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

$$^{1}C$$
 ^{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

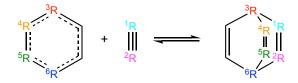
Cyclic_Ether_Formation

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}C ^{-2}Cb ^{-3}C ^{-1}C ^{-2}Cb

Intra_R_Add_Exocyclic

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

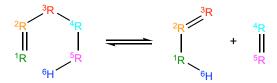
$R_Addition_MultipleBond$

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

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

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

Surface_Dissociation_to_Bidentate

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Surface_Dissociation_vdW

Surface_DoubleBond_to_Bidentate

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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_recombination

halocarbene_recombination_double

intra_H_migration

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

intra_NO2_ONO_conversion

intra_OH_migration

intra_halogen_migration

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

 $intra_substitutionCS_cyclization$

intra_substitutionCS_isomerization

 $intra_substitutionS_cyclization$

intra_substitutionS_isomerization

 ${\tt lone_electron_pair_bond}$