# 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

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

### 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

$$^{4}H$$
 $\downarrow$ 
 $^{3}R$ 
 $^{2}R$ 
 $^{1}NH_{2}$ 
 $^{3}R$ 
 $^{2}R$ 
 $^{3}R$ 
 $^{2}R$ 
 $^{4}H$ 
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#### 1,3\_sigmatropic\_rearrangement

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

## 1,4\_Cyclic\_birad\_scission

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

### 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

6\_membered\_central\_C-C\_shift

Baeyer-Villiger\_step1\_cat

Baeyer-Villiger\_step2

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

 ${\tt Baeyer-Villiger\_step2\_cat}$ 

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

 ${\tt Bimolec\_Hydroperoxide\_Decomposition}$ 

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

#### Birad\_R\_Recombination

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

Birad\_recombination

Br\_Abstraction

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

 ${\tt CO\_Disproportionation}$ 

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

Cl\_Abstraction

$$^{1}R$$
  $^{-2}CI$  +  $^{3}R$   $\stackrel{}{=}$   $^{1}R$  +  $^{2}CI$   $^{-3}R$ 

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

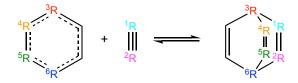
Cyclic\_Ether\_Formation

Cyclic\_Thioether\_Formation

### Cyclopentadiene\_scission

#### Diels\_alder\_addition

### Diels\_alder\_addition\_Aromatic



### Disproportionation

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

## Disproportionation-Y

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

#### F\_Abstraction

#### $H2_Loss$

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### 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

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

## ${\tt Intra\_Disproportionation}$

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

## Intra\_RH\_Add\_Endocyclic

## Intra\_RH\_Add\_Exocyclic

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

## $Intra\_R\_Add\_Endocyclic$

## Intra\_R\_Add\_ExoTetCyclic

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

### Intra\_R\_Add\_Exo\_scission

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

## Intra\_R\_Add\_Exocyclic

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

## Intra\_Retro\_Diels\_alder\_bicyclic

### Intra\_ene\_reaction

### Ketoenol

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

## Korcek\_step1

### Korcek\_step1\_cat

## Korcek\_step2

## Peroxyl\_Disproportionation

$$R_{-10}^{-20} + R_{-30}^{-40} + R_{-30}^{-40} + R_{-30}^{-40} + R_{-30}^{-40}$$

## 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

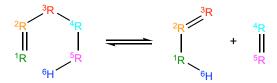
## $R\_Addition\_MultipleBond$

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

#### R\_Recombination

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

#### Retroene



### Singlet\_Carbene\_Intra\_Disproportionation

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

#### Singlet\_Val6\_to\_triplet

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

#### SubstitutionS

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

#### 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

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

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

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

 $Surface\_Adsorption\_Bidentate$ 

 ${\tt Surface\_Adsorption\_Dissociative}$ 

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

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

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

Surface\_Adsorption\_Double

Surface\_Adsorption\_Single

 ${\tt Surface\_Adsorption\_vdW}$ 

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

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

## ${\tt Surface\_EleyRideal\_Addition\_Multiple\_Bond}$

### Surface\_Migration

#### Surface\_vdW\_to\_Bidentate

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#### XY\_Addition\_MultipleBond

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

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

$$Y = F, Cl, Br$$

### XY\_elimination\_hydroxyl

halocarbene\_CO\_dimerization

$$^{3}O = ^{2}C = ^{1}C \xrightarrow{Y} ^{2}C = ^{3}O^{+} + R^{-1}C^{-}Y$$
 $Y = F, Cl, Br, I$ 

halocarbene\_recombination

halocarbene\_recombination\_double

$$R^{-1}C^{-R} + R^{-2}C^{-Y} \longrightarrow R^{-1}C = {}^{2}C^{-R}$$
 $Y = F, CI, Br, I$ 

intra\_H\_migration

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

intra\_NO2\_ONO\_conversion

 ${\tt intra\_OH\_migration}$ 

intra\_halogen\_migration

$$^{3}Y$$
  $\stackrel{}{-2}R$   $^{1}R$   $\stackrel{}{}$   $^{2}R$   $^{2}R$   $^{3}Y$   $Y = F, Cl, Br$ 

 $intra\_substitutionCS\_cyclization$ 

intra\_substitutionCS\_isomerization

 $intra\_substitutionS\_cyclization$ 

intra\_substitutionS\_isomerization

lone\_electron\_pair\_bond