# 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\_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

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

### 1,3\_NH3\_elimination

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

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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

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

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

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

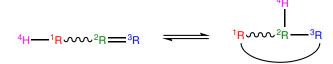
Intra\_Diels\_alder\_monocyclic

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

 ${\tt Intra\_Disproportionation}$ 

$$^{1}$$
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

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# 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

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

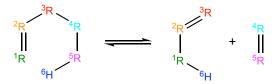
## $R\_Addition\_MultipleBond$

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

#### $R_{-}$ 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

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

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

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

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

Surface\_vdW\_to\_Bidentate

Image Not Available

XY\_Addition\_MultipleBond

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

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

$$Y = F, Cl, Br$$

intra\_H\_migration

intra\_NO2\_ONO\_conversion

intra\_OH\_migration

 $\verb"intra_substitutionCS_cyclization"$ 

intra\_substitutionCS\_isomerization

 $intra\_substitutionS\_cyclization$ 

intra\_substitutionS\_isomerization

ketoenol

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

lone\_electron\_pair\_bond