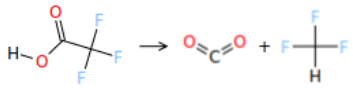
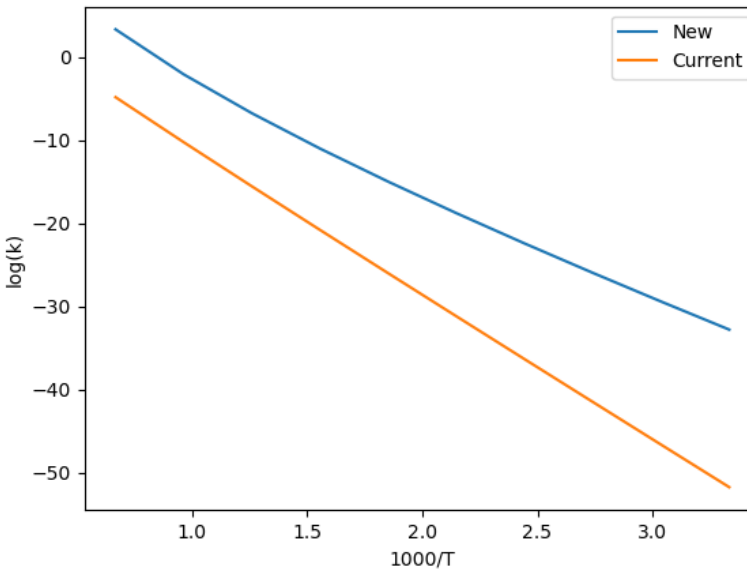
9 reactions matched to 1,3_Insertion_CO2

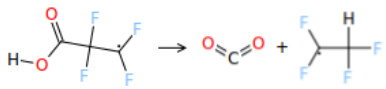
index: 44 

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

New Kinetics:
Arrhenius(A=(1.19e-45,'s^-1'), n=17.11, Ea=(41536.3,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusEP(A=(0.0347248,'m^3/(mol*s)'), n=2.50667, alpha=0, E0=(324.678,'kJ/mol'), comment="""Average of [From training reaction 2 used for CO2_Cdd;C_methane + Average of [From training reaction 3 used for CO2_Cdd;C_pri/NonDeC] + Average of [From training reaction 4 used for CO2_Cdd;C/H2/NonDeC]] Estimated using template [CO2_Cdd;Cs_H] for rate rule [CO2_Cdd;C_ter] Euclidian distance = 1.0 Multiplied by reaction path degeneracy 2.0 family: 1,3_Insertion_CO2""")

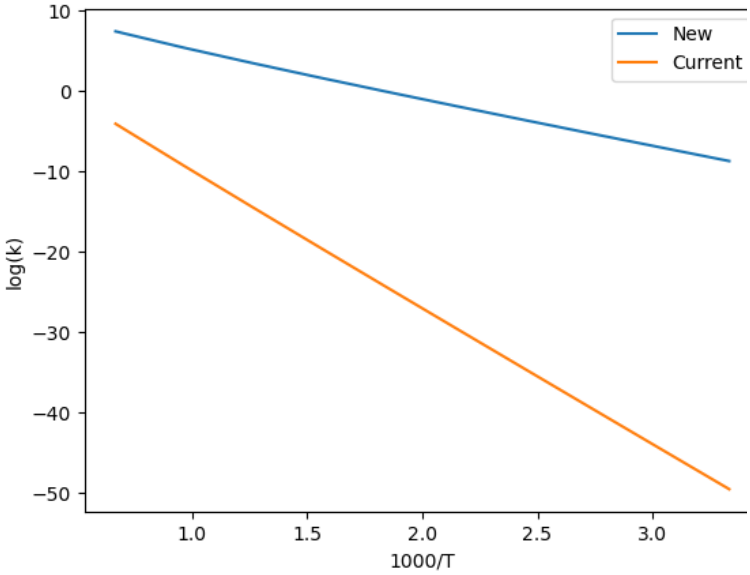


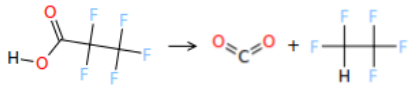
index: 96 

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

New Kinetics:
Arrhenius(A=(66.3,'s^-1'), n=2.87, Ea=(24236.8,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusEP(A=(10.2406,'m^3/(mol*s)'), n=1.86833, alpha=0, E0=(316.938,'kJ/mol'), comment="""Average of [From training reaction 1 used for CO2_Cdd;H2 + Average of [From training reaction 2 used for CO2_Cdd;C_methane + Average of [From training reaction 3 used for CO2_Cdd;C_pri/NonDeC] + Average of [From training reaction 4 used for CO2_Cdd;C/H2/NonDeC]]] Estimated using an average for rate rule [CO2_Cdd;R_H] Euclidian distance = 0 Multiplied by reaction path degeneracy 2.0 family: 1,3_Insertion_CO2""")



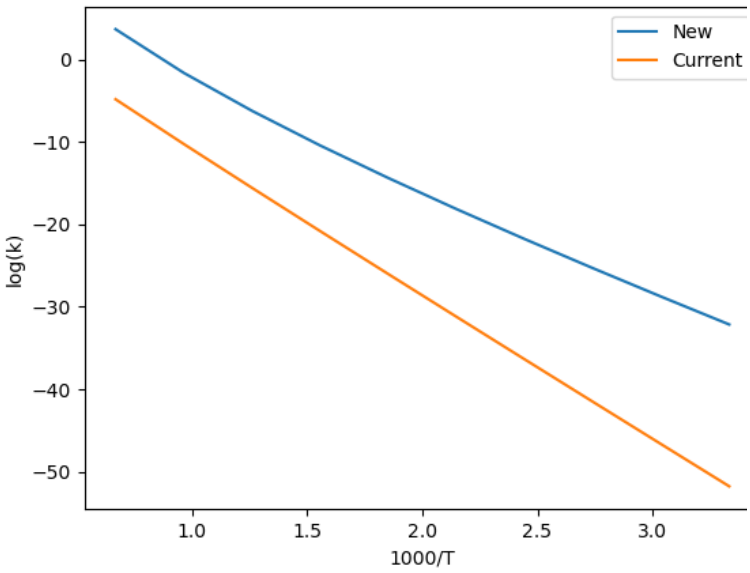
index: 100 

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

New Kinetics:
Arrhenius(A=(9.54e-42,'s^-1'), n=16.02, Ea=

(42280.7,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusEP(A=(0.0347248,'m^3/(mol*s)'), n=2.50667, alpha=0, E0=(324.678,'kJ/mol'), comment="""Average of [From training reaction 2 used for CO2_Cdd;C_methane + Average of [From training reaction 3 used for CO2_Cdd;C_pri/NonDeC] + Average of [From training reaction 4 used for CO2_Cdd;C/H2/NonDeC]] Estimated using template [CO2_Cdd;Cs_H] for rate rule [CO2_Cdd;C_ter] Euclidian distance = 1.0 Multiplied by reaction path degeneracy 2.0 family: 1,3_Insertion_CO2""")



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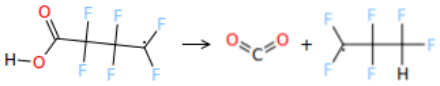
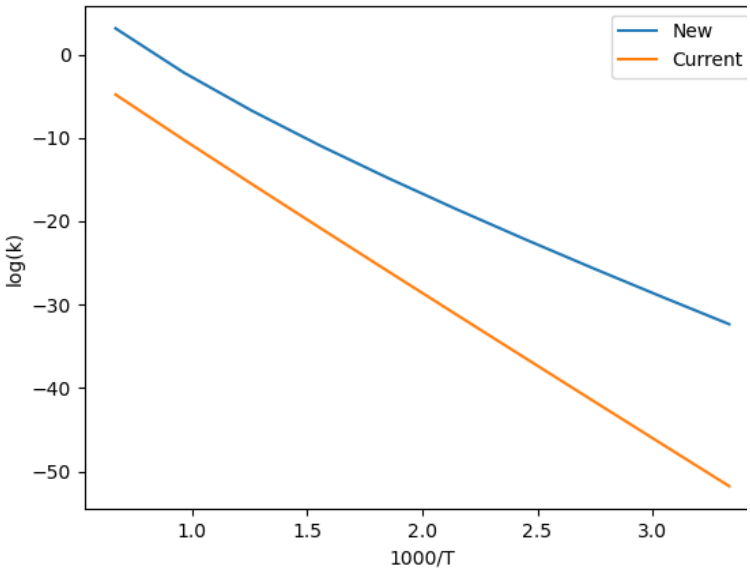


Note: Training reaction written in opposite direction from reaction family.

New Kinetics:
Arrhenius(A=(4.44e-44,'s^-1'), n=16.52, Ea=(41072.8,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusEP(A=(0.0347248,'m^3/(mol*s)'), n=2.50667, alpha=0, E0=(324.678,'kJ/mol'), comment="""Average of [From training reaction 2 used for CO2_Cdd;C_methane + Average of [From training reaction 3 used for CO2_Cdd;C_pri/NonDeC] + Average of [From training reaction 4 used for CO2_Cdd;C/H2/NonDeC]] Estimated using template [CO2_Cdd;Cs_H] for rate rule [CO2_Cdd;C_ter] Euclidian distance = 1.0 Multiplied by reaction path degeneracy 2.0 family: 1,3_Insertion_CO2""")



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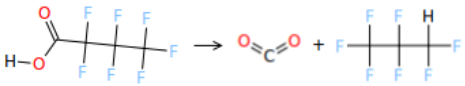
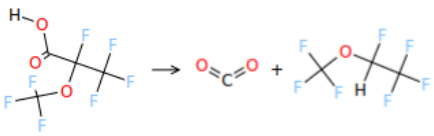


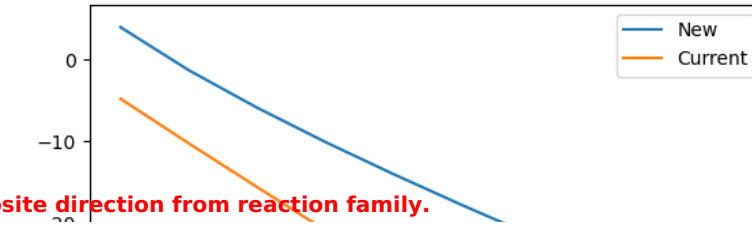
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:
Arrhenius(A=(2.18e-40,'s^-1'), n=15.66, Ea=(42257.3,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusEP(A=(0.0347248,'m^3/(mol*s)'), n=2.50667, alpha=0, E0=(324.678,'kJ/mol'), comment="""Average of [From training reaction 2 used for CO2_Cdd;C_methane + Average of [From training reaction 3 used for CO2_Cdd;C_pri/NonDeC] + Average of [From training reaction 4 used for CO2_Cdd;C/H2/NonDeC]] Estimated using template [CO2_Cdd;Cs_H] for rate rule [CO2_Cdd;C_ter] Euclidian distance = 1.0 Multiplied by reaction path degeneracy 2.0 family: 1,3_Insertion_CO2""")

index:
180

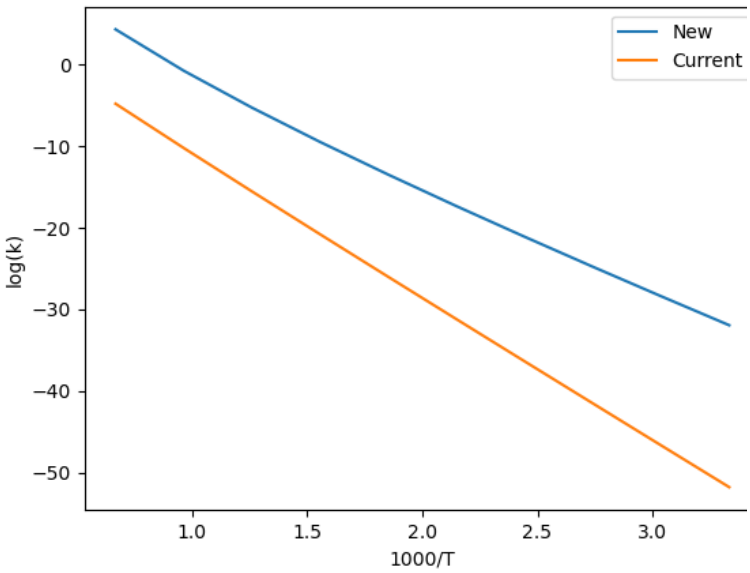




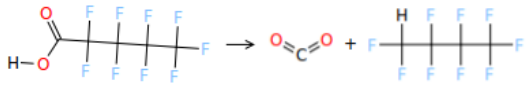
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:
Arrhenius(A=(6.99e-30,'s^-1'), n=12.69, Ea=
(46973.6,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusEP(A=(0.0347248,'m^3/(mol*s)'), n=2.50667,
alpha=0, E0=(324.678,'kJ/mol'), comment="""Average of
[From training reaction 2 used for CO2_Cdd;C_methane +
Average of [From training reaction 3 used for
CO2_Cdd;C_pri/NonDeC] + Average of [From training
reaction 4 used for CO2_Cdd;C/H2/NonDeC]] Estimated
using template [CO2_Cdd;Cs_H] for rate rule
[CO2_Cdd;C_ter] Euclidian distance = 1.0 Multiplied by
reaction path degeneracy 2.0 family:
1,3_Insertion_CO2""")



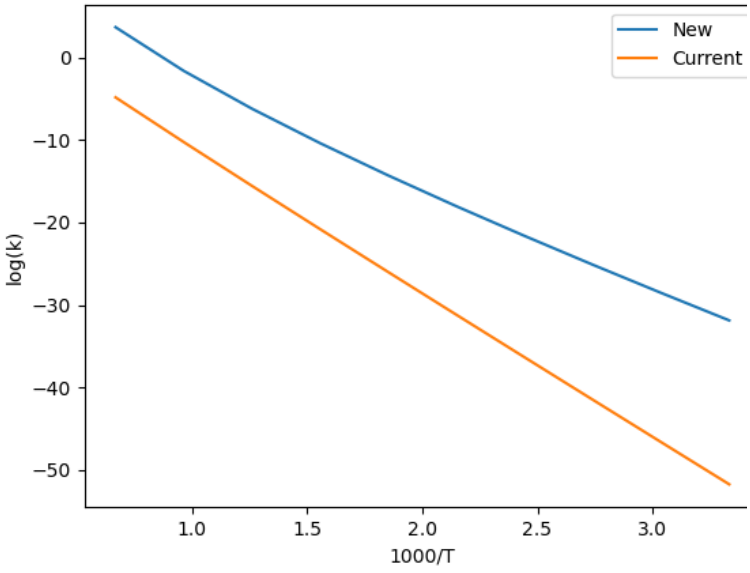
index:
206



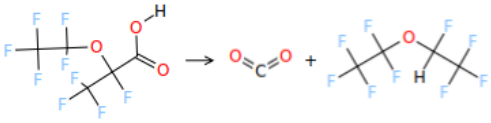
Note: Training reaction written in opposite direction from reaction family.

New Kinetics:
Arrhenius(A=(4.93e-43,'s^-1'), n=16.39, Ea=
(41420.4,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusEP(A=(0.0347248,'m^3/(mol*s)'), n=2.50667,
alpha=0, E0=(324.678,'kJ/mol'), comment="""Average of
[From training reaction 2 used for CO2_Cdd;C_methane +
Average of [From training reaction 3 used for
CO2_Cdd;C_pri/NonDeC] + Average of [From training
reaction 4 used for CO2_Cdd;C/H2/NonDeC]] Estimated
using template [CO2_Cdd;Cs_H] for rate rule
[CO2_Cdd;C_ter] Euclidian distance = 1.0 Multiplied by
reaction path degeneracy 2.0 family:
1,3_Insertion_CO2""")



index:
224

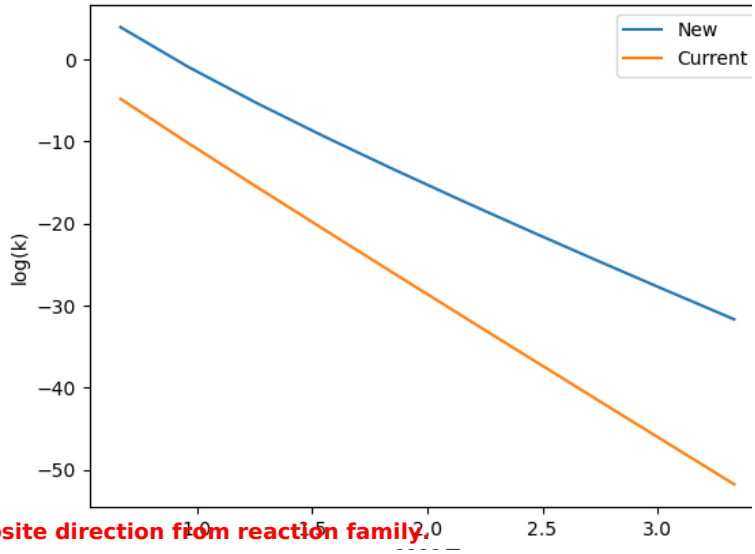


Note: Training reaction written in opposite direction from reaction family.

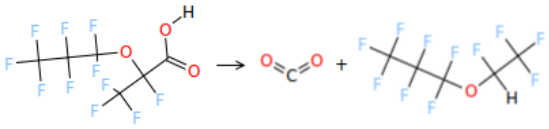
New Kinetics:
Arrhenius(A=(3.77e-25,'s^-1'), n=11.12, Ea=

(47765.6,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusEP(A=(0.0347248,'m^3/(mol*s)'), n=2.50667, alpha=0, E0=(324.678,'kJ/mol'), comment="""Average of [From training reaction 2 used for CO2_Cdd;C_methane + Average of [From training reaction 3 used for CO2_Cdd;C_pri/NonDeC] + Average of [From training reaction 4 used for CO2_Cdd;C/H2/NonDeC]] Estimated using template [CO2_Cdd;Cs_H] for rate rule [CO2_Cdd;C_ter] Euclidian distance = 1.0 Multiplied by reaction path degeneracy 2.0 family: 1,3_Insertion_CO2""")



index:
236



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

New Kinetics:
Arrhenius(A=(1.14e-22,'s^-1'), n=10.39, Ea=(48295.9,'cal/mol'), T0=(1,'K'))

Current Kinetics
ArrheniusEP(A=(0.0347248,'m^3/(mol*s)'), n=2.50667, alpha=0, E0=(324.678,'kJ/mol'), comment="""Average of [From training reaction 2 used for CO2_Cdd;C_methane + Average of [From training reaction 3 used for CO2_Cdd;C_pri/NonDeC] + Average of [From training reaction 4 used for CO2_Cdd;C/H2/NonDeC]] Estimated using template [CO2_Cdd;Cs_H] for rate rule [CO2_Cdd;C_ter] Euclidian distance = 1.0 Multiplied by reaction path degeneracy 2.0 family: 1,3_Insertion_CO2""")