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_XY_interchange

1,2_shiftC



1,2_shiftS

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

1,3_Insertion_CO2

1,3_Insertion_ROR

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

1,3_Insertion_RSR

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

1,3_NH3_elimination

$$^{4}H$$
 1
 ^{3}R
 ^{2}R
 $^{1}NH_{2}$
 ^{3}R
 ^{2}R
 ^{2}R
 ^{4}H
 0
 0
 0
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 1
 $^$

1,4_Cyclic_birad_scission

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

1,4_Linear_birad_scission

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

2+2_cycloaddition

Image Not Available

6_membered_central_C-C_shift

Baeyer-Villiger_step1_cat

$$[C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - O - 3O - 4H + R - 5C \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 5C - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H \end{bmatrix} + R - 8H \\ [C,H] = \begin{bmatrix} C,H$$

Baeyer-Villiger_step2

$${}^{2}[C,H] \xrightarrow{50} {}^{6}O \xrightarrow{7} {}^{7}C \xrightarrow{R} \qquad {}^{6}O \xrightarrow{1} \qquad {}^{7}C \xrightarrow{R} \qquad {}^{7}C \xrightarrow{$$

Baeyer-Villiger_step2_cat

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

${\tt Bimolec_Hydroperoxide_Decomposition}$

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

${\tt Birad_R_Recombination}$

Birad_recombination

Br_Abstraction

$$^{1}R$$
— ^{2}Br + ^{3}R ————— ^{1}R + ^{2}Br — ^{3}R

CO_Disproportionation

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

Cl_Abstraction

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

Concerted_Intra_Diels_alder_monocyclic_1,2_shiftH

 ${\tt Cyclic_Ether_Formation}$

Cyclic_Thioether_Formation

 ${\tt Cyclopentadiene_scission}$

Diels_alder_addition

Disproportionation

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

Disproportionation-Y

$${}^{1}R$$
 + ${}^{3}R$ $-{}^{2}R$ $-{}^{4}Y$ + ${}^{3}R$ $={}^{2}R$
 $Y = F. Cl. Br$

F_Abstraction

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

Intra_2+2_cycloaddition_Cd

Intra_5_membered_conjugated_C=C_C=C_addition

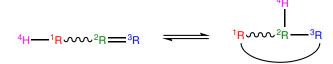
Intra_Diels_alder_monocyclic

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

 ${\tt Intra_Disproportionation}$

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

Intra_RH_Add_Endocyclic



Intra_RH_Add_Exocyclic



Intra_R_Add_Endocyclic

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

Intra_R_Add_ExoTetCyclic

Intra_R_Add_Exo_scission

Intra_R_Add_Exocyclic

Intra_Retro_Diels_alder_bicyclic

Intra_ene_reaction

Korcek_step1

Korcek_step1_cat

Korcek_step2

50
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10
 10

Peroxyl_Disproportionation

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

${\tt Peroxyl_Termination}$

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

R_Addition_COm

R_Addition_CSm

$$\frac{^{3}S}{10^{-3}S^{+}} + ^{2}R^{-1}C$$

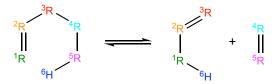
$R_Addition_MultipleBond$

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

R_{-} Recombination

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

Retroene



${\tt Singlet_Carbene_Intra_Disproportionation}$

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

Singlet_Val6_to_triplet

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

SubstitutionS

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

Substitution_O

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

Surface_Abstraction

Surface_Abstraction_Single_vdW

Surface_Abstraction_vdW

Surface_Addition_Single_vdW

$$^{2}R$$
 $\stackrel{}{=}$ ^{3}R ^{4}R ^{2}R ^{3}R ^{4}R ^{5}X ^{5}X

Surface_Adsorption_Abstraction_vdW

 $Surface_Adsorption_Bidentate$

Surface_Adsorption_Dissociative

 ${\tt Surface_Adsorption_Dissociative_Double}$

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

Surface_Adsorption_Double

Surface_Adsorption_Single

Surface_Adsorption_vdW

Surface_Bidentate_Dissociation

Surface_Dissociation

Surface_Dissociation_Beta

$$^{2}R$$
 ^{3}R ^{4}R ^{2}R ^{3}R ^{4}R ^{1}X ^{5}X ^{1}X ^{5}X

Surface_Dissociation_Double_vdW

$${\overset{2}{+}} {\overset{3}{+}} {\overset{1}{\times}} {\overset{4}{\times}} {\overset{4}{\times}} {\overset{2}{+}} {\overset{2}{+}} {\overset{3}{+}} {\overset{3$$

Surface_Dissociation_vdW

Surface_DoubleBond_to_Bidentate

Image Not Available

Surface_Dual_Adsorption_vdW

$${}^{2}R = {}^{3}R \qquad {}^{4}R = {}^{6}R \qquad = \qquad {}^{2}R = {}^{3}R = {}^{4}R \qquad + \qquad {}^{6}R \qquad \qquad {}^{1}X \qquad + \qquad {}^{6}R \qquad \qquad {}^{5}X$$

 ${\tt Surface_EleyRideal_Addition_Multiple_Bond}$

Surface_Migration

$$\begin{array}{c|cccc}
^{4}R & & ^{4}R \\
 & & & \\
^{2}R \longrightarrow ^{3}R & & & \\
 & & & \\
 & & & \\
^{1}X & & ^{1}X
\end{array}$$

Surface_vdW_to_Bidentate

Image Not Available

XY_Addition_MultipleBond

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

$$X = H, F, Cl, Br$$

$$Y = F, Cl, Br$$

halocarbene_recombination

$${}^{1}R + R^{-2}C-Y \xrightarrow{\qquad \qquad \qquad } {}^{1}C - {}^{1}R$$

$$Y = F, Cl, Br, I \qquad Y$$

halocarbene_recombination_double

intra H_migration

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

 $intra_NO2_ONO_conversion$

intra_OH_migration

 $intra_substitution CS_cyclization$

intra_substitutionCS_isomerization

intra_substitutionS_cyclization

intra_substitutionS_isomerization

ketoenol

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

lone_electron_pair_bond