# RMG-Py Reaction Families

# 1+2\_Cycloaddition

# 1,2-Birad\_to\_alkene

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

## 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

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

## 1,3\_Insertion\_RSR

$$^{3}R$$
  $-^{4}S$   $-^{8}R$  +  $^{1}R$   $=^{2}R$   $^{3}R$   $-^{1}R$   $-^{2}R$   $-^{4}S$   $-^{8}R$ 

### 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

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

## 2+2\_cycloaddition

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## 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

## $CO\_Disproportionation$

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

Concerted\_Intra\_Diels\_alder\_monocyclic\_1,2\_shiftH

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

## Cyclic\_Ether\_Formation

# Cyclic\_Thioether\_Formation

# ${\tt Cyclopentadiene\_scission}$

### Diels\_alder\_addition

# ${\tt Disproportionation}$

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

## HO2\_Elimination\_from\_PeroxyRadical

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

### H\_Abstraction

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

## Intra\_2+2\_cycloaddition\_Cd

## Intra\_5\_membered\_conjugated\_C=C\_C=C\_addition

# Intra\_Diels\_alder\_monocyclic

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

# Intra\_Disproportionation

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

# Intra\_RH\_Add\_Endocyclic

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

# Intra\_RH\_Add\_Exocyclic

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

## Intra\_R\_Add\_Endocyclic

# Intra\_R\_Add\_ExoTetCyclic

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

## Intra\_R\_Add\_Exo\_scission

$$^{1}$$
C $-^{3}$ C $-^{2}$ Cb  $\longrightarrow$   $^{3}$ C $-^{1}$ C $-^{2}$ Cb

# Intra\_R\_Add\_Exocyclic

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

# Intra\_Retro\_Diels\_alder\_bicyclic

## Intra\_ene\_reaction

# Korcek\_step1

## Korcek\_step1\_cat

# Korcek\_step2

$$^{2}$$
C  $^{3}$ C  $^{4}$ OH  $^{5}$ C  $^{2}$ C  $^{6}$ H  $^{4}$ C  $^{3}$ C  $^{6}$ H  $^{2}$ C  $^{6}$ H  $^{4}$ C  $^{3}$ C  $^{6}$ H  $^{4}$ C  $^{3}$ C  $^{6}$ H  $^{4}$ C  $^{6}$ H  $^{3}$ C  $^{6}$ H  $^{4}$ C  $^{6}$ H  $^{3}$ C  $^{6}$ H  $^{4}$ C  $^{6}$ H  $^{4}$ C  $^{6}$ H  $^{6}$ C  $^{6$ 

# 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

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

### R\_Addition\_COm

### R\_Addition\_CSm

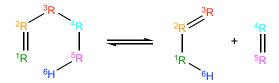
# $R\_Addition\_MultipleBond$

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

### R\_Recombination

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

#### Retroene



## Singlet\_Carbene\_Intra\_Disproportionation

## Singlet\_Val6\_to\_triplet

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

#### SubstitutionS

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

### Substitution\_O

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

### Surface\_Abstraction

### Surface\_Abstraction\_Beta

## Surface\_Abstraction\_Beta\_double\_vdW

$${}^{1}R - {}^{2}R - {}^{3}R$$
 ${}^{4}R$ 
 ${}^{1}R = {}^{2}R$ 
 ${}^{3}R - {}^{4}R$ 
 ${}^{5}\chi$ 
 ${}^{5}\chi$ 
 ${}^{5}\chi$ 
 ${}^{5}\chi$ 
 ${}^{5}\chi$ 
 ${}^{5}\chi$ 
 ${}^{6}\chi$ 

Surface\_Abstraction\_Single\_vdW

Surface\_Abstraction\_vdW

Surface\_Addition\_Single\_vdW

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

Surface\_Adsorption\_Abstraction\_vdW

 $Surface\_Adsorption\_Bidentate$ 

 ${\tt Surface\_Adsorption\_Dissociative}$ 

 ${\tt Surface\_Adsorption\_Dissociative\_Double}$ 

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

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

$$^{2}R$$
  $\xrightarrow{^{3}R}$   $^{2}R$   $^{2}R$   $^{3}R$   $^{1}X$   $^{4}X$   $^{4}X$   $^{4}X$   $^{1}X$   $^{4}X$ 

Surface\_Dissociation\_vdW

### Surface\_DoubleBond\_to\_Bidentate

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## Surface\_Dual\_Adsorption\_vdW

$$^{2}R$$
  $\xrightarrow{^{3}R}$   $^{4}R$   $\xrightarrow{^{6}R}$   $\xrightarrow{^{2}R}$   $^{3}R$   $\xrightarrow{^{4}R}$   $^{6}R$   $\xrightarrow{^{5}X}$   $\xrightarrow{^{1}X}$   $\xrightarrow{^{5}X}$ 

## Surface\_EleyRideal\_Addition\_Multiple\_Bond

## Surface\_Migration

### Surface\_vdW\_to\_Bidentate

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# $\verb"intra_H_migration"$

### intra\_NO2\_ONO\_conversion

## intra\_OH\_migration

$$^{1}R^{0}$$
  $^{2}O$   $^{3}OH$   $^{3}HO$   $^{1}R^{0}$ 

## $intra\_substitution CS\_cyclization$

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