# RMG-Py Reaction Families

# 1+2\_Cycloaddition

# 1,2-Birad\_to\_alkene

$$^{1}R^{\cdot} - ^{2}R^{\cdot} \longrightarrow ^{1}R = ^{2}F$$

## 1,2\_Insertion\_CO

#### 1,2\_Insertion\_carbene

#### 1,2\_NH3\_elimination

## 1,2\_shiftC

## 1,2\_shiftS

$$10 - 29 - 38$$
  $29 - 38 - 10$ 

#### 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

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

# 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

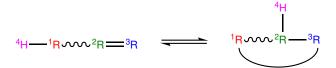
 ${\tt Intra\_5\_membered\_conjugated\_C=C\_C=C\_addition}$ 

# 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

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

# ${\tt Intra\_R\_Add\_Endocyclic}$

$$\frac{1}{R} w^2 R = {}^{3}R \qquad \qquad \frac{1}{R} w^2 R - {}^{3}R$$

# 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

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

#### R\_Addition\_COm

#### R\_Addition\_CSm

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

#### $R_Addition_MultipleBond$

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

#### R\_Recombination

#### Retroene

## Singlet\_Carbene\_Intra\_Disproportionation

# Singlet\_Val6\_to\_triplet

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

SubstitutionS

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

Substitution\_O

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

Surface\_Abstraction

Surface\_Abstraction\_vdW

Surface\_Addition\_Single\_vdW

$${\overset{2}{R}} = {\overset{3}{R}} \qquad {\overset{4}{R}} \qquad {\overset{2}{R}} = {\overset{2}{R}} - {\overset{3}{R}} - {\overset{4}{R}} \qquad + \qquad \\ {\overset{1}{\chi}} \qquad {\overset{5}{\chi}} \qquad {\overset{5}{\chi}} \qquad {\overset{5}{\chi}}$$

Surface\_Adsorption\_Abstraction\_vdW

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

 $Surface\_Adsorption\_Bidentate$ 

 ${\tt Surface\_Adsorption\_Dissociative}$ 

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