H migration in closed-shell molecules intra_H_migration_suprafacial ketoenol cpd_H_migration	R1=C: $a = 1.35$ R2=C: $b = 1.35$ R1=O: $a = 1.20$ R2=O: $b = 1.20$	⊘ OH ₹ ∕ ○ O
Reverse Diels-Alder Diels_alder_addition	a = 2.2 $b = 2.2$	
Intra Diels-Alder Intra_Diels_alder_R	a = 1.8 $b = 2.2$	
Endocyclic closed-shell cyclization Intra_RH_Add_Endocyclic_F Intra_RH_Add_Endocyclic_R	a = 2.0 $b = 1.3$ $c = 1.3$ $d = 1.4$ $e = 1.8$	
Exocyclic closed-shell cyclization Intra_RH_Add_Exocyclic_F Intra_RH_Add_Exocyclic_R	$ \begin{array}{c c} d & a = 2.0 \\ b = 1.9 \\ c & c = 1.4 \\ d = 1.4 \\ e = 1.3 \end{array} $	
Generalized Korcek step 2 reaction Korcek_step2	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
Patro and reaction	(a b) a = 1.35	

b = 1.35

c = 2.0

a = b = scan

a = 2.2

b = 2.2

R1 = H

a = 1.7

b = 1.09

c = 2.2

R1 = 0: b = 1.3

R1 = C: b = 1.45R2 = H: c = d = 1.3

R2 = C, O: c = d = 2.0

R1=C: a = 1.35

R2=C: b = 1.35

R1=O: a = 1.20

R2=0: b = 1.20

a = 1.3

b = 1.3c = 2.0

 $R_1 - R_2 - R_3$

C-C-C: a = 2.20 C-C-H: a = 1.79 C-C-O: a = 2.04 O-C-C: a = 2.12

O-C-H: a = 1.84

O-C-O: a = 2.04 C-O-C: a = 2.04 C-O-H: a = 1.42 C-O-O: a = 2.04 O-O-C: a = 2.04

Ri=C, Rj=C: Ri-Rj = 1.80 Ri=C, Rj=O: Ri-Rj = 1.68

Ri=C, Rj=H: Ri-Rj = 1.31

Ri=O, Rj=O: Ri-Rj = 1.78 Ri=O, Rj=H: Ri-Rj = 1.14

R1 ---- R2

a = 2.0

R1 = O

a = 1.67

b = 1.8

c = 1.9

Rn = C

a = 1.67

b = 2.2

c = 1.9

R₃ b

Template geometries

Example

Reaction

Retro-ene reaction

r12_cycloaddition

r22_cycloaddition

r12_insertion_R

Reverse 1,2 cycloaddition

Reverse 2,2 cycloaddition

Reverse 1,2 R insertion

Reverse 1,3 insertion

r13_insertion_CO2

r13_insertion_ROR

r13_insertion_RSR

intra R migration

intra_OH_migration

intra H migration

12_shift_S_F

12_shift_S_R

HO₂ elimination

Radical β-scission

Radical α-scission R_Addition_COm3_R R_Addition_CSm3_R

addition

addition

Exocyclic intramolecular radical

Endocyclic intramolecular radical

(note that this reaction type does not

include a saddle point search, KinBot

only lists the energies of the products.

homolytic_scissions keyword)

Intra_R_Add_ExoTetCyclic_F
Intra_R_Add_Exocyclic_F

Intra_R_Add_Endocyclic_F

Cyclization-elimination

Cyclic Ether Formation

Homolytic scission

Invoked with the

R_Addition_MultipleBond

HO2_Elimination_from_PeroxyRadical

R migration in radicals

Retro Ene