RMG-Py Reaction Families

1+2_Cycloaddition

1,2-Birad_to_alkene

$$^{1}\text{R}^{\cdot}$$
 $^{2}\text{R}^{\cdot}$ ^{1}R ^{2}R

1,2_Insertion_CO

1,2_Insertion_carbene

1,2_NH3_elimination

1,2_shiftC

1,2_shiftS

$$1c_{-2}s_{-3}$$
 $2s_{-3}$ $3R_{-1}c_{-3}$

1,3_Insertion_CO2

1,3_Insertion_ROR

$$^{3}R-^{4}O-R + ^{1}R=^{2}R = ^{3}R-^{1}R-^{2}R-^{4}O-R$$

1,3_Insertion_RSR

$$^{3}R$$
 $-^{4}S$ $-^{R}$ + ^{1}R $=^{2}R$ ^{3}R $-^{1}R$ $-^{2}R$ $-^{4}S$ $-^{R}$

1,3_NH3_elimination

1,4_Cyclic_birad_scission

$$^{2}R$$
 ^{-1}R ^{4}R ^{-3}R ^{2}R ^{-1}R ^{4}R ^{-3}R

1,4_Linear_birad_scission

$${}^{1}R - {}^{2}R - {}^{3}R - {}^{4}R$$
 \longrightarrow ${}^{1}R = {}^{2}R + {}^{3}R = {}^{4}R$

2+2_cycloaddition_CCO

2+2_cycloaddition_CO

2+2_cycloaddition_CS

2+2_cycloaddition_Cd

6_membered_central_C-C_shift

Baeyer-Villiger_step1_cat

Baeyer-Villiger_step2

$${}^{2}[C,H]$$
 ${}^{5}O$
 ${}^{6}O$
 ${}^{7}C$
 R
 ${}^{1}C$
 ${}^{2}[C,H]$
 ${}^{3}O$
 ${}^{2}[C,H]$
 ${}^{4}H$
 ${}^{8}O$

Baeyer-Villiger_step2_cat

$${}^{2}[C,H]$$
 ${}^{5}O$
 ${}^{6}O$
 ${}^{10}H$
 ${}^{9}O$
 ${}^{7}C$
 R
 ${}^{1}C$
 ${}^{1}C$

Bimolec_Hydroperoxide_Decomposition

$$R - \frac{10}{10} - \frac{20}{10} + R - \frac{40}{10} - \frac{3}{10} + R - \frac{20}{10} + \frac{20}$$

Birad_R_Recombination

$${}^{1}R^{'} + {}^{2}R : \longrightarrow {}^{1}R - {}^{2}R^{'}$$

Birad_recombination

${\tt CO_Disproportionation}$

$$^{1}R + ^{2}O = ^{3}C - ^{4}H = ^{1}R - ^{4}H + ^{2}O = ^{3}C$$

Concerted_Intra_Diels_alder_monocyclic_1,2_shiftH

$${}^{1}C = {}^{2}C - {}^{3}C = {}^{4}C - {}^{5}C = {}^{6}C - {}^{7}H$$

${\tt Cyclic_Ether_Formation}$

1
R 2 O $^{-3}$ OR \longrightarrow 1 R 2 O + 3 OF.

Cyclic_Thioether_Formation

 ${\tt Cyclopentadiene_scission}$

Diels_alder_addition

Disproportionation

$${}^{1}R + {}^{3}R - {}^{2}R - {}^{4}H \longrightarrow {}^{1}R - {}^{4}H + {}^{3}R = {}^{2}R$$

HO2_Elimination_from_PeroxyRadical

$$^{5}H$$
— ^{1}R — ^{2}R — ^{3}O — ^{4}O — ^{5}H + ^{1}R = ^{2}R

H_Abstraction

$$^{1}R$$
 ^{-2}H + ^{3}R \longrightarrow ^{1}R + ^{2}H ^{-3}R

Intra_2+2_cycloaddition_Cd

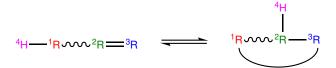
 ${\tt Intra_5_membered_conjugated_C=C_C=C_addition}$

Intra_Diels_alder_monocyclic

Intra_Disproportionation

$$^{1}R^{4}H^{-2}R^{-4}H$$
 $^{4}H^{-1}R^{3}R^{-2}R$

Intra_RH_Add_Endocyclic



Intra_RH_Add_Exocyclic

$$^{4}H$$
— ^{1}R ^{2}R = ^{3}R
 ^{1}R ^{2}R - ^{3}R - ^{4}H

${\tt Intra_R_Add_Endocyclic}$

$$^{1}\dot{R}$$
 ^{2}R ^{3}R ^{1}R ^{3}R

Intra_R_Add_ExoTetCyclic

1
R 2 R $^{-3}$ R $^{-3}$ R $^{-3}$ R $^{-1}$ R $^{-3}$

Intra_R_Add_Exo_scission

Intra_R_Add_Exocyclic

$$\frac{1}{R}$$
 $\frac{1}{R}$ $\frac{1}{R}$ $\frac{1}{R}$ $\frac{3}{R}$

Intra_Retro_Diels_alder_bicyclic

Intra_ene_reaction

Korcek_step1

Korcek_step1_cat

$Korcek_step2$

Peroxyl_Disproportionation

$$R - {}^{1}O - {}^{2}O \cdot + R - {}^{3}O - {}^{4}O \cdot \longrightarrow R - {}^{1}O \cdot + R - {}^{3}O \cdot + {}^{2}O - {}^{4}O$$

Peroxyl_Termination

$$^{4}H$$
 ^{-1}R ^{-2}O ^{-3}O $^{+}$ R ^{-5}O ^{-6}O ^{-6}O ^{-6}O ^{-6}O

R_Addition_COm

R_Addition_CSm

$${}^{3}S_{1C} = {}^{3}S^{+} + {}^{2}R = {}^{2}R = {}^{1}C^{-}$$

$R_Addition_MultipleBond$

$$^{2}R$$
 = ^{1}R + ^{3}R = ^{2}R - ^{1}R - ^{3}R

R_Recombination

$$^{1}R$$
 + ^{2}R \longrightarrow ^{1}R $-^{2}R$

${\tt Singlet_Carbene_Intra_Disproportionation}$

$$\bigcirc ^{1}C$$
 $\bigcirc ^{2}C$ $\bigcirc ^{3}H$ $\bigcirc ^{3}H$ $\bigcirc ^{1}C$ $\bigcirc ^{2}C$

Singlet_Val6_to_triplet

$$^{1}(O/S) = ^{2}(O/S)$$
 $^{1}(O/S) - ^{2}(O/S)$

SubstitutionS

$$R - {}^{1}S - {}^{2}R + {}^{3}R^{.} = R - {}^{1}S - {}^{3}R + {}^{2}R^{.}$$

Substitution_O

$$R - {}^{1}O - {}^{2}R + {}^{3}R^{i} \longrightarrow R - {}^{1}O - {}^{3}R + {}^{2}R^{i}$$

Surface_Abstraction

Surface_Adsorption_Bidentate

$$^{1}R = ^{2}R$$
+
 $^{3}X + ^{4}X$
 $^{1}R - ^{2}R$
 $^{3}X + ^{4}X$

Surface_Adsorption_Dissociative

 $Surface_Adsorption_Double$

Surface_Adsorption_Single

 $Surface_Adsorption_vdW$

Surface_Bidentate_Dissociation

Surface_Dissociation

Surface_Dissociation_vdW

Surface_Recombination

intra_H_migration

$$^{3}H$$
 ^{2}R ^{1}R ^{1}R ^{2}R ^{3}H

intra_NO2_ONO_conversion

intra_OH_migration

intra_substitutionCS_cyclization

intra_substitutionCS_isomerization

3
R· 2 S $-^{1}$ C \longrightarrow 1 C $-^{3}$ R· 2 S

intra_substitutionS_cyclization

intra_substitutionS_isomerization

ketoenol

$${}^{1}R = {}^{2}R - {}^{2}O - {}^{4}R$$
 \longrightarrow ${}^{4}R - {}^{1}R - {}^{2}R = {}^{2}C$

 ${\tt lone_electron_pair_bond}$