RMG-Py Reaction Families

1+2_Cycloaddition

$^1R{=}^2R$ + ^3R ⮂ $^1R{-}^2R$ / ^3R (triangle)
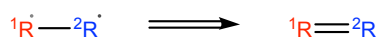
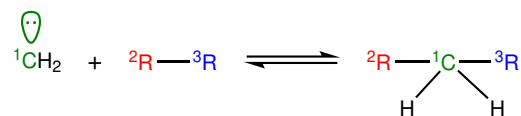## 1,2-Birad_to_alkene

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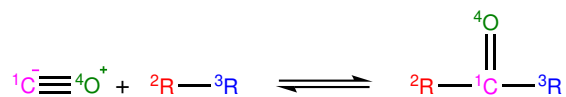
1,2_Insertion_CO

$^1\bar{C}{\equiv}^4\overset{+}{O}$ + $^2R{-}^3R$ ⮂ $^2R{-}^1C{-}^3R$ with ^4O double bonded to ^1C

1,2_Insertion_carbene

$^1CH_2$ + $^2R{-}^3R$ ⮂ $^2R{-}^1C{-}^3R$ with H, H on ^1C

1,2_NH3_elimination

$^4H{-}^2N(^3N){-}^1NH_2$ ⮂ $^3N{=}^2N$ + $^4H{-}^1NH_2$

1,2_shiftC

$H{-}^1C(H)(H){-}^2C{-}^3\dot{C}$ ⮂ $^2\dot{C}{-}^3C{-}^1C(H)(H){-}H$

1,2_shiftS

$^1C{-}^2S{-}^3\dot{R}$ ⮂ $^2\dot{S}{-}^3R{-}^1C$

1,3_Insertion_CO2

$$^2O\!=\!^1C\!=\!O \quad + \quad ^3R\!-\!^4R \quad \rightleftharpoons \quad ^3R\!-\!^1\overset{\overset{\displaystyle O}{\|}}{C}\!-\!^2O\!-\!^2R$$

1,3_Insertion_ROR

$$^3R\!-\!^4O\!-\!R \quad + \quad ^1R\!=\!^2R \quad \rightleftharpoons \quad ^3R\!-\!^1R\!-\!^2R\!-\!^4O\!-\!R$$
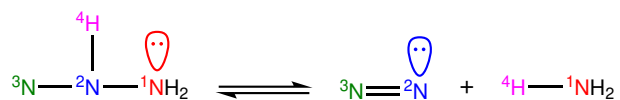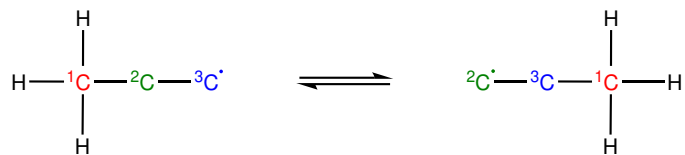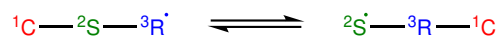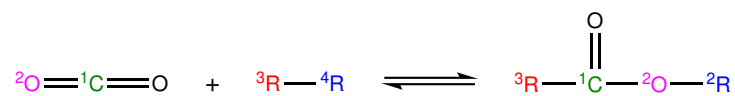
1,3_Insertion_RSR

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

1,3_NH3_elimination

$$^3R\!-\!^2R\!-\!^1NH_2 \ (\overset{4H}{\underset{}{|}}) \quad \rightleftharpoons \quad ^3R\!=\!^2R \quad + \quad ^4H\!-\!^1NH_2$$
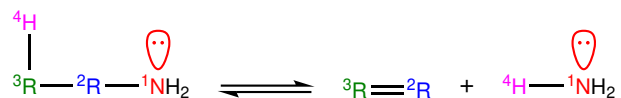
1,4_Cyclic_birad_scission

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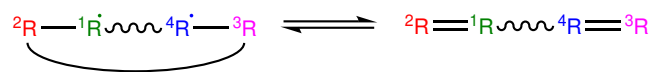
1,4_Linear_birad_scission

$$^1\dot{R}\!-\!^2R\!-\!^3R\!-\!^4\dot{R} \quad \rightleftharpoons \quad ^1R\!=\!^2R \quad + \quad ^3R\!=\!^4R$$
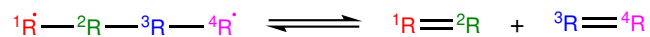
2+2_cycloaddition

Image Not Available

6_membered_central_C-C_shift
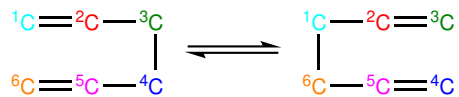
$$\begin{array}{c} ^1C\!=\!^2C\!-\!^3C \\ | \\ ^6C\!=\!^5C\!-\!^4C \end{array} \quad \rightleftharpoons \quad \begin{array}{c} ^1C\!-\!^2C\!=\!^3C \\ | \\ ^6C\!-\!^5C\!=\!^4C \end{array}$$

Baeyer-Villiger_step1_cat

^{2}O

^{1}C

[C,H]   [C,H]

+   R—O—^{3}O—^{4}H   +   R—^{5}C

^{6}O

^{7}O—^{8}H

[C,H] ^{3}O—O

^{1}C   R

[C,H] ^{2}O—^{8}H

+   R—^{5}C

^{6}O—^{4}H

^{7}O

Baeyer-Villiger_step2

^{2}[C,H] ^{5}O—^{6}O

^{1}C ^{7}C—R

[C,H] ^{3}O—^{4}H ^{8}O

[C,H] ^{5}O

^{1}C ^{2}[C,H]

^{3}O

+

^{6}O

^{7}C—R

^{4}H—^{8}O

Baeyer-Villiger_step2_cat

^{2}[C,H] ^{5}O—^{6}O

^{1}C   R

[C,H] ^{3}O—^{4}H

+ ^{10}H—^{9}O

^{7}C—R

^{8}O

[C,H] ^{5}O

^{1}C ^{2}[C,H]

^{3}O

+   R—^{6}O—^{10}H   +

^{9}O

^{7}C—R

^{4}H—^{8}O
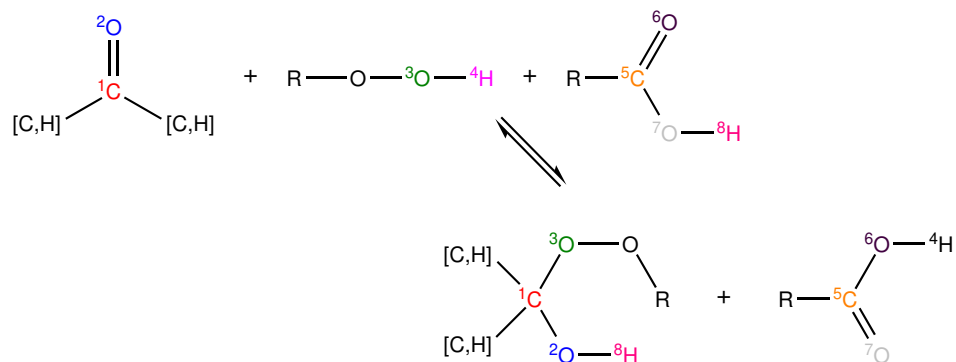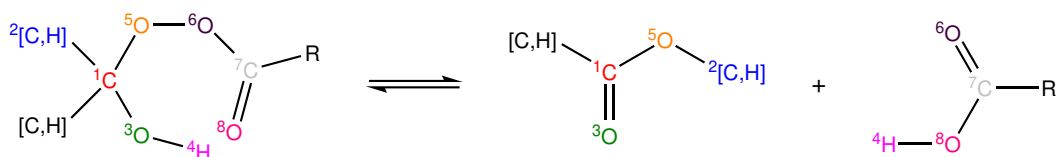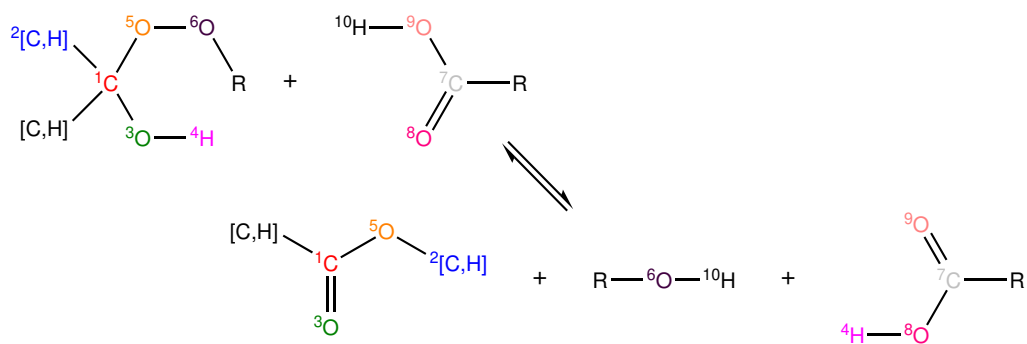
Bimolec_Hydroperoxide_Decomposition

R—^{1}O—^{2}O—H   +   R—O—^{4}O—^{3}H   ⇌   R—^{1}O·   + ^{2}O (H, ^{3}H)   +   R—O—^{4}O·
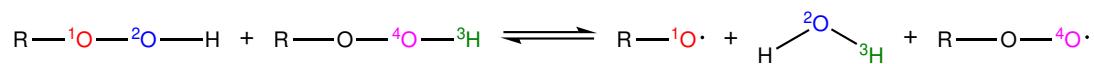
Birad_R_Recombination

^{1}R·   + ^{2}R :   ⇌ ^{1}R—^{2}R·

Birad_recombination

^{1}R⌇^{2}R   ⇌ ^{1}R⌇^{2}R

3
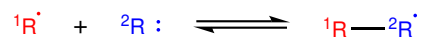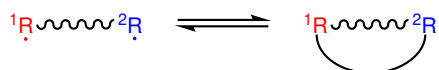
CO_Disproportionation

$$^1R\bullet \;+\; ^2O{=}^3C{-}^4H \;\rightleftharpoons\; ^1R{-}^4H \;+\; ^2O{\equiv}^3C$$
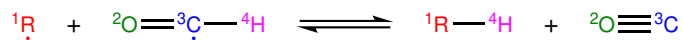
Concerted_Intra_Diels_alder_monocyclic_1,2_shiftH

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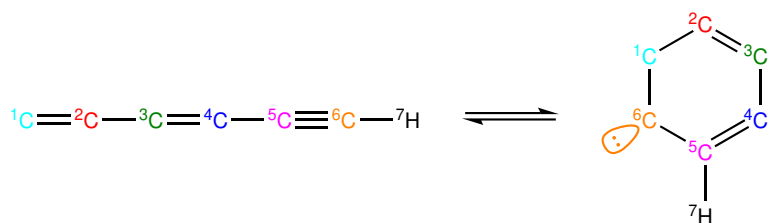
Cyclic_Ether_Formation

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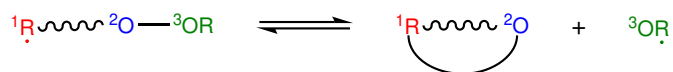
Cyclic_Thioether_Formation

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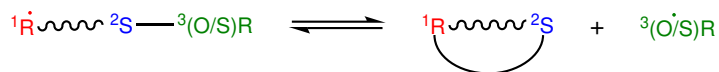
Cyclopentadiene_scission

$$\rightleftharpoons\; {:}^2C{-}^3C{=}^4C{-}^5C{=}^1C$$
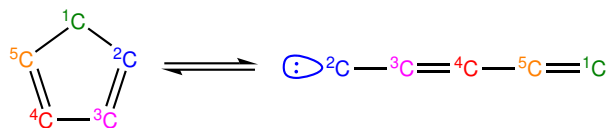
Diels_alder_addition

Disproportionation

$$^1R\bullet \;+\; ^3\dot{R}{-}^2R{-}^4H \;\rightleftharpoons\; ^1R{-}^4H \;+\; ^3R{=}^2R$$
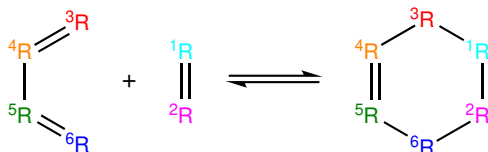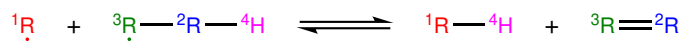
HO2_Elimination_from_PeroxyRadical

$$^5H{-}^1R{-}^2R{-}^3O{-}^4\dot{O} \;\rightleftharpoons\; ^3\dot{O}{-}^4O{-}^5H \;+\; ^1R{=}^2R$$

H_Abstraction

$$^1R-^2H \;+\; ^3R\!\cdot \;\; \rightleftharpoons \;\; ^1R\!\cdot \;+\; ^2H-^3R$$
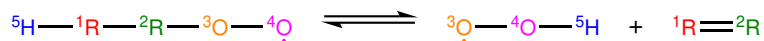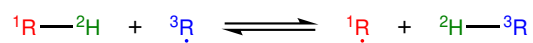
Intra_2+2_cycloaddition_Cd

$$\begin{array}{cc} ^1C & ^3C \\[-2pt] \| & \| \\[-2pt] ^2C & - ^4C \end{array} \;\;\rightleftharpoons\;\; \begin{array}{cc} ^1C & - ^3C \\[-2pt] | & | \\[-2pt] ^2C & = ^4C \end{array}$$
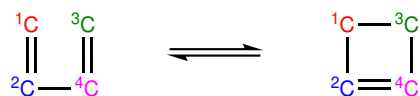
Intra_5_membered_conjugated_C=C_C=C_addition

$$^1C=^5C=^4C-^3C=^2C \;\;\rightleftharpoons\;\;$$
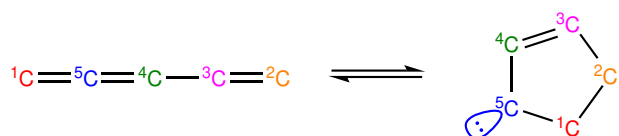
Intra_Diels_alder_monocyclic

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

Intra_Disproportionation

$$^1R\!\cdot\!\sim\!^3R\!\cdot-^2R-^4H \;\;\rightleftharpoons\;\; ^4H-^1R\!\sim\!^3R=^2R$$
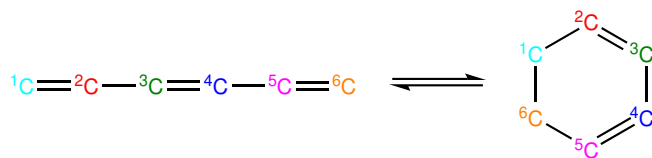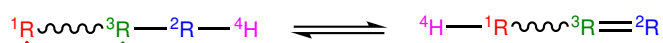
Intra_RH_Add_Endocyclic

$$^4H-^1R\!\sim\!^2R=^3R \;\;\rightleftharpoons\;\;$$
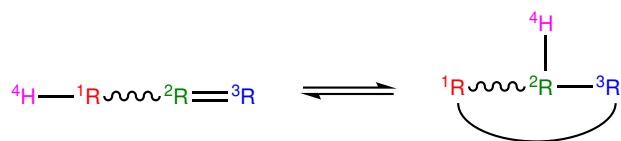
Intra_RH_Add_Exocyclic

$$^4H-^1R\!\sim\!^2R=^3R \;\;\rightleftharpoons\;\; ^1R\!\sim\!^2R-^3R-^4H$$
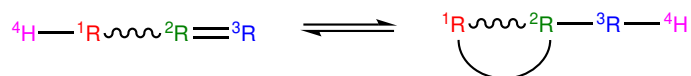
Intra_R_Add_Endocyclic

$$^1R\!\cdot\!\sim\!^2R=^3R \;\;\rightleftharpoons\;\; ^1R\!\sim\!^2R\!\cdot-^3R$$

5
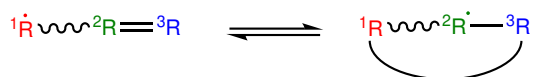
Intra_R_Add_ExoTetCyclic

$$^1\dot{R} \sim\sim ^2R — ^3R \quad \rightleftharpoons \quad ^1R \sim\sim ^2R \quad + \quad ^3\dot{R}$$
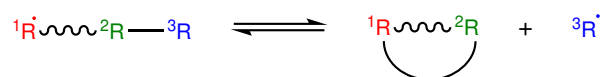
Intra_R_Add_Exo_scission

$$^1\dot{C} — ^3C — ^2Cb \quad \rightleftharpoons \quad ^3\dot{C} — ^1C — ^2Cb$$
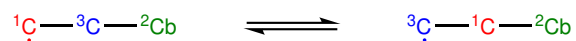
Intra_R_Add_Exocyclic

$$^1\dot{R} \sim\sim ^2R = ^3R \quad \rightleftharpoons \quad ^1R \sim\sim ^2R — ^3\dot{R}$$
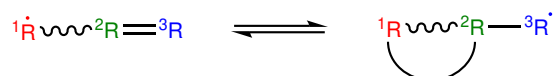
Intra_Retro_Diels_alder_bicyclic

$$^1R = ^2R — ^3R = ^4R \sim\sim ^5R = ^6R$$
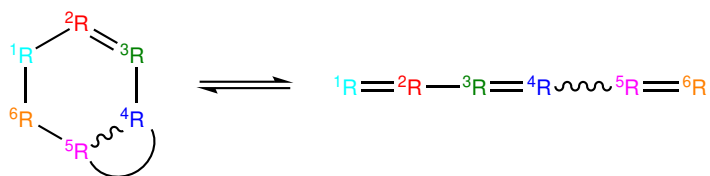
Intra_ene_reaction

Korcek_step1

6
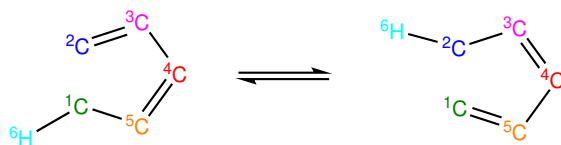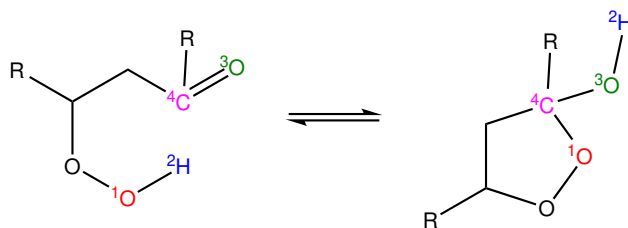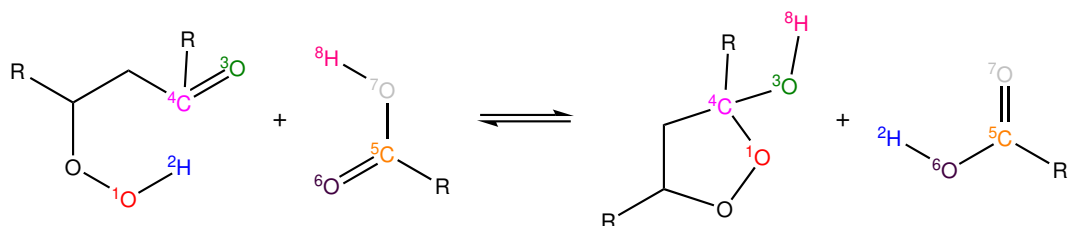
Korcek_step1_cat

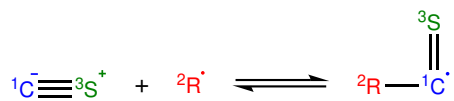## Korcek_step2
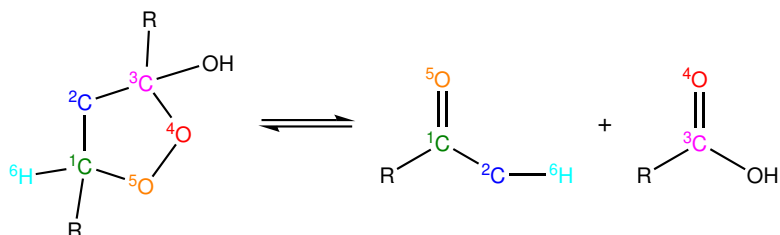
Peroxyl_Disproportionation

R—^{1}O—^{2}O· + R—^{3}O—^{4}O· ⇌ R—^{1}O· + R—^{3}O· + ^{2}O—^{4}O

Peroxyl_Termination

^{4}H—^{1}R—^{2}O—^{3}O· + R—^{5}O—^{6}O· ⇌ ^{1}R═^{2}O + R—^{5}O—^{4}H + ^{3}O—^{6}O
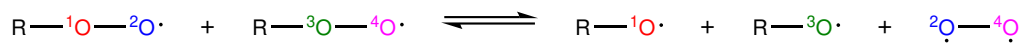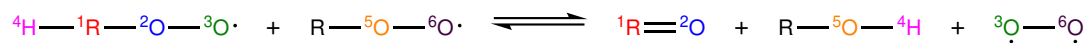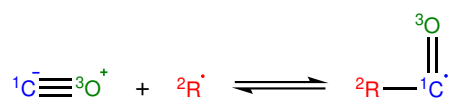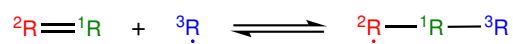
R_Addition_COm

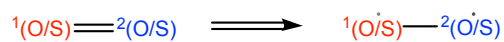## R_Addition_CSm

R_Addition_MultipleBond

R_Recombination

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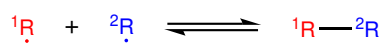
Retroene
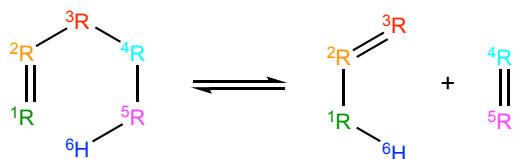
Singlet_Carbene_Intra_Disproportionation

$$\overset{\dots}{\bigcirc}{}^1C\!-\!^2C\!-\!^3H \ \rightleftharpoons \ ^3H\!-\!^1C\!=\!^2C$$
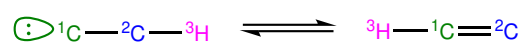
Singlet_Val6_to_triplet

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

SubstitutionS

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

Substitution_O

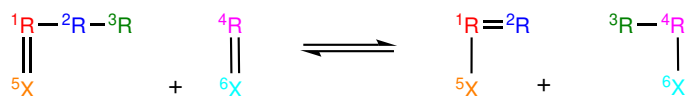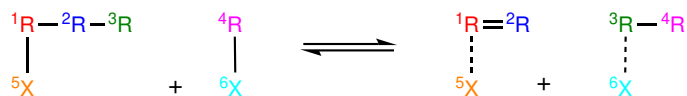$$R\!-\!^1O\!-\!^2R \ + \ ^3\dot{R} \ \rightleftharpoons \ R\!-\!^1O\!-\!^3R \ + \ ^2\dot{R}$$
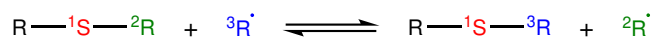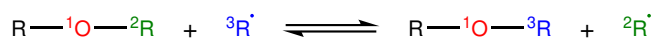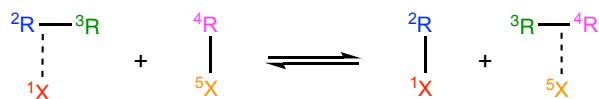
Surface_Abstraction
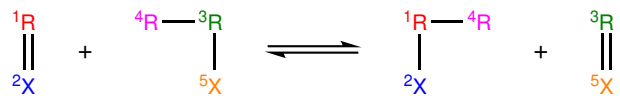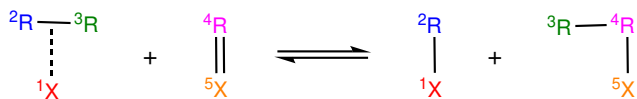

Surface_Abstraction_Beta
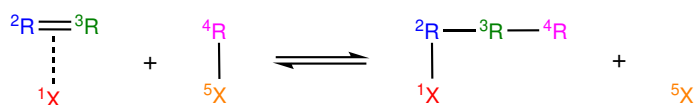

Surface_Abstraction_Beta_double_vdW
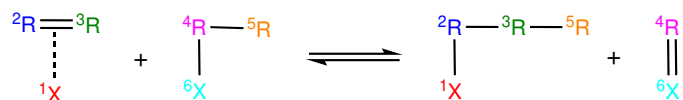
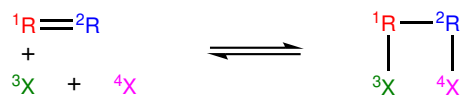## Surface_Abstraction_Single_vdW

Surface_Abstraction_vdW

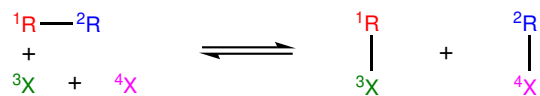## Surface_Addition_Single_vdW

Surface_Adsorption_Abstraction_vdW
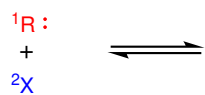

Surface_Adsorption_Bidentate

Surface_Adsorption_Dissociative

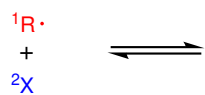## Surface_Adsorption_Dissociative_Double
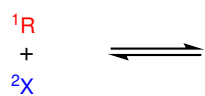
`Surface_Adsorption_Double`

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

`Surface_Adsorption_Single`

^{1}R ·
\+
^{2}X
$\rightleftharpoons$
^{1}R
$|$
^{2}X

`Surface_Adsorption_vdW`

^{1}R
\+
^{2}X
$\rightleftharpoons$
^{1}R
$\vdots$
^{2}X

`Surface_Bidentate_Dissociation`

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

`Surface_Dissociation`

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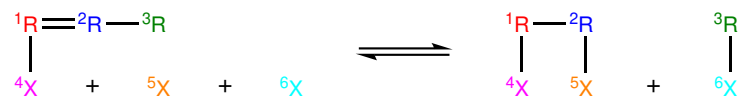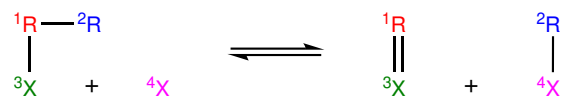
`Surface_Dissociation_Beta`

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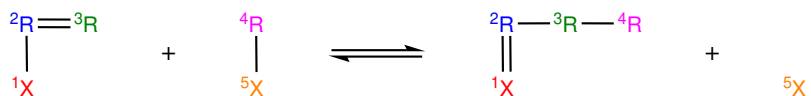
`Surface_Dissociation_Double_vdW`

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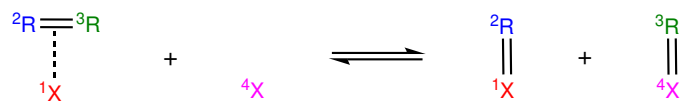
`Surface_Dissociation_vdW`

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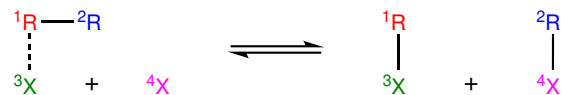
Surface_DoubleBond_to_Bidentate

Image Not Available

Surface_Dual_Adsorption_vdW

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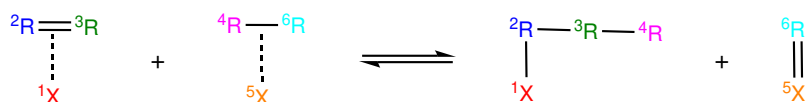
Surface_EleyRideal_Addition_Multiple_Bond

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

Surface_Migration

^{4}R, $^{2}R - ^{3}R$ with ^{1}X $\rightleftharpoons$ ^{4}R, $^{2}R - ^{3}R$ with ^{1}X
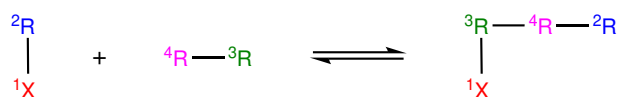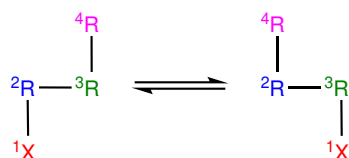
Surface_vdW_to_Bidentate

Image Not Available

intra_H_migration

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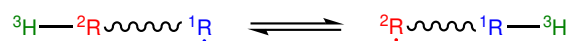
intra_NO2_ONO_conversion

$^{1}R - ^{2}N^{+} - ^{3}O^{-}$, O $\rightleftharpoons$ $^{2}N - ^{3}O - ^{1}R$, O
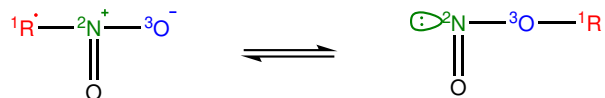
intra_OH_migration

$^{1}R \sim ^{2}O - ^{3}OH$ $\rightleftharpoons$ $^{3}HO - ^{1}R \sim ^{2}O$
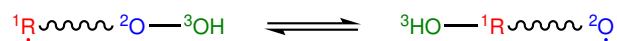
intra_substitutionCS_cyclization

$^{3}R \sim ^{1}C - ^{2}S$ $\rightleftharpoons$ $^{3}R \sim ^{1}C$ + ^{2}S
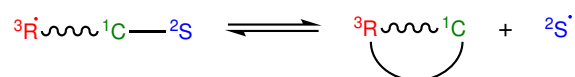
intra_substitutionCS_isomerization

$$^3R \sim ^2S - ^1C \quad \rightleftharpoons \quad ^1C - ^3R \sim ^2S$$
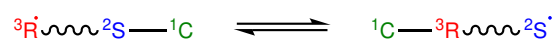
intra_substitutionS_cyclization

$$^3R \sim ^1S - ^2R \quad \rightleftharpoons \quad ^3R \sim ^1S \quad + \quad ^2R$$
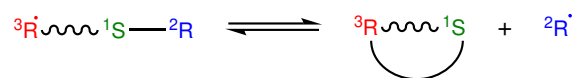
intra_substitutionS_isomerization

$$^3R \sim ^2R - ^1S \quad \rightleftharpoons \quad ^1S - ^3R \sim ^2R$$

ketoenol

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

lone_electron_pair_bond