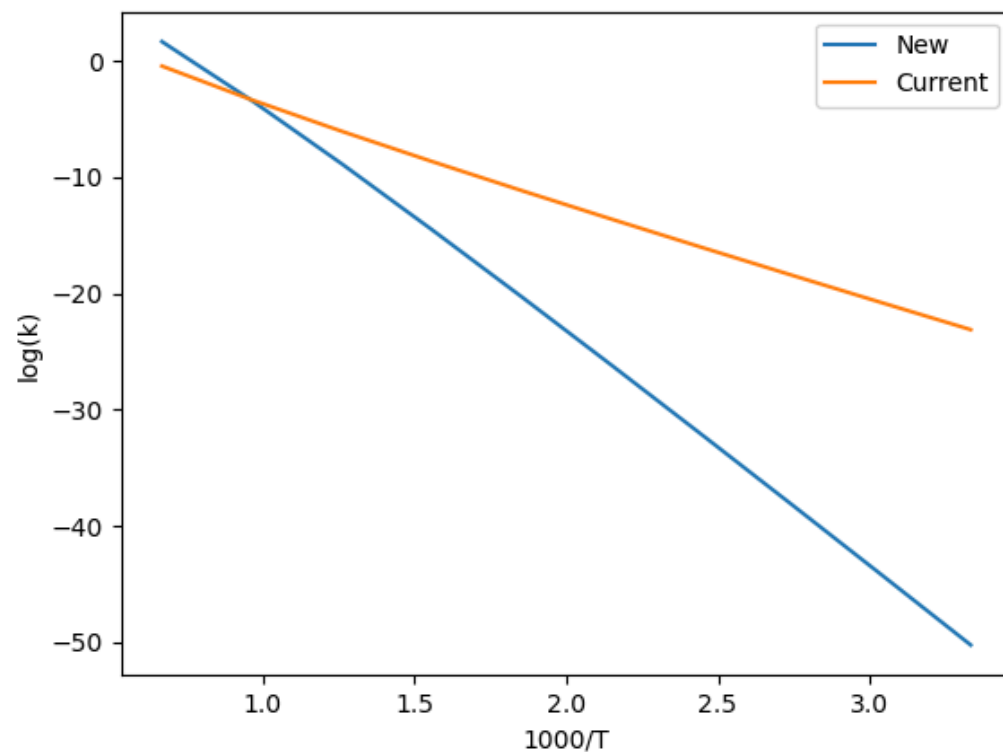1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

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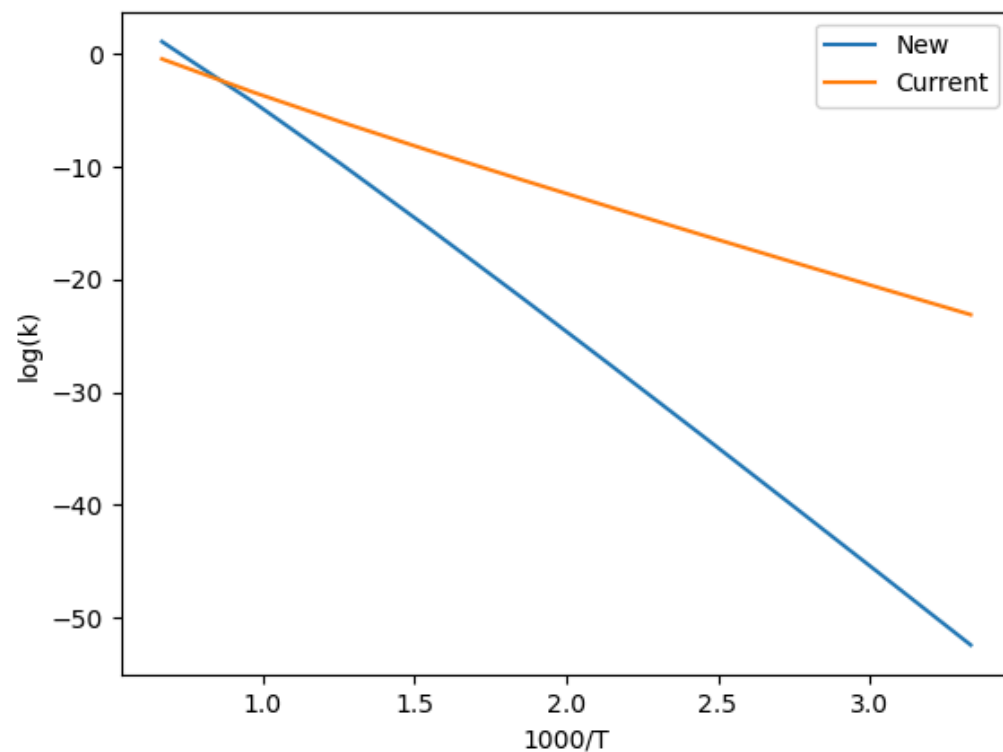**Note: Training reaction written in opposite direction from reaction family.**

New Kinetics:
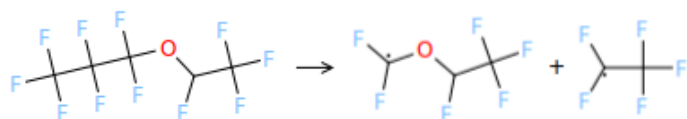Arrhenius(A=(1.46e+42,'s^-1'), n=-8.27, Ea=(101700,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
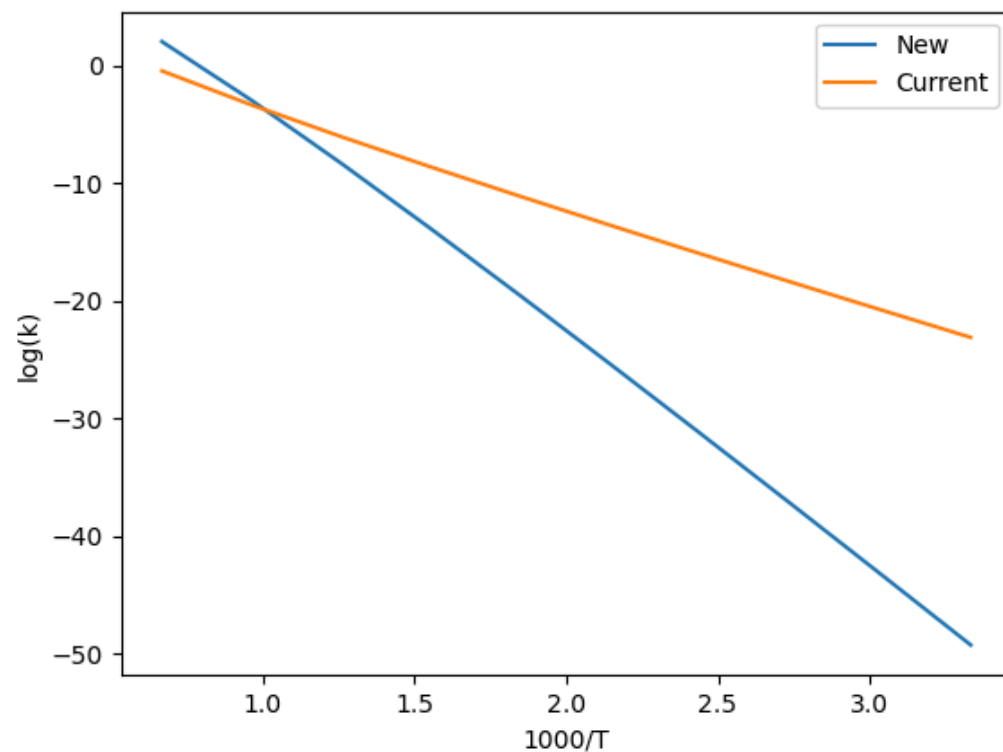>F_Ext-2CF-R_Ext-4R!H-R""")

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

New Kinetics:
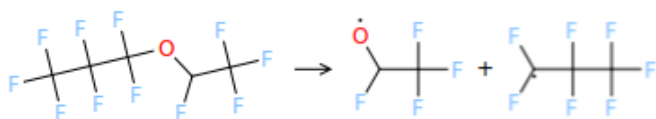Arrhenius(A=(2.05e+43,'s^-1'), n=-8.49, Ea=(98240,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
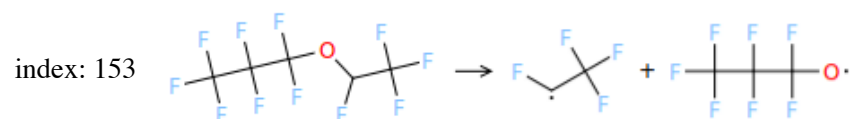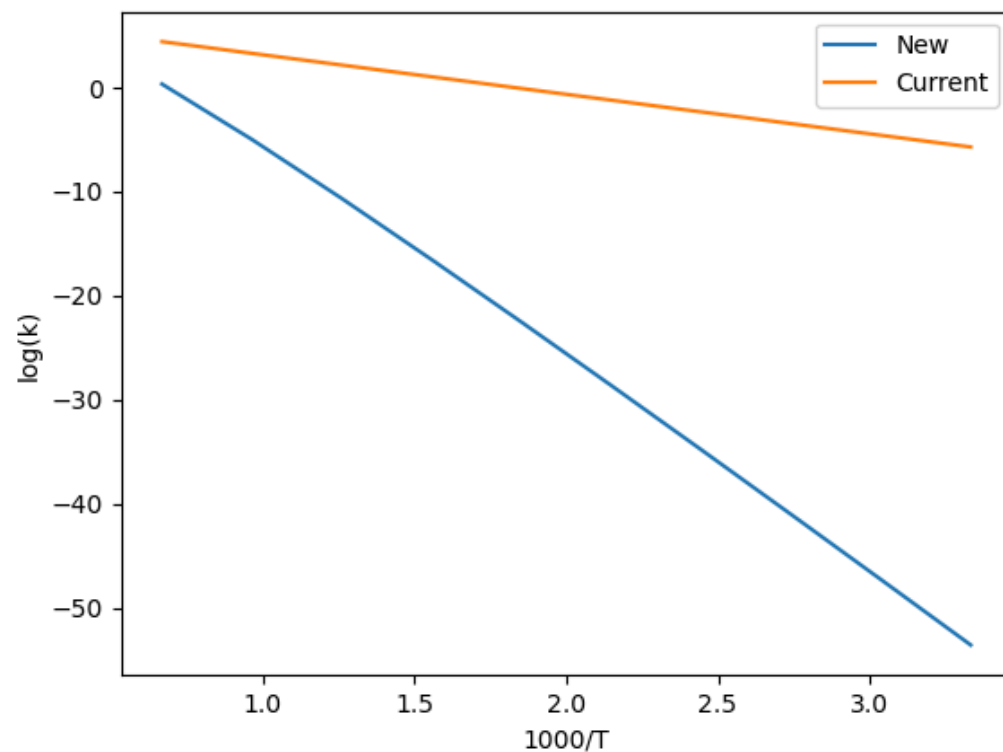1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
>F_Ext-2CF-R_Ext-4R!H-R""")

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

New Kinetics:
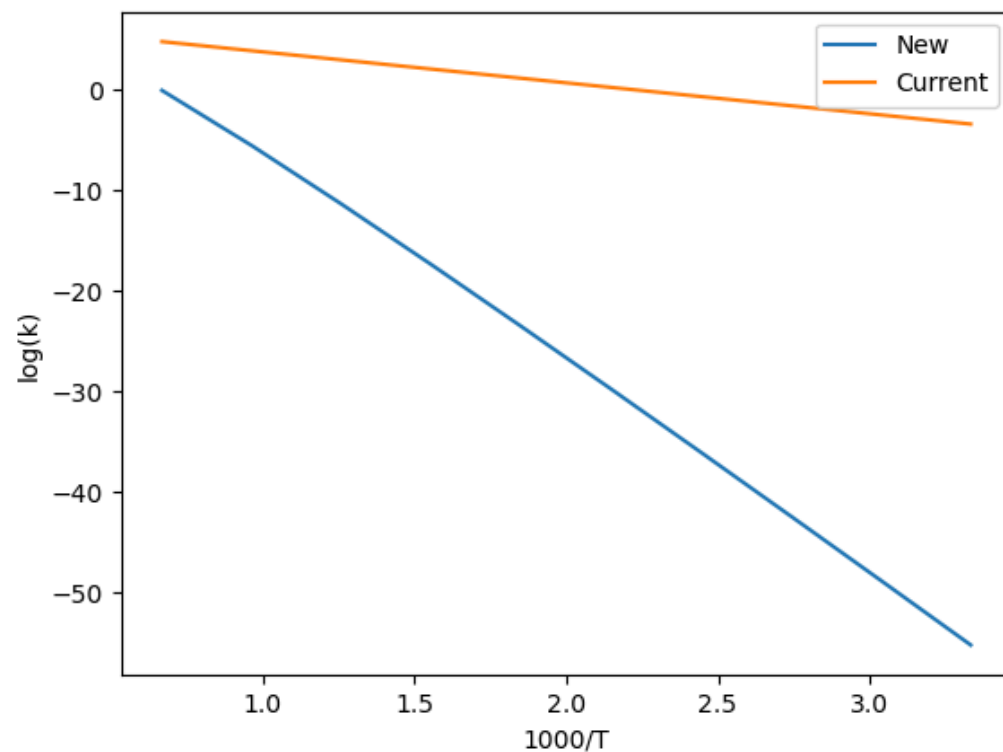Arrhenius(A=(1.59e+41,'s^-1'), n=-8.17, Ea=(102300,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(9.04e+06,'m^3/(mol*s)'), n=2.17087e-08, w0=
(179,'kJ/mol'), E0=(72.7054,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-
3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
R_2R->C_Ext-2C-R_Ext-2C-R""")

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

New Kinetics:
Arrhenius(A=(5.38e+39,'s^-1'), n=-7.75, Ea=(104000,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(7.38316e+06,'m^3/(mol*s)'), n=1.31229e-07, w0=
(179,'kJ/mol'), E0=(58.9141,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'),
uncertainty=RateUncertainty(mu=-0.016021952005170214,
var=0.3543710496450803, Tref=1000.0, N=2, data_mean=0.0,
correlation='Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS-
>Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
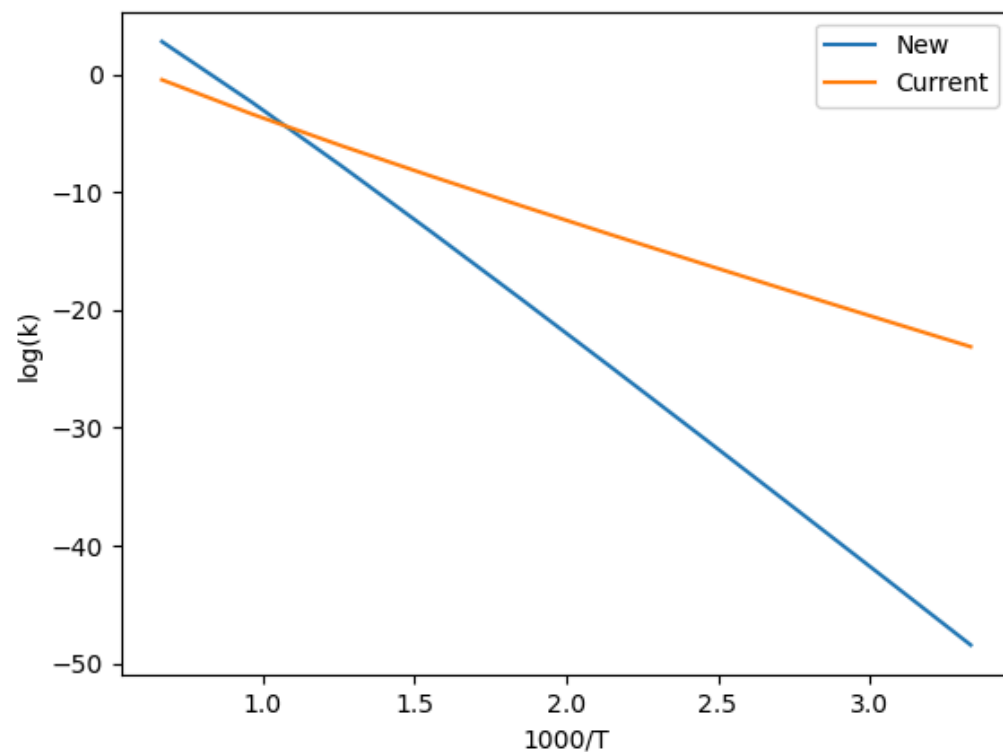>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
R_2R->C""")

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

New Kinetics:
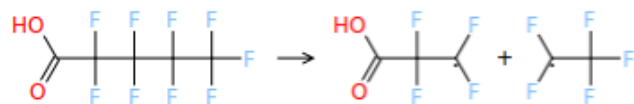Arrhenius(A=(1.5e+38,'s^-1'), n=-6.74, Ea=(95990,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
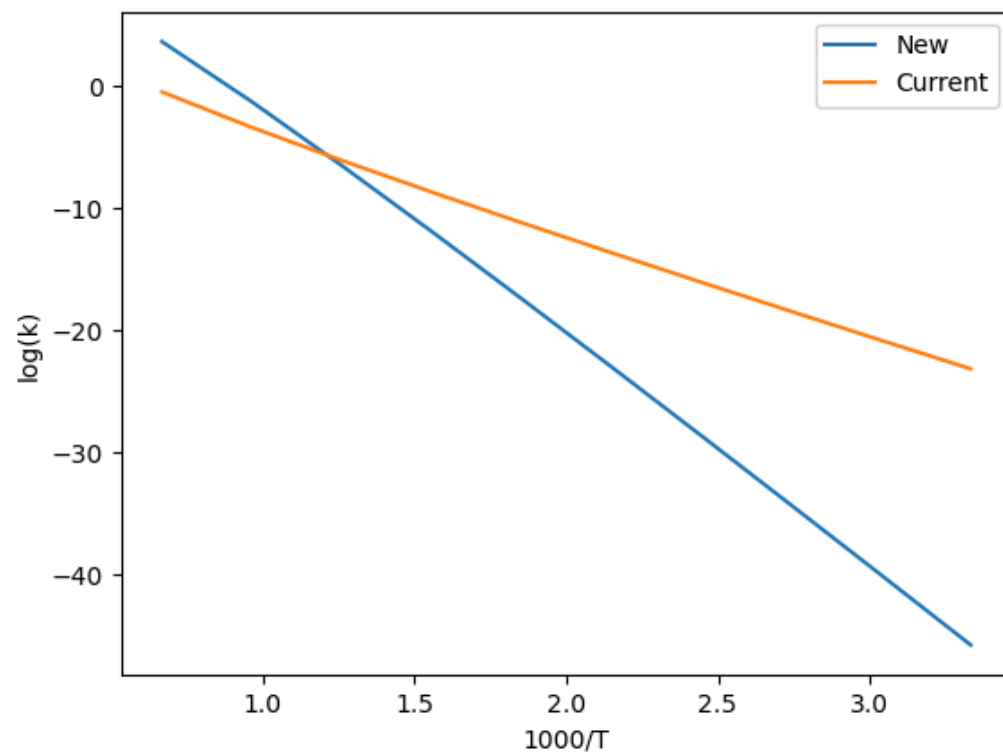>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
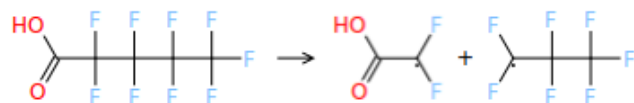
New Kinetics:
Arrhenius(A=(1.45e+39,'s^-1'), n=-6.91, Ea=(93040,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
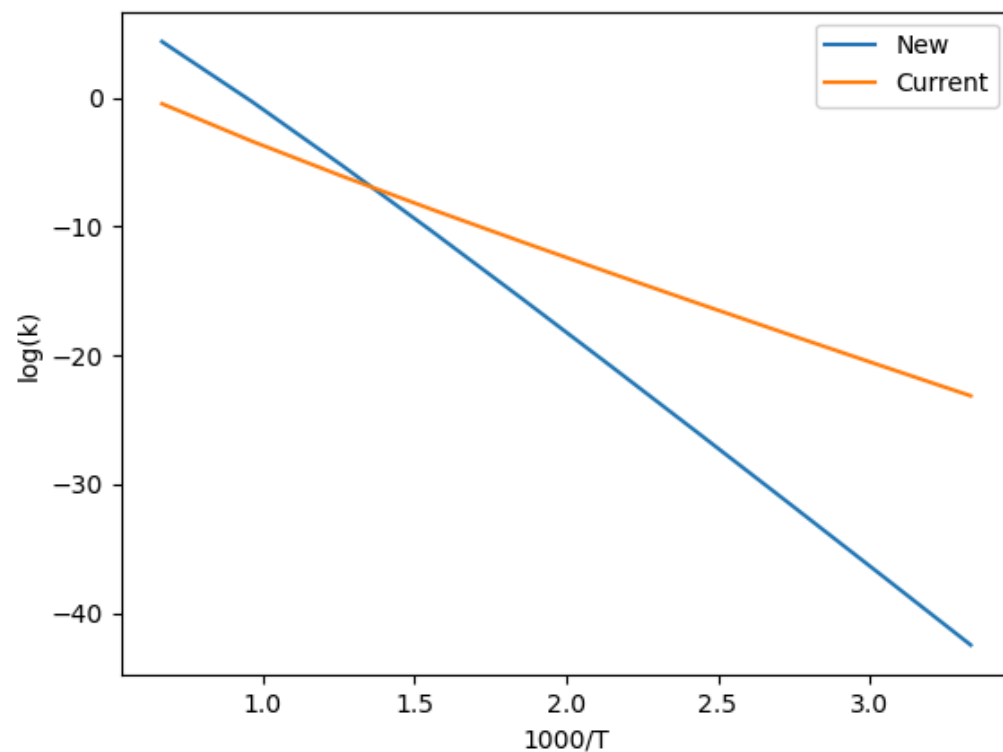>F_Ext-2CF-R_Ext-4R!H-R""")

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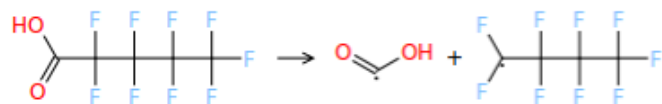**Note: Training reaction written in opposite direction from reaction family.**

New Kinetics:
Arrhenius(A=(5.26e+38,'s^-1'), n=-6.76, Ea=(88450,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
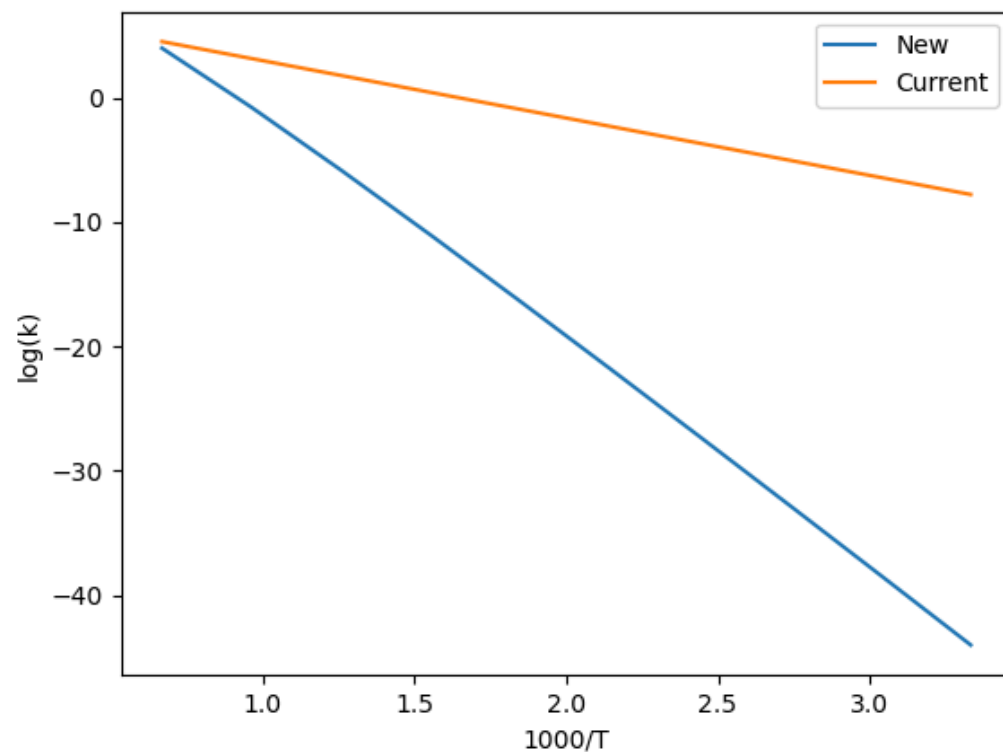>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
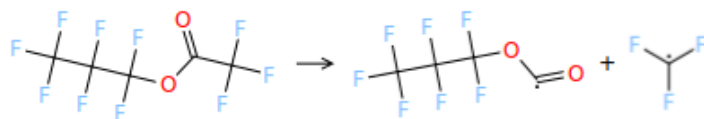
New Kinetics:
Arrhenius(A=(5.3e+38,'s^-1'), n=-6.78, Ea=(90500,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(4e+07,'m^3/(mol*s)'), n=0, w0=(173,'kJ/mol'), E0=
(88.2769,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_4R!H->O',), comment="""Estimated from node Root_N-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
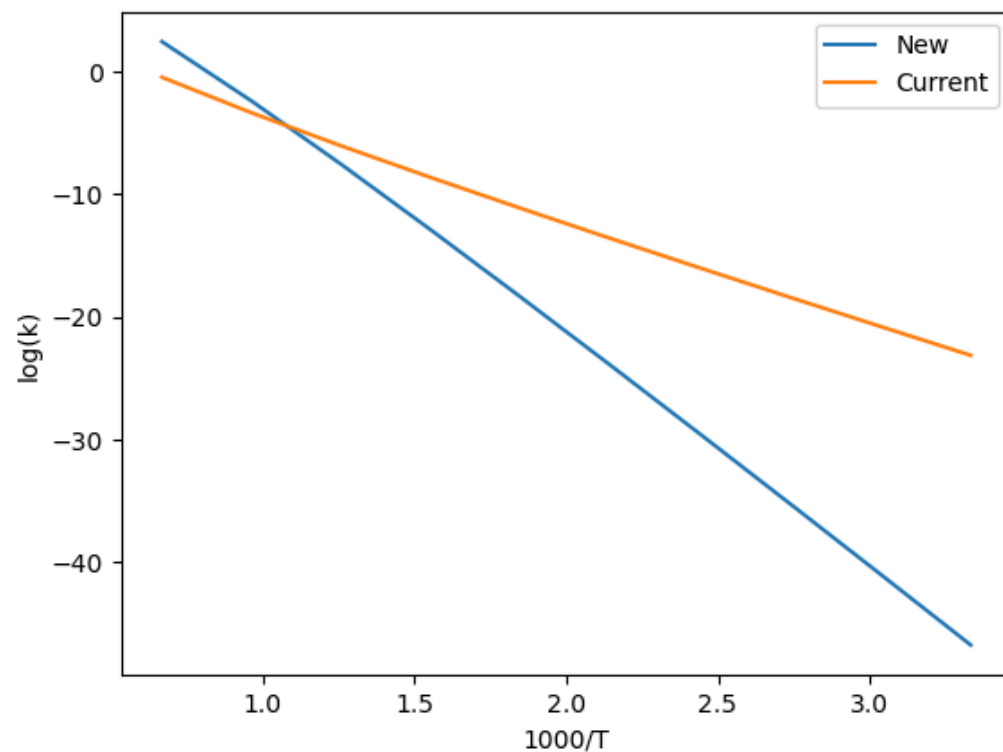2CF-R_4R!H->O""")

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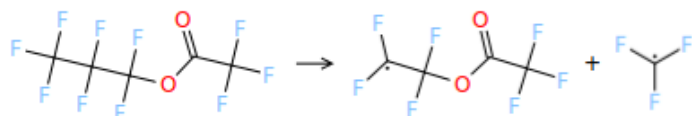**Note: Training reaction written in opposite direction from reaction family.**

New Kinetics:
Arrhenius(A=(4.76e+39,'s^-1'), n=-7.44, Ea=(93320,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
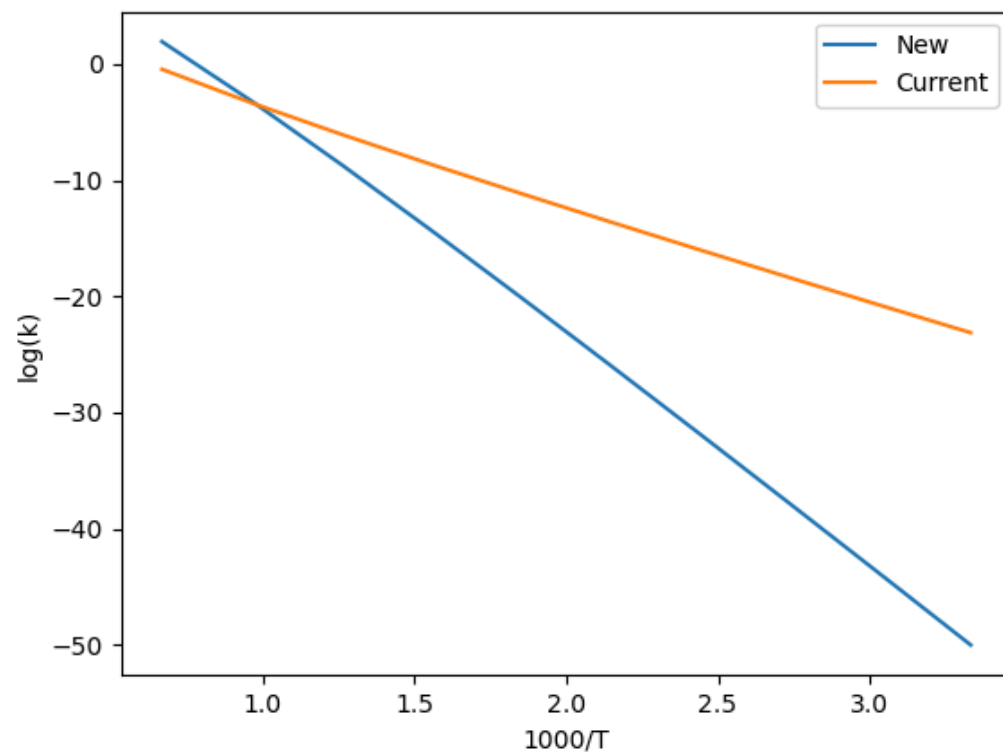>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
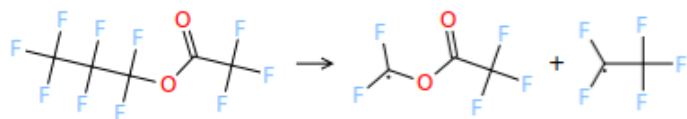
New Kinetics:
Arrhenius(A=(1.01e+41,'s^-1'), n=-7.79, Ea=(98430,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
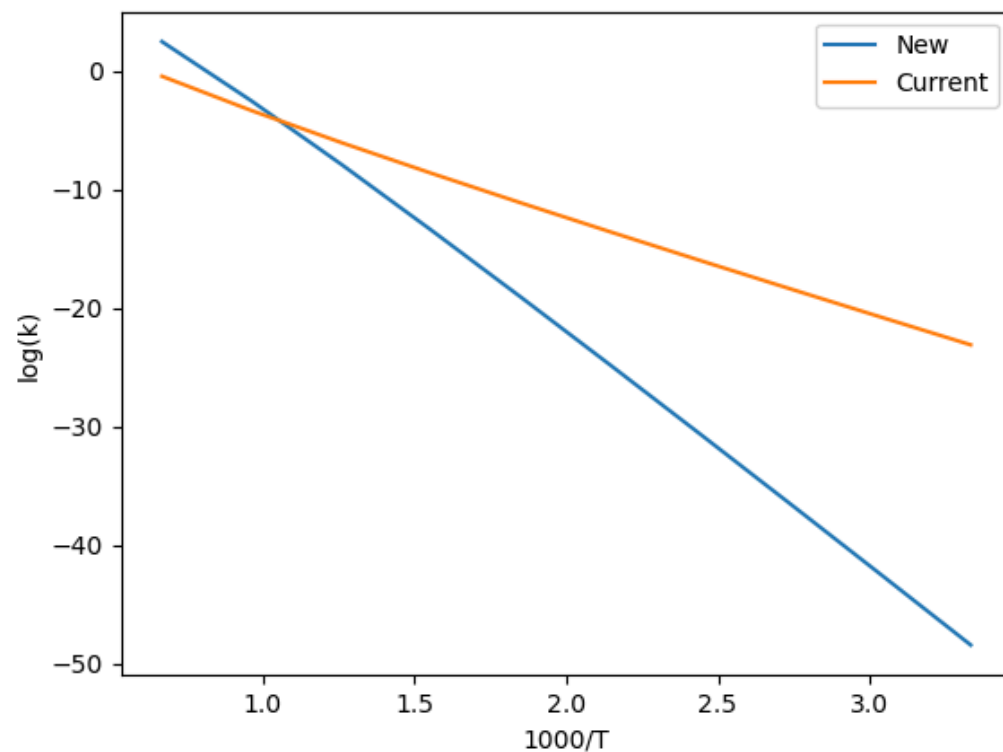>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
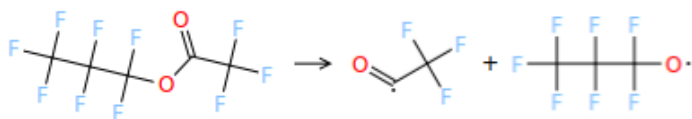
New Kinetics:
Arrhenius(A=(1.59e+41,'s^-1'), n=-7.76, Ea=(96690,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
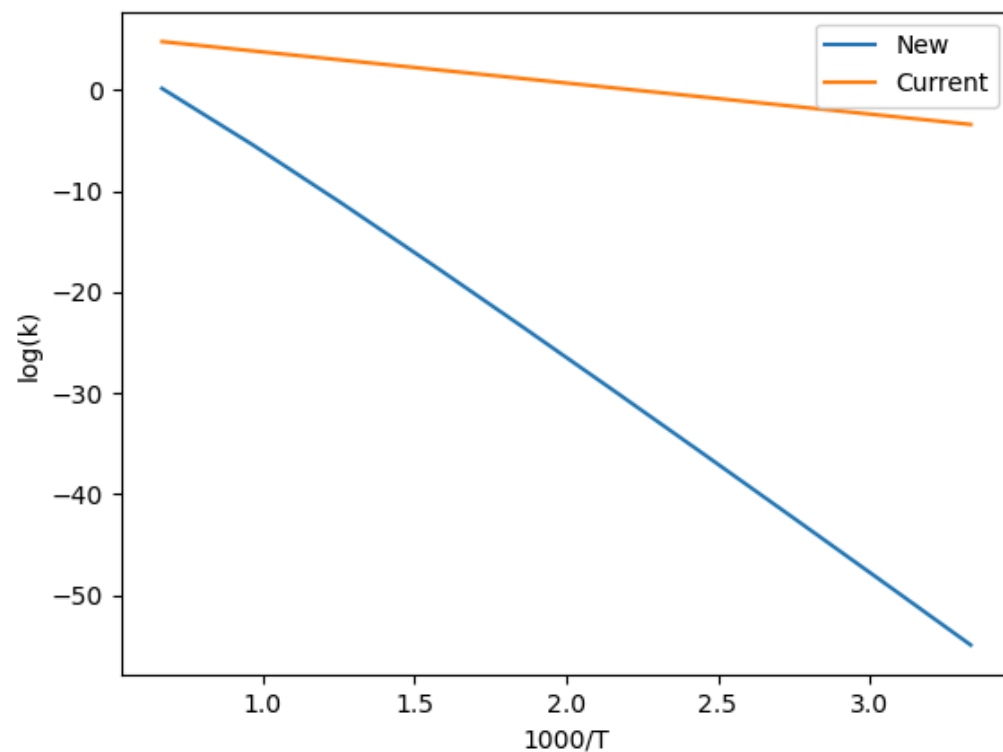>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
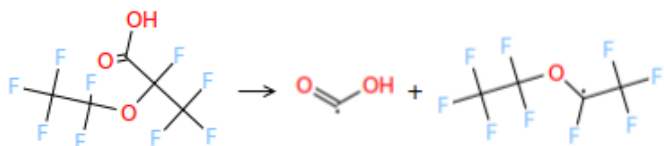
New Kinetics:
Arrhenius(A=(1.69e+38,'s^-1'), n=-7.24, Ea=(103300,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(7.38316e+06,'m^3/(mol*s)'), n=1.31229e-07, w0=
(179,'kJ/mol'), E0=(58.9141,'kJ/mol'), Tmin=(300,'K'), Tmax=(2000,'K'),
uncertainty=RateUncertainty(mu=-0.016021952005170214,
var=0.3543710496450803, Tref=1000.0, N=2, data_mean=0.0,
correlation='Root_N-1R->H_N-1BrCClFINOPSSi->N_N-1BrCClFOS-
>Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-R_2R->C',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
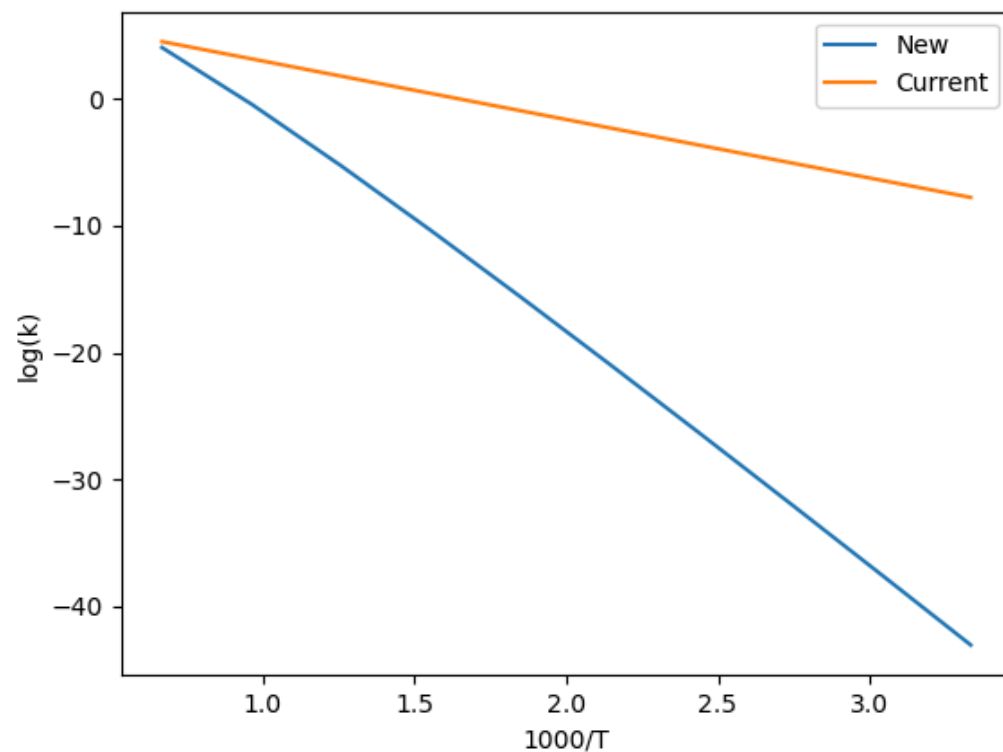>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
R_2R->C""")

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Note: Training reaction written in opposite direction from reaction family.
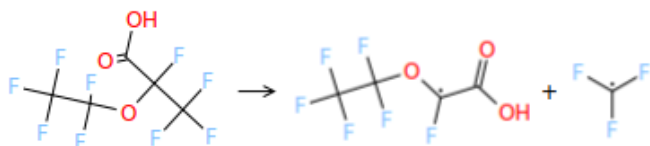
New Kinetics:
Arrhenius(A=(4.73e+46,'s^-1'), n=-9.2, Ea=(91920,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(4e+07,'m^3/(mol*s)'), n=0, w0=(173,'kJ/mol'), E0=
(88.2769,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_4R!H->O',), comment="""Estimated from node Root_N-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_4R!H->O""")

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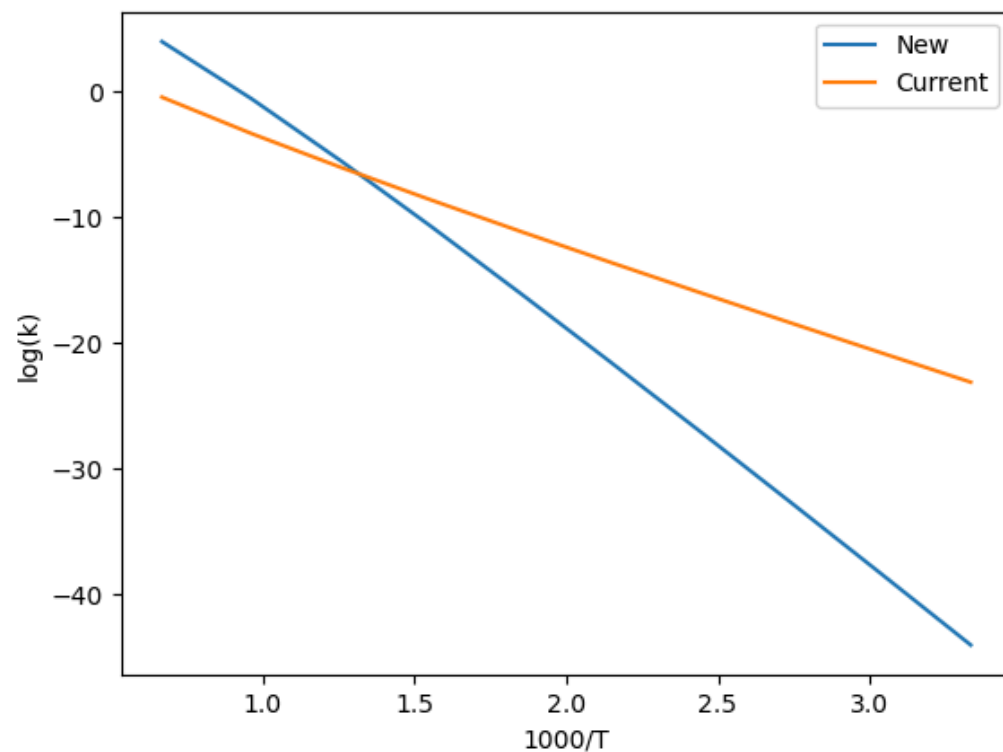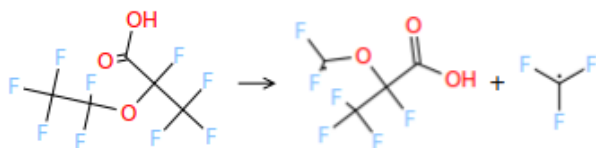**Note: Training reaction written in opposite direction from reaction family.**

New Kinetics:
Arrhenius(A=(3.11e+47,'s^-1'), n=-9.41, Ea=(93640,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
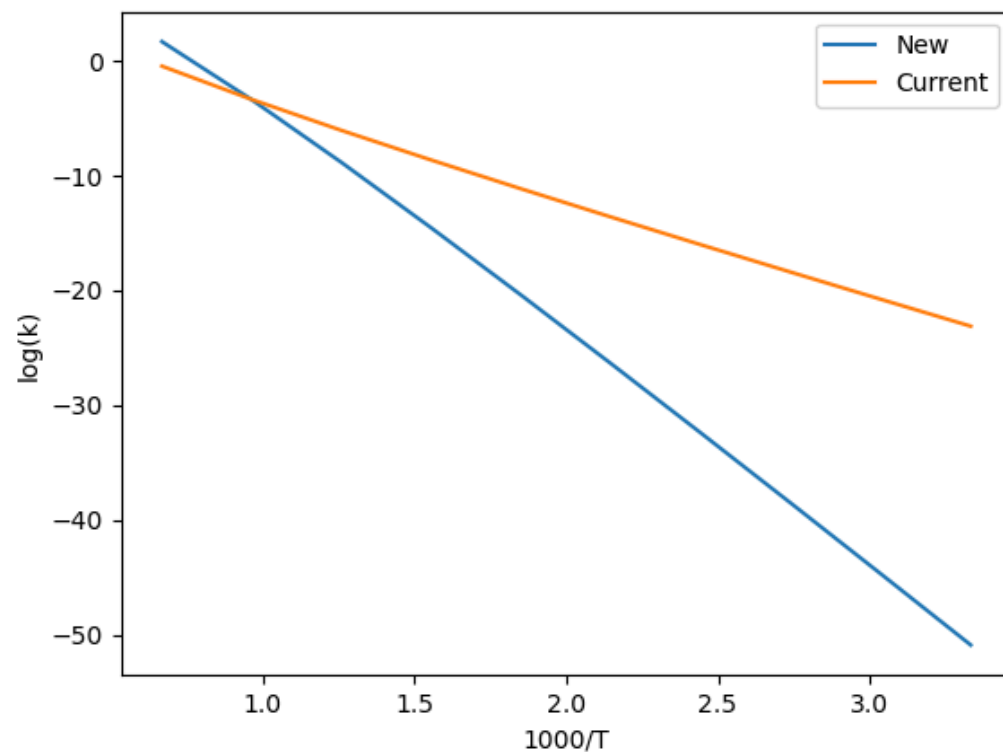>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
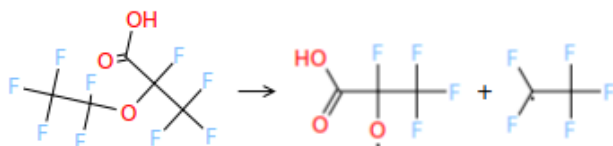
New Kinetics:
Arrhenius(A=(3.4e+46,'s^-1'), n=-9.46, Ea=(101600,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
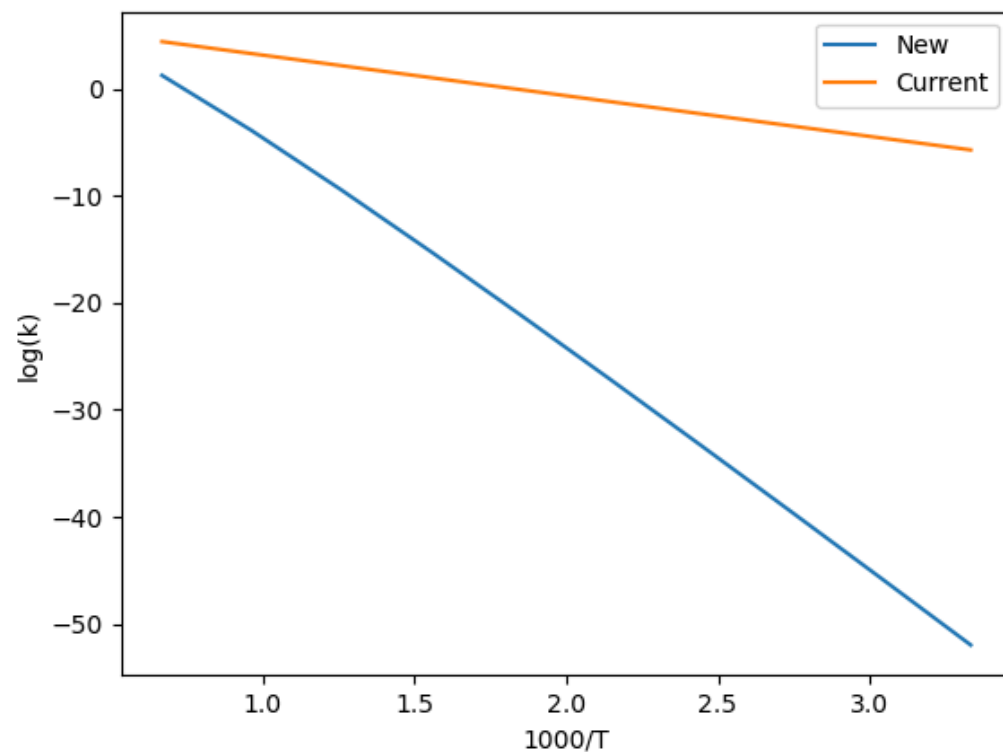>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
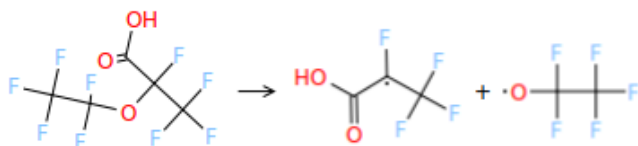
New Kinetics:
Arrhenius(A=(1.29e+45,'s^-1'), n=-9.11, Ea=(102300,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(9.04e+06,'m^3/(mol*s)'), n=2.17087e-08, w0=
(179,'kJ/mol'), E0=(72.7054,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-
3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
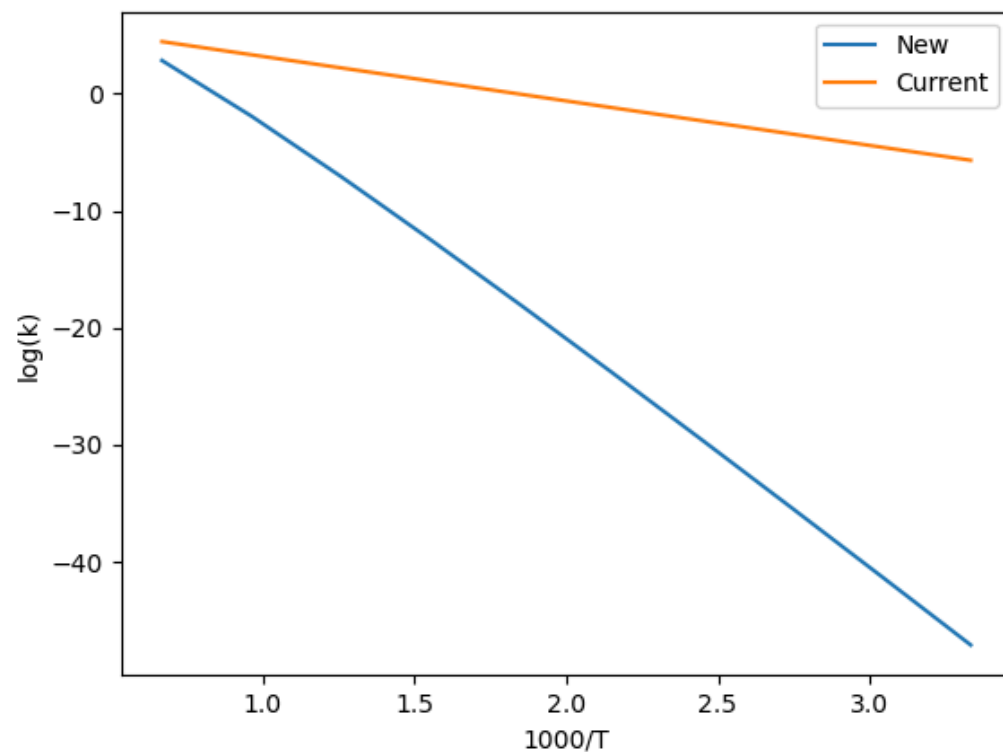R_2R->C_Ext-2C-R_Ext-2C-R""")

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Note: Training reaction written in opposite direction from reaction family.
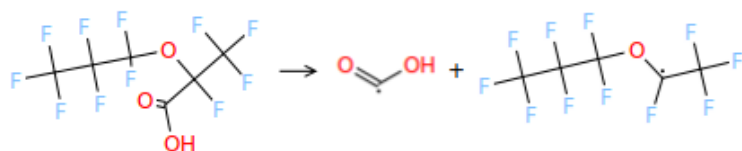
New Kinetics:
Arrhenius(A=(8.28e+46,'s^-1'), n=-9.44, Ea=(96930,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(9.04e+06,'m^3/(mol*s)'), n=2.17087e-08, w0=
(179,'kJ/mol'), E0=(72.7054,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-
3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
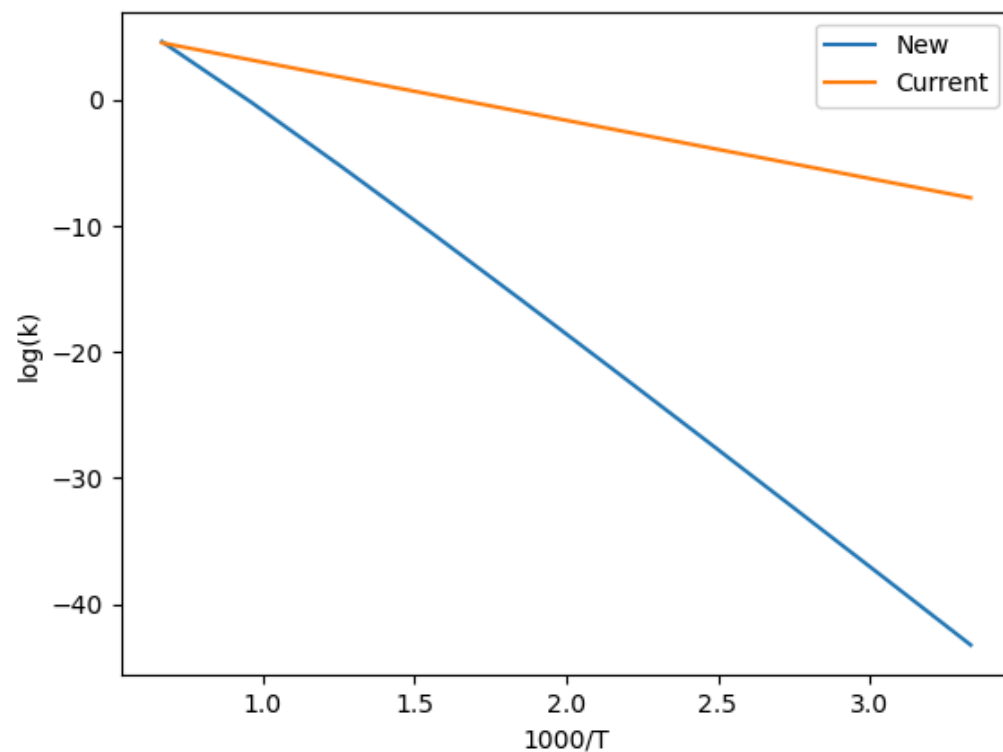R_2R->C_Ext-2C-R_Ext-2C-R""")

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Note: Training reaction written in opposite direction from reaction family.
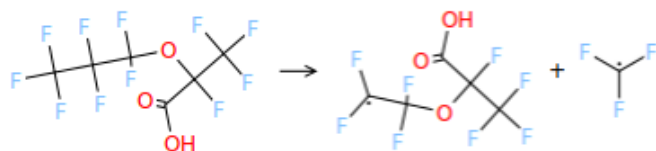
New Kinetics:
Arrhenius(A=(1.27e+36,'s^-1'), n=-5.82, Ea=(89150,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(4e+07,'m^3/(mol*s)'), n=0, w0=(173,'kJ/mol'), E0=
(88.2769,'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-1R->H_N-
1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_4R!H->O',), comment="""Estimated from node Root_N-1R->H_N-
1BrCCIFINOPSSi->N_N-1BrCCIFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
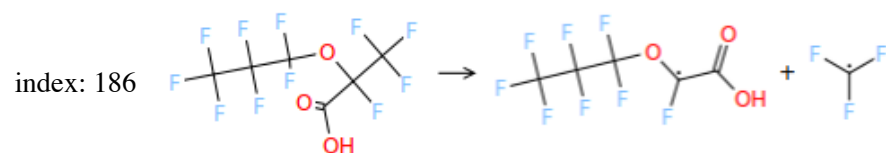inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_4R!H->O""")

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

New Kinetics:
Arrhenius(A=(2.9e+37,'s^-1'), n=-6.48, Ea=(97680,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
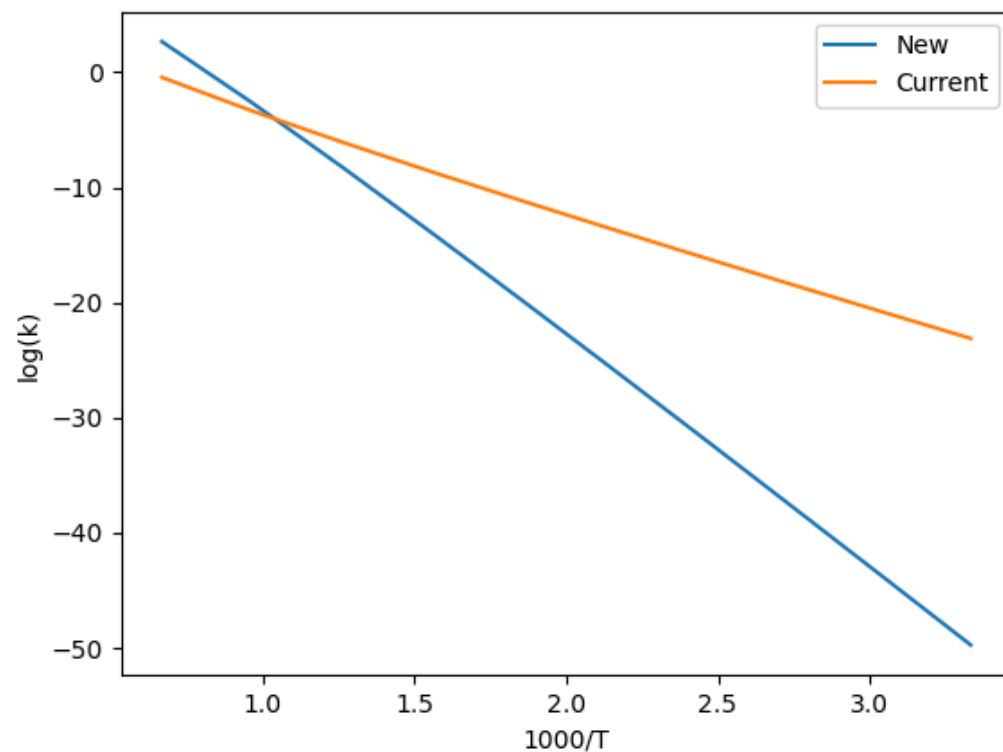1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
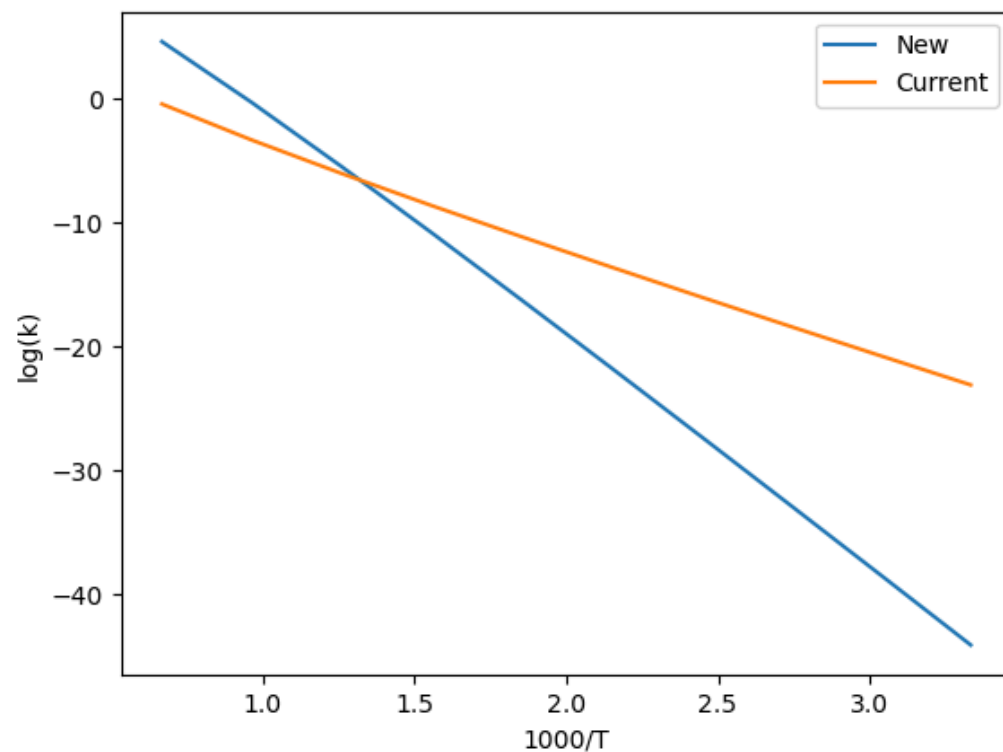>F_Ext-2CF-R_Ext-4R!H-R""")

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

New Kinetics:
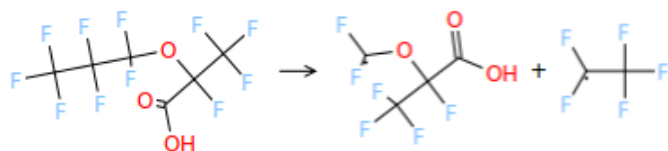Arrhenius(A=(8.48e+36,'s^-1'), n=-6.02, Ea=(90780,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
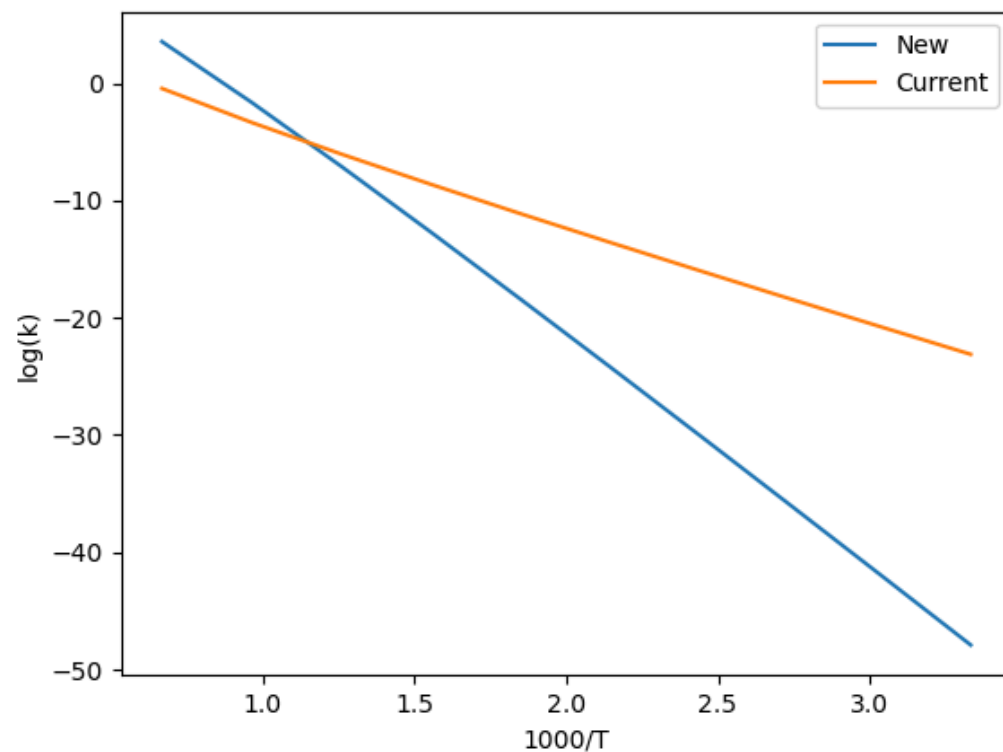>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
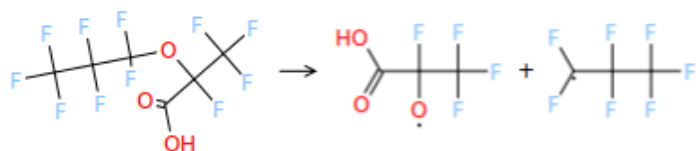
New Kinetics:
Arrhenius(A=(6.52e+37,'s^-1'), n=-6.39, Ea=(95950,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(2.63131e-11,'m^3/(mol*s)'), n=4.71246, w0=
(173,'kJ/mol'), E0=(139.101,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-1BrCFS-
inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H->F_Ext-
2CF-R_Ext-4R!H-R',), comment="""Estimated from node Root_N-1R-
>H_N-1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_N-1BrCFOS->O_N-
1BrCFS-inRing_1BrCFS->C_N-2R->S_N-2BrCF->Br_Ext-1C-R_3R!H-
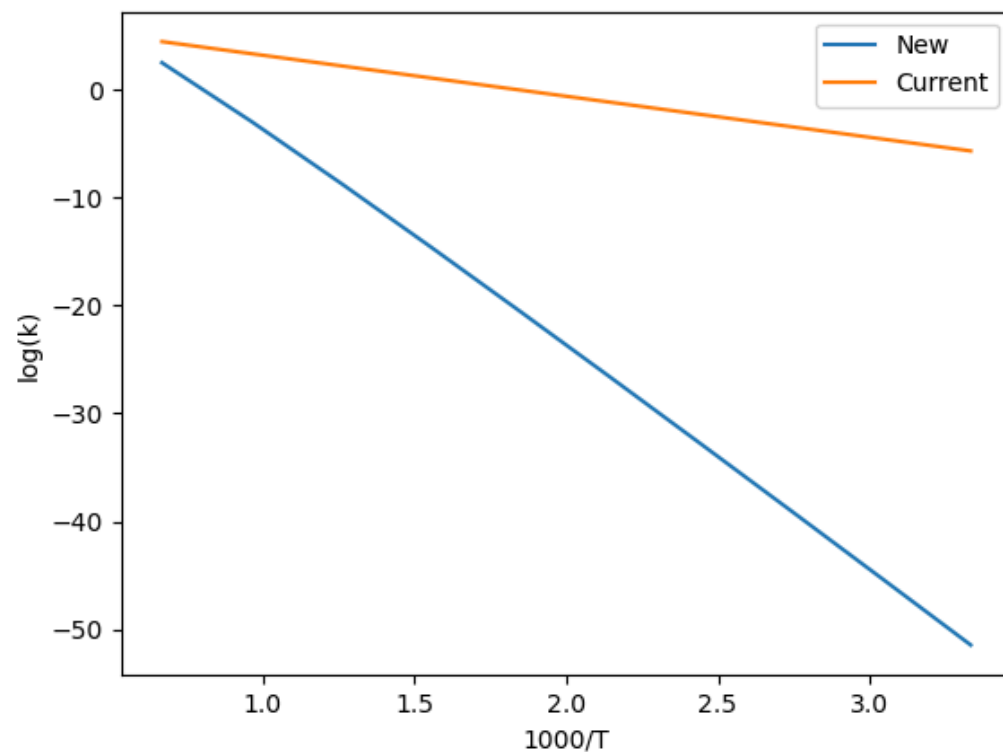>F_Ext-2CF-R_Ext-4R!H-R""")

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Note: Training reaction written in opposite direction from reaction family.
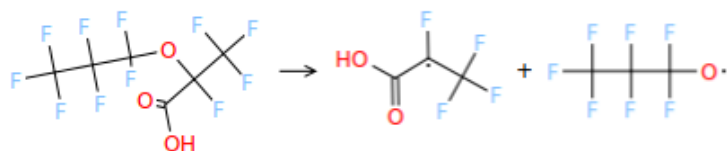
New Kinetics:
Arrhenius(A=(2.32e+37,'s^-1'), n=-6.39, Ea=(100200,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusBM(A=(9.04e+06,'m^3/(mol*s)'), n=2.17087e-08, w0=
(179,'kJ/mol'), E0=(72.7054,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-
3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
R_2R->C_Ext-2C-R_Ext-2C-R""")

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

New Kinetics:

Arrhenius(A=(3.7e+36,'s^-1'), n=-6.09, Ea=(94240,'cal/mol'), T0=(1,'K'))

Current Kinetics

ArrheniusBM(A=(9.04e+06,'m^3/(mol*s)'), n=2.17087e-08, w0=
(179,'kJ/mol'), E0=(72.7054,'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-1R->H_N-
1BrCClFINOPSSi->N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-
3R!H->O_Ext-2R-R_2R->C_Ext-2C-R_Ext-2C-R',),
comment="""Estimated from node Root_N-1R->H_N-1BrCClFINOPSSi-
>N_N-1BrCClFOS->Cl_1BrCFOS->O_Ext-1O-R_N-3R!H->O_Ext-2R-
R_2R->C_Ext-2C-R_Ext-2C-R""")