RMG-Py Reaction Families

1+2_Cycloaddition

$$^1R={}^2R \quad + \quad {}^3R \quad \Longrightarrow \quad {}^1R-{}^2R \atop {}^3R$$
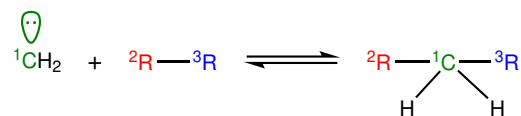
1,2-Birad_to_alkene

$$^1\dot{R}-{}^2\dot{R} \quad \Longrightarrow \quad {}^1R={}^2R$$
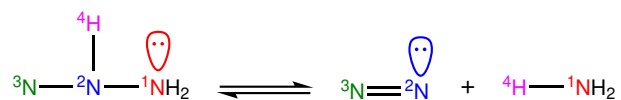
1,2_Insertion_CO

$$^1\bar{C}\equiv{}^4\overset{+}{O} + {}^2R-{}^3R \quad \Longrightarrow \quad {}^2R-\underset{}{\overset{^4O}{{}^1C}}-{}^3R$$

1,2_Insertion_carbene

$$^1CH_2 \quad + \quad {}^2R-{}^3R \quad \Longrightarrow \quad {}^2R-\underset{H \quad H}{{}^1C}-{}^3R$$

1,2_NH3_elimination
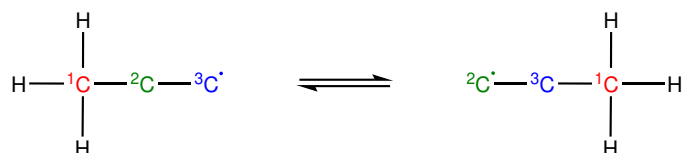
$$^3N-\overset{^4H}{{}^2N}-{}^1NH_2 \quad \Longrightarrow \quad {}^3N={}^2N \quad + \quad {}^4H-{}^1NH_2$$

1,2_XY_interchange

$$^1X-{}^2R-{}^3R-{}^4Y \quad \Longrightarrow \quad {}^4Y-{}^1R-{}^2R-{}^1X$$

X = F, Cl, Br, I, O
Y = F, Cl, Br, I

1,2_shiftC

$$H-\underset{H}{\overset{H}{{}^1C}}-{}^2C-{}^3\dot{C} \quad \Longrightarrow \quad {}^2\dot{C}-{}^3C-\underset{H}{\overset{H}{{}^1C}}-H$$

1,2_shiftS

$^1C - {}^2S - {}^3R^{\bullet} \quad \rightleftharpoons \quad {}^2S^{\bullet} - {}^3R - {}^1C$

1,3_Insertion_CO2

$^2O={}^1C=O \quad + \quad {}^3R - {}^4R \quad \rightleftharpoons \quad {}^3R - {}^1C(=O) - {}^2O - {}^2R$

1,3_Insertion_ROR

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

1,3_Insertion_RSR

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

1,3_NH3_elimination

$^3R - {}^2R - {}^1NH_2$ (with ^4H) $\quad \rightleftharpoons \quad {}^3R={}^2R \quad + \quad {}^4H - {}^1NH_2$
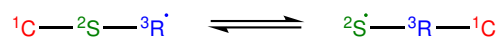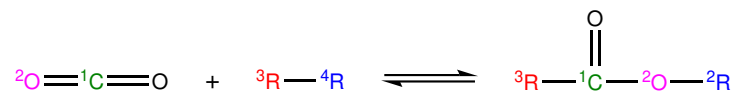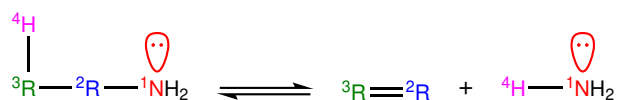
1,3_sigmatropic_rearrangement

$^1R={}^2R - {}^3R - {}^4R \quad \rightleftharpoons \quad {}^4R - {}^1R - {}^2R={}^3R$
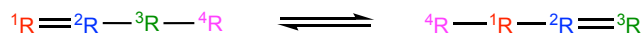
1,4_Cyclic_birad_scission

$^2R - {}^1R^{\bullet} \sim {}^4R^{\bullet} - {}^3R \quad \rightleftharpoons \quad {}^2R={}^1R \sim {}^4R={}^3R$
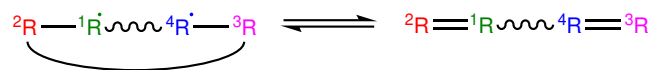
1,4_Linear_birad_scission

$^1R^{\bullet} - {}^2R - {}^3R - {}^4R^{\bullet} \quad \rightleftharpoons \quad {}^1R={}^2R \quad + \quad {}^3R={}^4R$

2+2_cycloaddition

$^1C={}^2R \quad + \quad {}^3R={}^4R \quad \rightleftharpoons \quad {}^1C - {}^3R / {}^2R - {}^4R$ (ring)
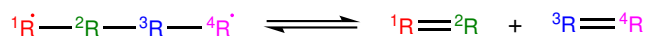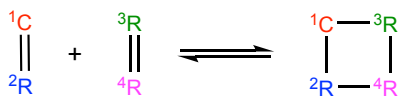
6_membered_central_C-C_shift
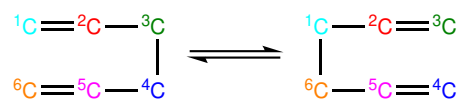
$^1C=^2C-^3C$ ... $^6C=^5C-^4C$ ⇌ $^1C-^2C=^3C$ ... $^6C-^5C=^4C$

Baeyer-Villiger_step1_cat

^2O ... ^1C ... [C,H] [C,H] + R—O—^3O—^4H + R—^5C(=^6O)—^7O—^8H ⇌

[C,H][C,H]^1C(^3O—O—R)(^2O—^8H) + R—^5C(—^6O—^4H)(=^7O)

Baeyer-Villiger_step2

[C,H]^2[C,H]^1C(—^5O—^6O—^7C(R)(=^8O))(^3O—^4H)([C,H]) ⇌ [C,H]^1C(—^5O—^{2}[C,H])(=^3O) + ^6O=^7C(R)(^4H—^8O)

Baeyer-Villiger_step2_cat

^{2}[C,H] [C,H]^1C(—^5O—^6O—R)(^3O—^4H) + ^{10}H—^9O—^7C(R)(=^8O) ⇌

[C,H]^1C(—^5O—^{2}[C,H])(=^3O) + R—^6O—^{10}H + ^9O=^7C(R)(^4H—^8O)
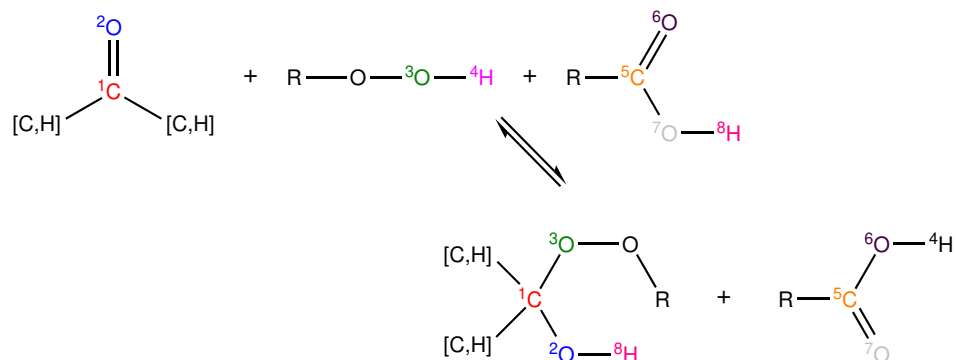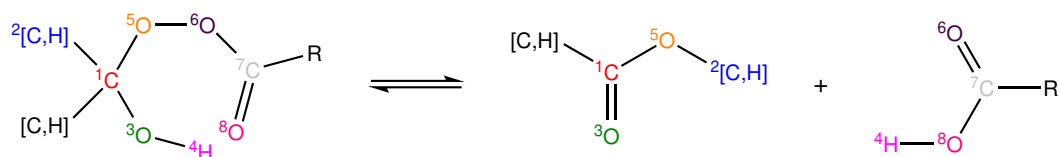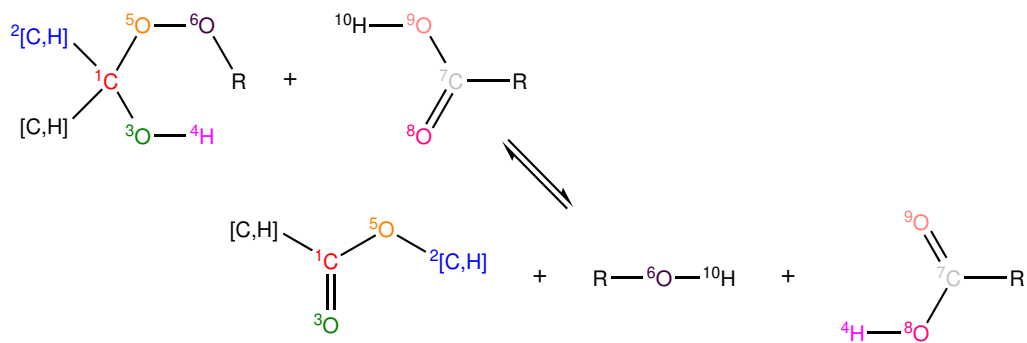
Bimolec_Hydroperoxide_Decomposition
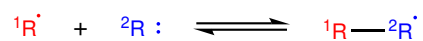
R—^1O—^2O—H + R—O—^4O—^3H ⇌ R—^1O· + ^2O(H)(^3H) + R—O—^4O·

Birad_R_Recombination

$$^1R^{\bullet} \ + \ ^2R: \ \rightleftharpoons \ ^1R\!-\!^2R^{\bullet}$$

Birad_recombination

$$^1\dot{R}\sim\sim\sim^2\dot{R} \ \rightleftharpoons \ ^1R\sim\sim\sim^2R$$

Br_Abstraction

$$^1R\!-\!^2Br \ + \ ^3\dot{R} \ \rightleftharpoons \ ^1\dot{R} \ + \ ^2Br\!-\!^3R$$

CO_Disproportionation

$$^1\dot{R} \ + \ ^2O\!=\!^3\dot{C}\!-\!^4H \ \rightleftharpoons \ ^1R\!-\!^4H \ + \ ^2O\!\equiv\!^3C$$

Cl_Abstraction

$$^1R\!-\!^2Cl \ + \ ^3\dot{R} \ \rightleftharpoons \ ^1\dot{R} \ + \ ^2Cl\!-\!^3R$$
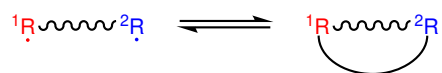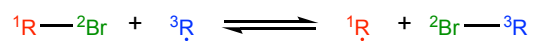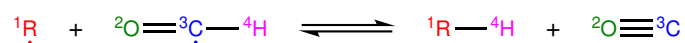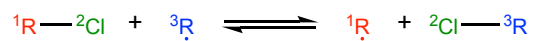
Concerted_Intra_Diels_alder_monocyclic_1,2_shiftH

$$^1C\!=\!^2C\!-\!^3C\!=\!^4C\!-\!^5C\!\equiv\!^6C\!-\!^7H \ \rightleftharpoons$$
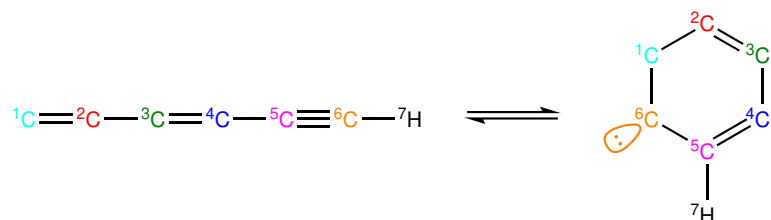
Cyclic_Ether_Formation

$$^1\dot{R}\sim\sim\sim^2O\!-\!^3OR \ \rightleftharpoons \ ^1R\sim\sim\sim^2O \ + \ ^3O\dot{R}$$
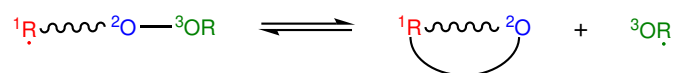
Cyclic_Thioether_Formation

$$^1\dot{R}\sim\sim\sim^2S\!-\!^3(O/S)R \ \rightleftharpoons \ ^1R\sim\sim\sim^2S \ + \ ^3(O/\dot{S})R$$
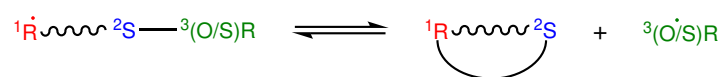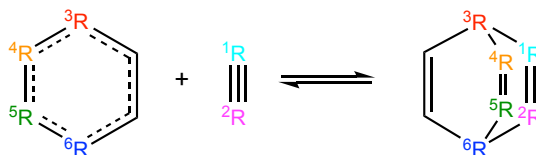
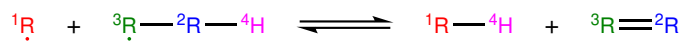## Cyclopentadiene_scission
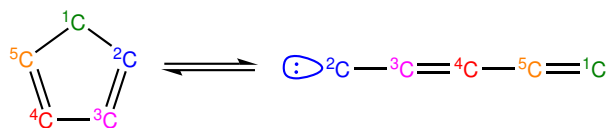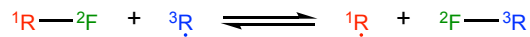

Diels_alder_addition
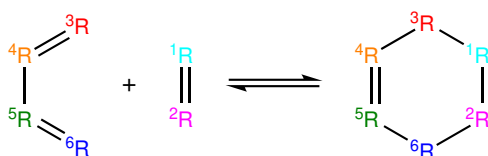
Diels_alder_addition_Aromatic

Disproportionation
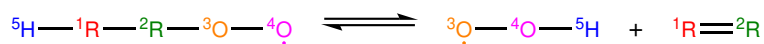

Disproportionation-Y
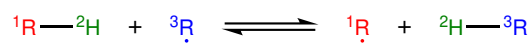

$Y = F, Cl, Br$
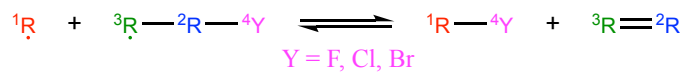
F_Abstraction

H2_Loss

Image Not Available

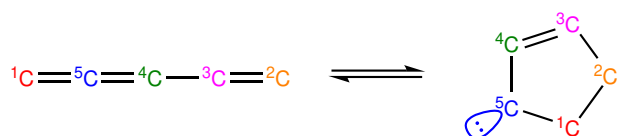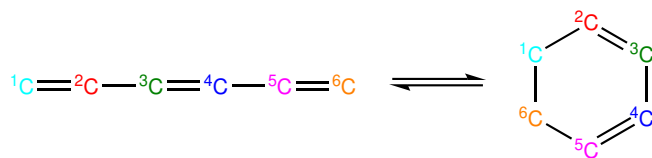## HO2_Elimination_from_PeroxyRadical

H_Abstraction

^1R—^2H + $^3R\cdot$ ⇌ $^1R\cdot$ + ^2H—^3R

Intra_2+2_cycloaddition_Cd

^1C=^2C—^4C=^3C (four-membered ring) ⇌ ^1C—^3C / ^2C=^4C
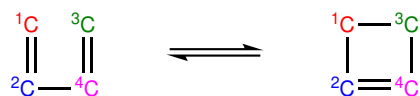
Intra_5_membered_conjugated_C=C_C=C_addition

^1C=^5C=^4C—^3C=^2C ⇌ (five-membered ring: ^3C, ^4C, ^2C, ^5C, ^1C)

Intra_Diels_alder_monocyclic

^1C=^2C—^3C=^4C—^5C=^6C ⇌ (six-membered ring: ^2C, ^1C, ^3C, ^6C, ^4C, ^5C)

Intra_Disproportionation

$^1R\cdot$〰$^3R\cdot$—^2R—^4H ⇌ ^4H—^1R〰^3R=^2R
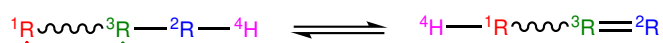
Intra_RH_Add_Endocyclic

^4H—^1R〰^2R=^3R ⇌ ^1R〰^2R(^4H)—^3R (ring)
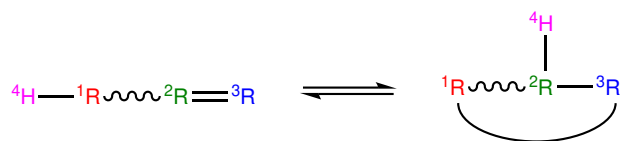
Intra_RH_Add_Exocyclic

^4H—^1R〰^2R=^3R ⇌ ^1R〰^2R—^3R—^4H (ring)
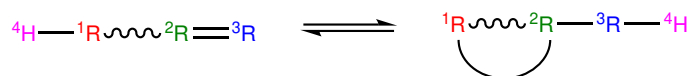
Intra_R_Add_Endocyclic

$^1R\cdot$〰^2R=^3R ⇌ ^1R〰$^2R\cdot$—^3R (ring)
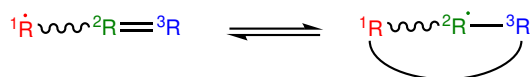
Intra_R_Add_ExoTetCyclic

$^1R \cdots ^2R - ^3R \quad \rightleftharpoons \quad ^1R \cdots ^2R \quad + \quad ^3R$
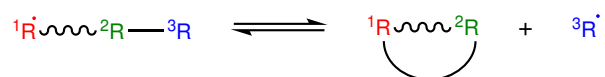
Intra_R_Add_Exo_scission

$^1C - ^3C - ^2Cb \quad \rightleftharpoons \quad ^3C - ^1C - ^2Cb$
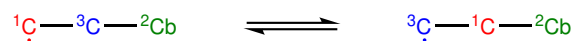
Intra_R_Add_Exocyclic

$^1R \cdots ^2R = ^3R \quad \rightleftharpoons \quad ^1R \cdots ^2R - ^3R$
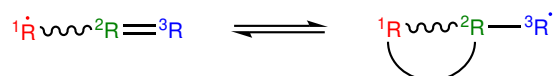
Intra_Retro_Diels_alder_bicyclic

$^1R \quad ^2R = ^3R \quad ^6R \quad ^4R \quad ^5R \quad \rightleftharpoons \quad ^1R = ^2R - ^3R = ^4R \cdots ^5R = ^6R$

Intra_ene_reaction

$^2C = ^3C \quad ^4C \quad ^1C - ^5C \quad ^6H \quad \rightleftharpoons \quad ^6H - ^2C \quad ^3C = ^4C \quad ^1C = ^5C$

Ketoenol

$^1R = ^2R - ^3O - ^4H \quad \rightleftharpoons \quad ^4H - ^1R - ^2R = ^3O$

Korcek_step1

$R, R, ^3O, ^4C, ^2H, ^1O \quad \rightleftharpoons \quad ^2H, R, ^3O, ^4C, ^1O, R$

Korcek_step1_cat

$R-^1O-^2H$ ... (reaction scheme with labeled atoms)

Korcek_step2

(reaction scheme with labeled atoms: ^2C, ^3C, ^1C, ^4O, ^5O, ^6H, OH → ^5O, ^1C, ^2C, ^6H, ^4O, ^3C, OH)
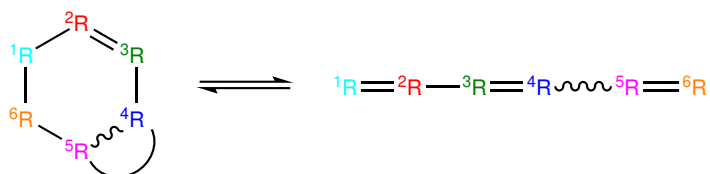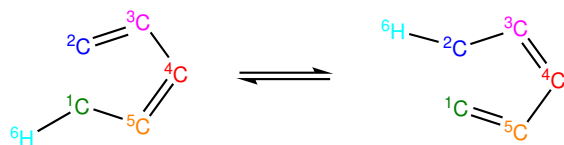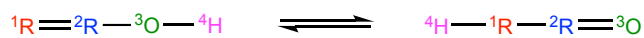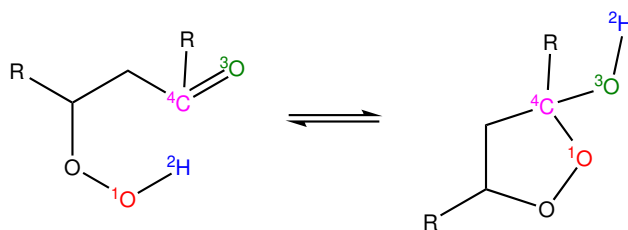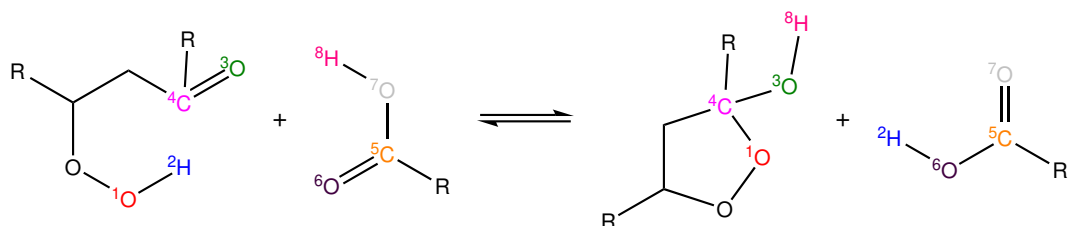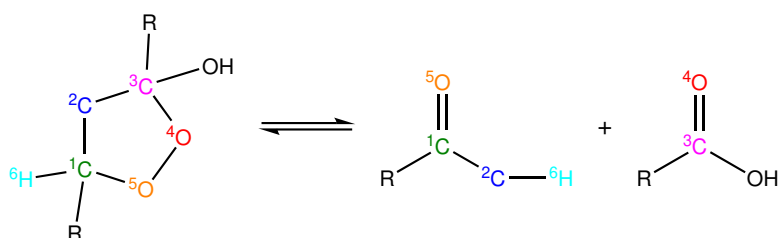
Peroxyl_Disproportionation

$R-^1O-^2O\cdot \ + \ R-^3O-^4O\cdot \ \rightleftharpoons \ R-^1O\cdot \ + \ R-^3O\cdot \ + \ ^2\underset{\cdot}{O}-^4\underset{\cdot}{O}$

Peroxyl_Termination

$^4H-^1R-^2O-^3O\cdot \ + \ R-^5O-^6O\cdot \ \rightleftharpoons \ ^1R=^2O \ + \ R-^5O-^4H \ + \ ^3\underset{\cdot}{O}-^6\underset{\cdot}{O}$

R_Addition_COm

$^1\overset{-}{C}\equiv{}^3\overset{+}{O} \ + \ ^2R\cdot \ \rightleftharpoons \ ^2R-^1\underset{\cdot}{C}{=}^3O$

R_Addition_CSm

$^1\overset{-}{C}\equiv{}^3\overset{+}{S} \ + \ ^2R\cdot \ \rightleftharpoons \ ^2R-^1\underset{\cdot}{C}{=}^3S$
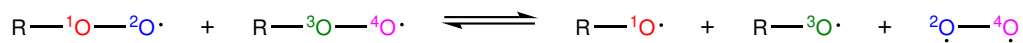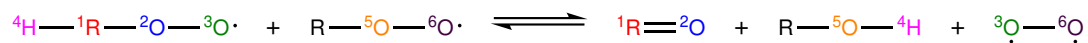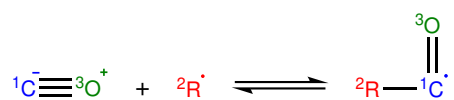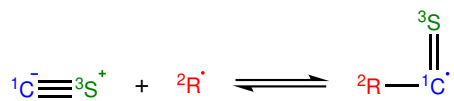
R_Addition_MultipleBond

$^2R{=}^1R \ + \ ^3\underset{\cdot}{R} \ \rightleftharpoons \ ^2\underset{\cdot}{R}-^1R-^3R$

R_Recombination

$$^1\dot{R} + {}^2\dot{R} \rightleftharpoons {}^1R\!-\!{}^2R$$
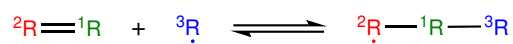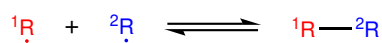
Retroene
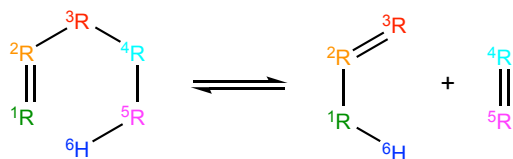
Singlet_Carbene_Intra_Disproportionation

$$\ddot{C}\,{}^1C\!-\!{}^2C\!-\!{}^3H \rightleftharpoons {}^3H\!-\!{}^1C\!=\!{}^2C$$
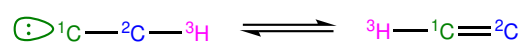
Singlet_Val6_to_triplet

$$^1(O/S)\!=\!{}^2(O/S) \longrightarrow {}^1(O\dot{/}S)\!-\!{}^2(O\dot{/}S)$$

SubstitutionS

$$R\!-\!{}^1S\!-\!{}^2R + {}^3\dot{R} \rightleftharpoons R\!-\!{}^1S\!-\!{}^3R + {}^2\dot{R}$$

Substitution_O

$$R\!-\!{}^1O\!-\!{}^2R + {}^3\dot{R} \rightleftharpoons R\!-\!{}^1O\!-\!{}^3R + {}^2\dot{R}$$
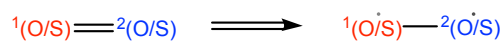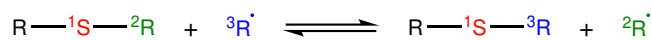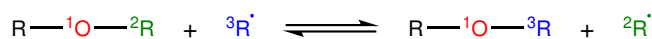
Surface_Abstraction
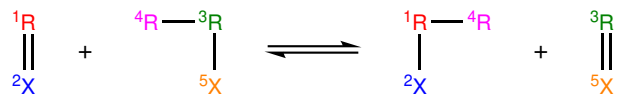
Surface_Abstraction_Single_vdW

Surface_Abstraction_vdW

Surface_Addition_Single_vdW

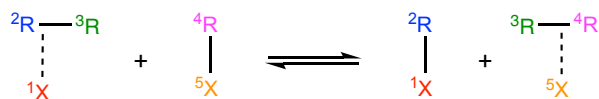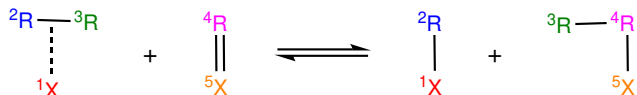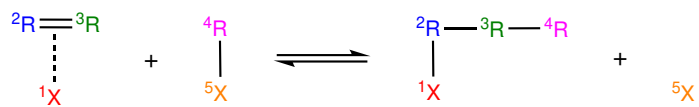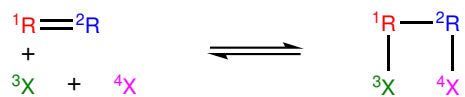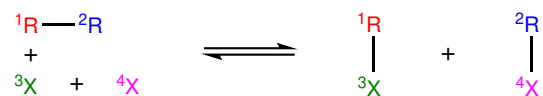$$^{2}R = {}^{3}R \quad + \quad {}^{4}R \quad \rightleftharpoons \quad {}^{2}R - {}^{3}R - {}^{4}R \quad + \quad$$
$$^{1}X \qquad\qquad {}^{5}X \qquad\qquad\qquad {}^{1}X \qquad\qquad\qquad {}^{5}X$$

Surface_Adsorption_Abstraction_vdW

$$^{2}R = {}^{3}R \quad + \quad {}^{4}R - {}^{5}R \quad \rightleftharpoons \quad {}^{2}R - {}^{3}R - {}^{5}R \quad + \quad {}^{4}R$$
$$^{1}X \qquad\qquad {}^{6}X \qquad\qquad\qquad {}^{1}X \qquad\qquad\qquad {}^{6}X$$
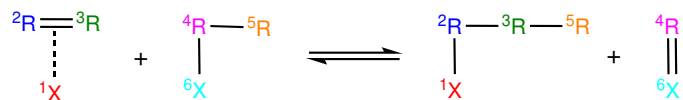
Surface_Adsorption_Bidentate

$$^{1}R = {}^{2}R$$
$$+$$
$$^{3}X \quad + \quad {}^{4}X \qquad \rightleftharpoons \qquad {}^{1}R - {}^{2}R$$
$$^{3}X \qquad {}^{4}X$$

Surface_Adsorption_Dissociative

$$^{1}R - {}^{2}R$$
$$+$$
$$^{3}X \quad + \quad {}^{4}X \qquad \rightleftharpoons \qquad {}^{1}R \qquad + \qquad {}^{2}R$$
$$^{3}X \qquad\qquad {}^{4}X$$

Surface_Adsorption_Dissociative_Double

$$^{2}R = {}^{3}R$$
$$+ \qquad\qquad + \qquad\qquad \rightleftharpoons \qquad {}^{2}R \quad + \quad {}^{3}R$$
$$^{1}X \qquad\qquad {}^{4}X \qquad\qquad\qquad {}^{1}X \qquad\qquad {}^{4}X$$

Surface_Adsorption_Double

$$^{1}R :$$
$$+ \qquad \rightleftharpoons \qquad {}^{1}R$$
$$^{2}X \qquad\qquad {}^{2}X$$
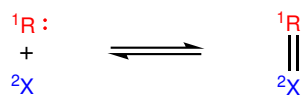
Surface_Adsorption_Single

$$^{1}R \cdot$$
$$+ \qquad \rightleftharpoons \qquad {}^{1}R$$
$$^{2}X \qquad\qquad {}^{2}X$$
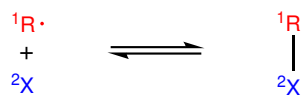
Surface_Adsorption_vdW

$$^1R + {}^2X \rightleftharpoons {}^1R\cdots{}^2X$$
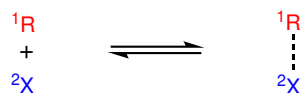
Surface_Bidentate_Dissociation

$$^1R={}^2R-{}^3R \quad {}^4X \ + \ {}^5X \ + \ {}^6X \rightleftharpoons {}^1R-{}^2R \quad {}^4X \quad {}^5X \ + \ {}^3R \quad {}^6X$$

Surface_Dissociation

$$^1R-{}^2R \quad {}^3X \ + \ {}^4X \rightleftharpoons {}^1R \quad {}^3X \ + \ {}^2R \quad {}^4X$$
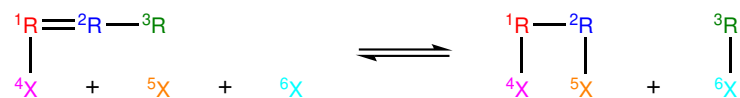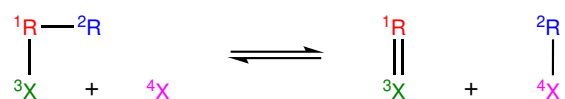
Surface_Dissociation_Beta

$$^2R={}^3R \quad {}^1X \ + \ {}^4R \quad {}^5X \rightleftharpoons {}^2R-{}^3R-{}^4R \quad {}^1X \ + \ {}^5X$$
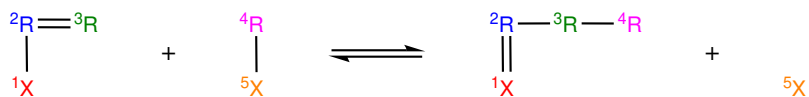
Surface_Dissociation_Double_vdW

$$^2R={}^3R \quad {}^1X \ + \ {}^4X \rightleftharpoons {}^2R \quad {}^1X \ + \ {}^3R \quad {}^4X$$
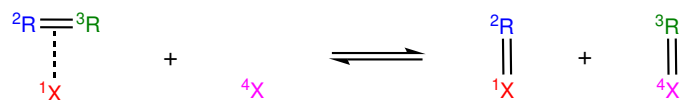
Surface_Dissociation_vdW

$$^1R-{}^2R \quad {}^3X \ + \ {}^4X \rightleftharpoons {}^1R \quad {}^3X \ + \ {}^2R \quad {}^4X$$
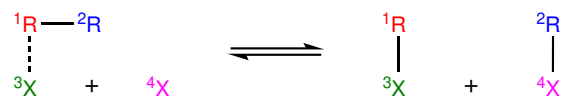
Surface_DoubleBond_to_Bidentate

Image Not Available

Surface_Dual_Adsorption_vdW

$$^2R={}^3R \quad {}^1X \ + \ {}^4R-{}^6R \quad {}^5X \rightleftharpoons {}^2R-{}^3R-{}^4R \quad {}^1X \ + \ {}^6R \quad {}^5X$$
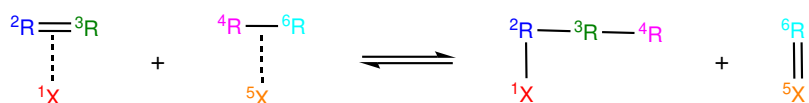
Surface EleyRideal Addition Multiple Bond

^2R | ^1X + ^4R—^3R ⇌ ^3R—^4R—^2R / ^1X
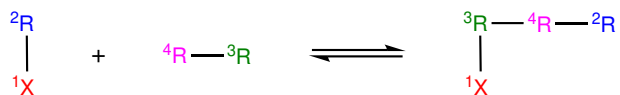
Surface Migration

^4R | ^2R—^3R | ^1X ⇌ ^4R | ^2R—^3R | ^1X
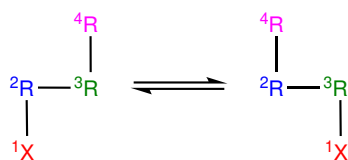
Surface_vdW_to_Bidentate

Image Not Available

XY Addition MultipleBond

^1R=^2R + ^3X—^4Y ⇌ ^3X—^1R—^2R—^4Y

X = H, F, Cl, Br
Y = F, Cl, Br
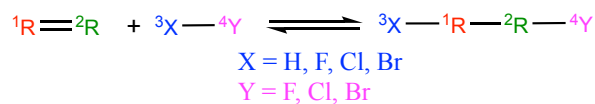
XY elimination hydroxyl

R—^2R(—^3R)(—^1X)—^4C(—R)(—^5O—^6Y) ⇌ ^2R=^3R + ^4C=^5O + ^1X—^6Y

X = H, F, Cl, Br
Y = H, F, Cl, Br

halocarbene recombination

^{1}R• + R-^2C-Y ⇌ •^2C(—R)—^1R / Y

Y = F, Cl, Br, I
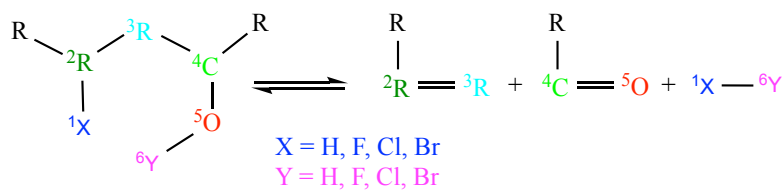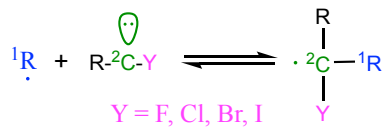
halocarbene recombination double

R-^1C-R + R-^2C-Y ⇌ (R)(R)^1C=^2C(R)(Y)

Y = F, Cl, Br, I

intra_H_migration

$$^3H - ^2R \www ^1\dot{R} \rightleftharpoons ^2\dot{R} \www ^1R - ^3H$$
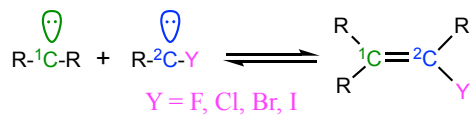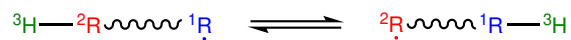
intra_NO2_ONO_conversion

$$^1\dot{R} - ^2N^+ - ^3O^- \rightleftharpoons N - ^3O - ^1R$$
$$\quad\quad \| \quad\quad\quad\quad\quad\quad\quad \|$$
$$\quad\quad O \quad\quad\quad\quad\quad\quad\quad O$$
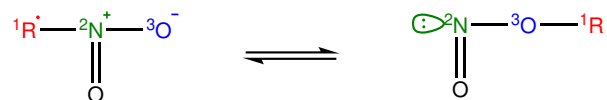
intra_OH_migration

$$^1\dot{R} \wwww ^2O - ^3OH \rightleftharpoons ^3HO - ^1R \wwww ^2\dot{O}$$
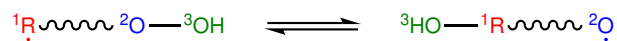
intra_halogen_migration

$$^3Y - ^2R \wwww ^1\dot{R} \rightleftharpoons ^2\dot{R} \wwww ^1R - ^3Y$$
$$Y = F, Cl, Br$$
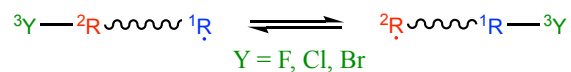
intra_substitutionCS_cyclization

$$^3\dot{R} \wwww ^1C - ^2S \rightleftharpoons ^3R \wwww ^1C \;\;+\;\; ^2\dot{S}$$
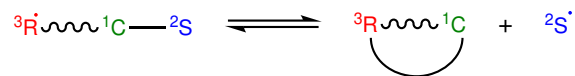
intra_substitutionCS_isomerization

$$^3\dot{R} \wwww ^2S - ^1C \rightleftharpoons ^1C - ^3R \wwww ^2\dot{S}$$
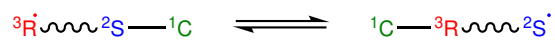
intra_substitutionS_cyclization

$$^3\dot{R} \wwww ^1S - ^2R \rightleftharpoons ^3R \wwww ^1S \;\;+\;\; ^2\dot{R}$$
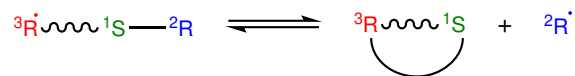
intra_substitutionS_isomerization

$$^3\dot{R} \wwww ^2R - ^1S \rightleftharpoons ^1S - ^3R \wwww ^2\dot{R}$$

lone_electron_pair_bond