

Reaction plus calculation example list

Type of chemical reaction	Case	Characteristic of chemical reaction	Calculatable software	
			Pro	Express
Nucleophilic addition	Michael addition	Regioselectivity	○	○
Cycloaddition	Diels-Alder reaction	Stereoselectivity	○	○
	[3+2] cycloaddition of benzyne and azide (Igawa et al.)	Regioselectivity	○	○
	Cycloaddition of allyl sulfide by Sn catalyst by Sn catalyst (Hirabayashi et al.)	Typical metal Chalcogen	○	○
Insertion	CO ₂ fixation by UV irradiation (Ishida et al.)	Cycloaddition	○	○
	CO ₂ fixation by Cu catalyst (Tsuji et al.)	Transition metal	○	△
Electrophilic substitution	Kolbe-Schmitt reaction	Regioselectivity	○	○
Rearrangement	Beckmann rearrangement	Transferability of substituent	○	○
Coupling	Mizoroki-Heck reaction	Transition metal Cis-trans selectivity	○	○
	Transmetalation by Migita-Kosugi-Stille reaction	Transition metal Transmetalation	○	○
	Pd catalyst for cross-coupling (Gorelsky et al.)	Transition metal Regioselectivity	○	○
Metathesis	Wittig reaction	Phosphorous ylide	○	○
Cleavage Decomposition	Cleavage of uni-substituted cyclobutene (Frey et al.)	Cis-trans selectivity	○	○
	Fragmentation process of p-benzoquinone+ in mass spectrometry (Sugimura et al.)	Radical cation	○	○
Radical	Homolytic ring-closing reaction of diradical molecule (Abe et al.)	Open shell singlet state Reaction of open shell to closed shell	○	×
Typical element	Generation of borylzincate (Uchiyama et al.)	Cleavage of boron-boron bond Typical metal	○	×
	Si cluster isomerization (Iwamoto et al.)	Isomerization Typical element cluster	○	×
Formal intramolecular	Indole synthesis by Zn catalyst (Ilies et al.)	Typical metal	○	×
	Formal rearrangement of en-aldimin (Momiyama et al.)	Complex multi-step reaction	○	×
Heterogeneous	Formic acid decomposition process on zinc oxide surface	Metal oxide	○	×
Other	Bowl type inversion of Pd norcorrole (Shinokubo et al.)	Inversion of bowl-shaped molecular	○	○
	Encapsulation process of Ar atom into fullerene (Murata et al.)	Endohedral fullerene Molecular surgery	○	×