

Summary

February 11, 2016

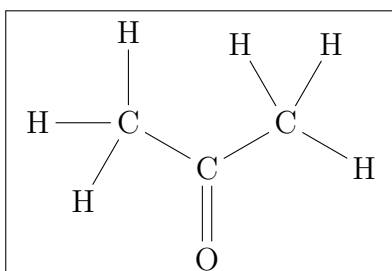
Contents

0.1	Input Graphs	3
0.1.1	propanone	3
0.1.2	propenol	3
0.1.3	butenol	3
0.1.4	butanone	4
0.1.5	2-pentenol	4
0.1.6	2-pentanone	5
0.1.7	3-pentenol	5
0.1.8	3-pentanone	5
0.1.9	3-methylbutenol	6
0.1.10	3-methylbutanone	6
0.1.11	methanal	7
0.1.12	ethanal	7
0.1.13	propanal	7
0.2	Input Rules	8
0.2.1	2.2.1 Aldol-Reaktion (saeurekatalytisch) main	8
0.2.2	2.2.1 Aldol-Reaktion (saeurekatalytisch) Keto-Enol-Tautomerisation	9
0.2.3	1.1. Chlorierung Alkane	9
0.2.4	1.2.1 Arndt-Eistert-Synthese	10
0.2.5	1.2.2 cannizzaro-Reaktion	11
0.2.6	1.2.3. Claisen-Kondensation	12
0.2.7	1.2.4. Grignard-Reaktion 1	13
0.2.8	1.2.4. Grignard-Reaktion 2	14
0.2.9	1.2.4. Grignard-Reaktion 1	16
0.2.10	1.2.4. Grignard-Reaktion 4	17
0.2.11	1.2.5 Knoevenagel-Reaktion Esterspaltung	18
0.2.12	1.2.5 Knoevenagel-Reaktion hin	19
0.2.13	1.2.5 Knoevenagel-Reaktion rueck	20
0.2.14	1.2.6 Prileschajew-Oxidation 1	21
0.2.15	br-naexchange	22
0.2.16	1.2.7 Wurz-Reaktion c-bondformation	23
0.2.17	1.2.8 Wurz-Fittig-Synthese	24
0.2.18	1.3.1 Kerhalogenierung von Aromaten	25
0.2.19	2.1.1 Aldol-Reaktion (basekatalysiert)	26
0.2.20	2.1.2 Mannich Reaktion	27
0.2.21	2.2.1 Aldol-Reaktion (saeurekatalytisch) main	28
0.2.22	2.2.1 Aldol-Reaktion (saeurekatalytisch) Keto-Enol-Tautomerisation	29
0.2.23	2.2.2 Baeyer-Villiger-Oxidation	29
0.2.24	2.2.3 cyanhydrinbildung aldehyd	30
0.2.25	2.2.3 cyanhydrinbildung ketone	31
0.2.26	2.2.4 Perkin-Reaktion	32

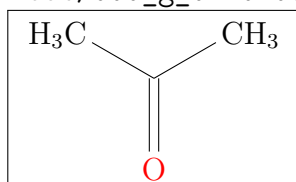
0.2.27	2.3.1 AcyloinKondensation	33
0.2.28	2.3.2. Pinakol-Kopplung	35
0.2.29	3.1.1 Lossen-Abbau	35
0.2.30	3.2 Bimolekulare Eliminierung, E2	36
0.2.31	4.1 Wagner-Meerwein-Umlagerung	37
0.2.32	4.2. Pinakol Umlagerung 1	38
0.2.33	4.2. Pinakol Umlagerung 2	39
0.2.34	4.3. Fries-Umlagerung Para 1	40
0.2.35	4.3. Fries-Umlagerung Para 2	41
0.2.36	4.3. Fries-Umlagerung Ortho 3	42
0.2.37	4.3. Fries-Umlagerung Ortho 4	43
0.2.38	4.4. Keto-Enol-Tautomerie 1	44
0.2.39	4.4. Keto-Enol-Tautomerie 2	45
0.2.40	4.5. Beckmann-Umlagerung 1	46
0.2.41	4.5. Beckmann-Umlagerung 2	46
0.2.42	4.6 Benzilsaureumlagerung	47
0.2.43	4.7. Claisen-Umlagerung 1	48
0.2.44	4.7. Claisen-Umlagerung 2	49
0.2.45	4.7. Claisen-Umlagerung 3	50
0.2.46	4.7. Claisen-Umlagerung 4	51
0.2.47	4.7. Claisen-Umlagerung 5	52
0.2.48	4.7. Claisen-Umlagerung 6	54
0.2.49	5.1 Erlenmaeyer-Ploechl-Azlacton-Synthese	55
0.2.50	Wittig1	57
0.2.51	5.3 Wolff-Kishner-Rule	58
0.2.52	DG Hyper, dg_0	59
0.2.53	DG NonHyper, dg_0	60

0.1 Input Graphs

0.1.1 propanone

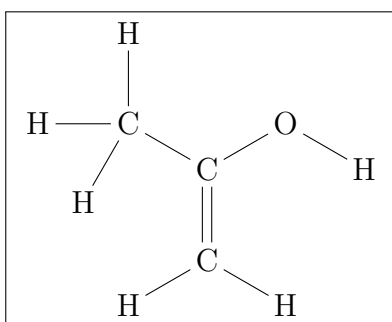


File: out/000_g_0.10100000

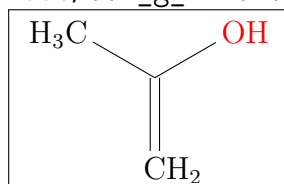


File: out/000_g_0.11110100

0.1.2 propenol

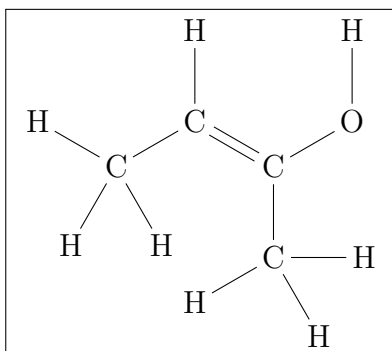


File: out/001_g_1.10100000

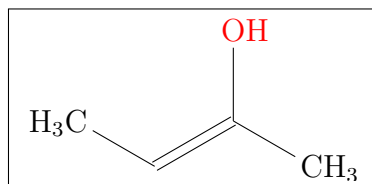


File: out/001_g_1.11110100

0.1.3 butenol

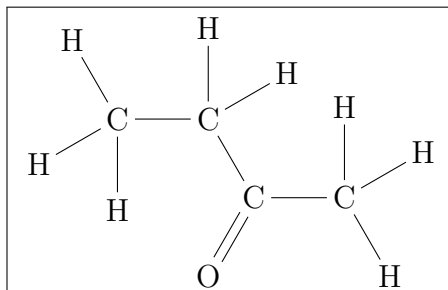


File: out/002_g_2.10100000

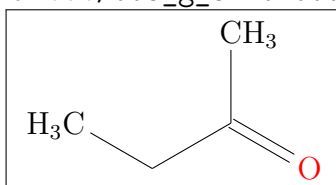


File: out/002_g_2.11110100

0.1.4 butanone

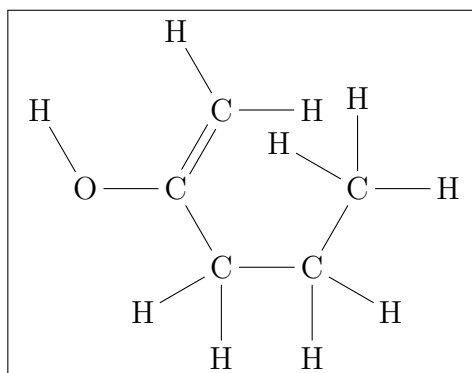


File: out/003_g_3.10100000

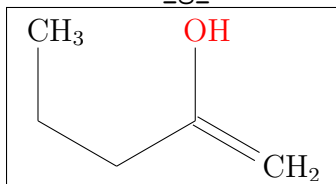


File: out/003_g_3.11110100

0.1.5 2-pentenol

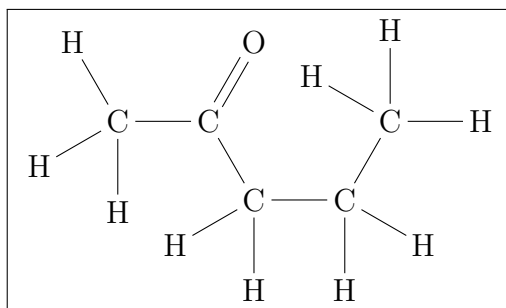


File: out/004_g_4.10100000

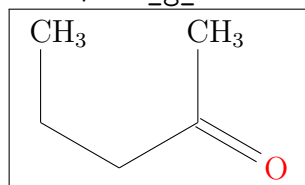


File: out/004_g_4.11110100

0.1.6 2-pentanone

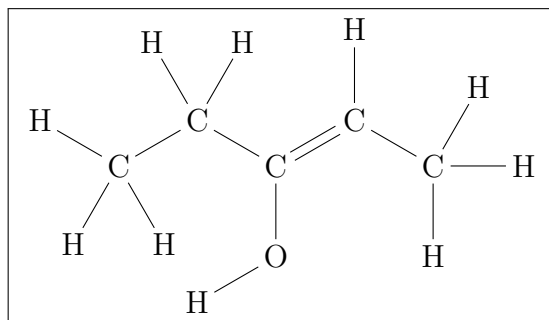


File: out/005_g_5.10100000

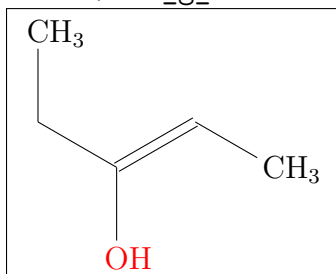


File: out/005_g_5.11110100

0.1.7 3-pentenol

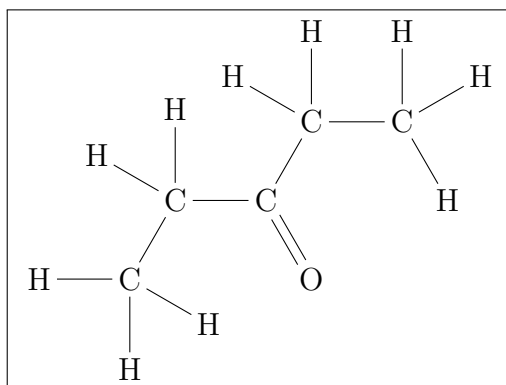


File: out/006_g_6.10100000

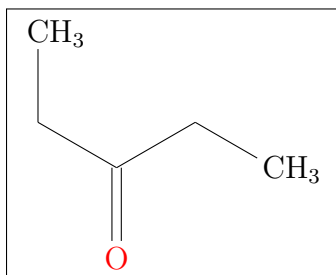


File: out/006_g_6.11110100

0.1.8 3-pentanone

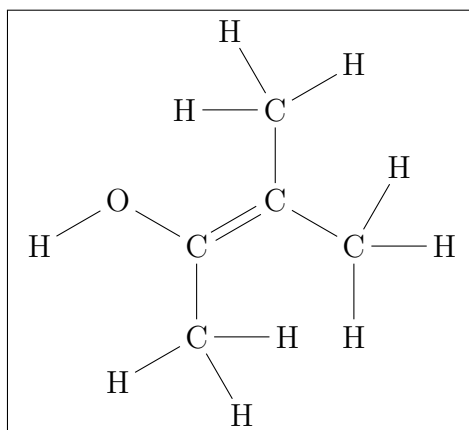


File: out/007_g_7.10100000

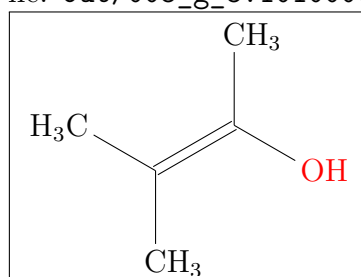


File: out/007_g_7.11110100

0.1.9 3-methylbutenol

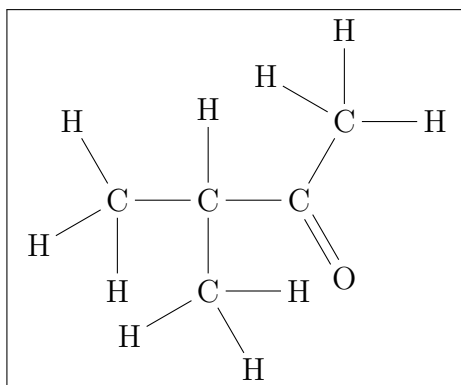


File: out/008_g_8.10100000

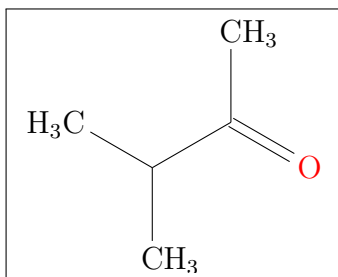


File: out/008_g_8.11110100

0.1.10 3-methylbutanone

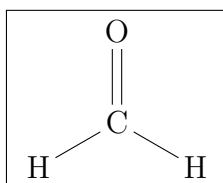


File: out/009_g_9.10100000

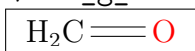


File: out/009_g_9.11110100

0.1.11 methanal

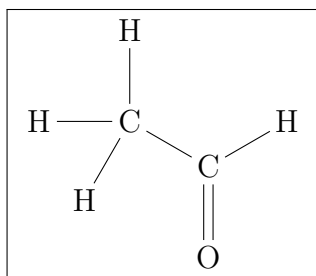


File: out/010_g_10.10100000

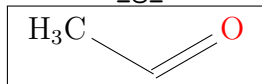


File: out/010_g_10.11110100

0.1.12 ethanal

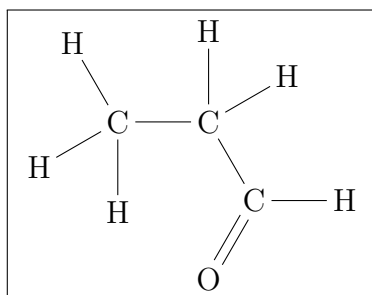


File: out/011_g_11.10100000

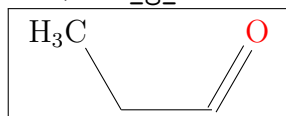


File: out/011_g_11.11110100

0.1.13 propanal



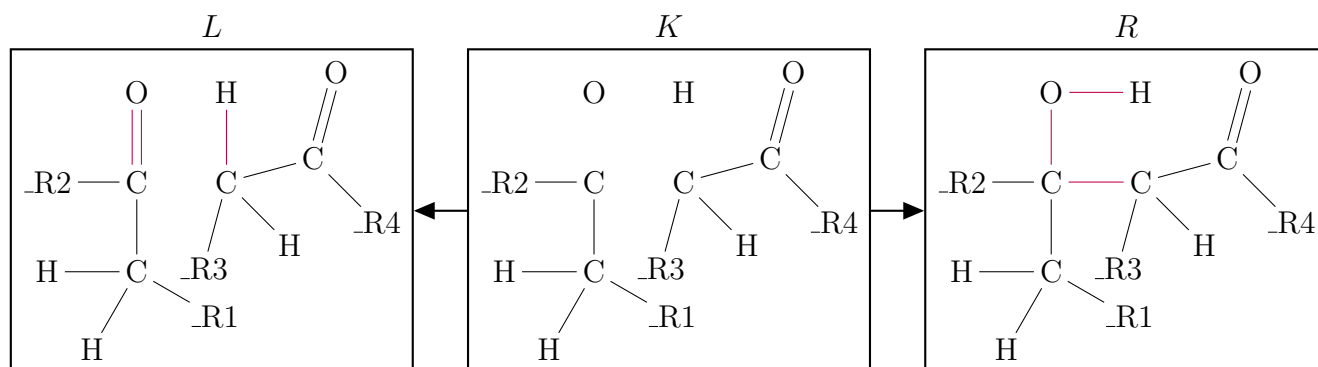
File: out/012_g_12.10100000



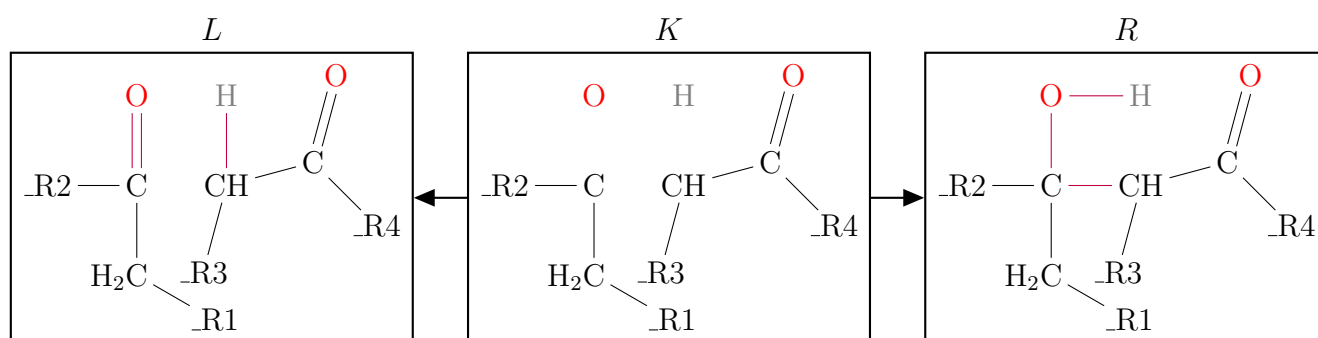
File: out/012_g_12.11110100

0.2 Input Rules

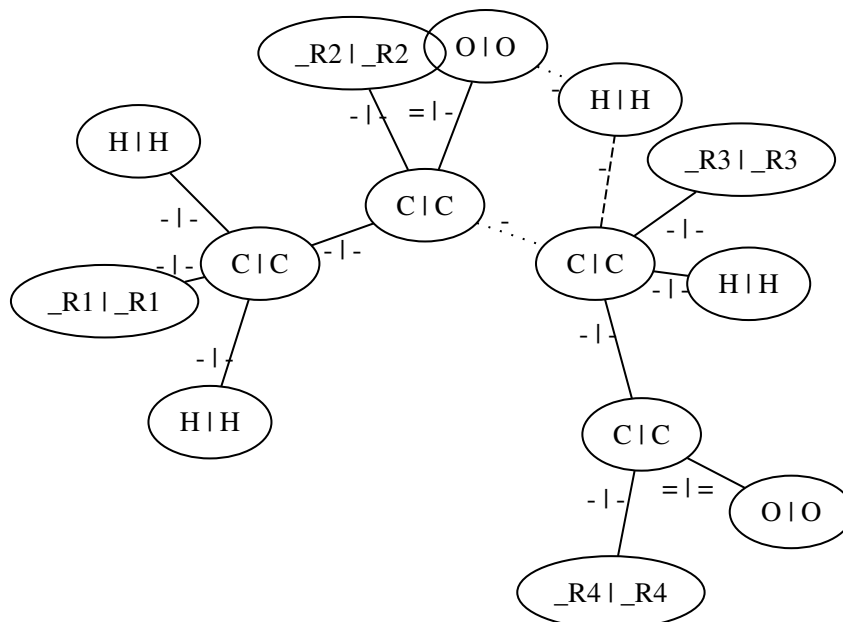
0.2.1 2.2.1 Aldol-Reaktion (saeurekatalytisch) main



Files: out/014_r_0.10100000.{L, K, R}

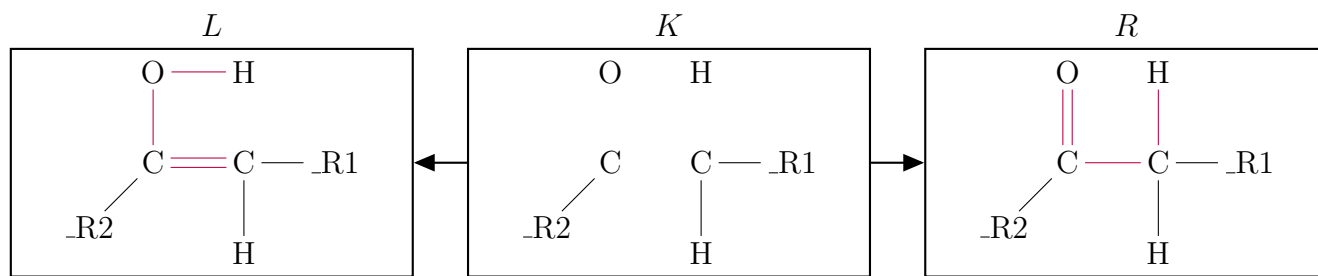


Files: out/015_r_0.11100100.{L, K, R}

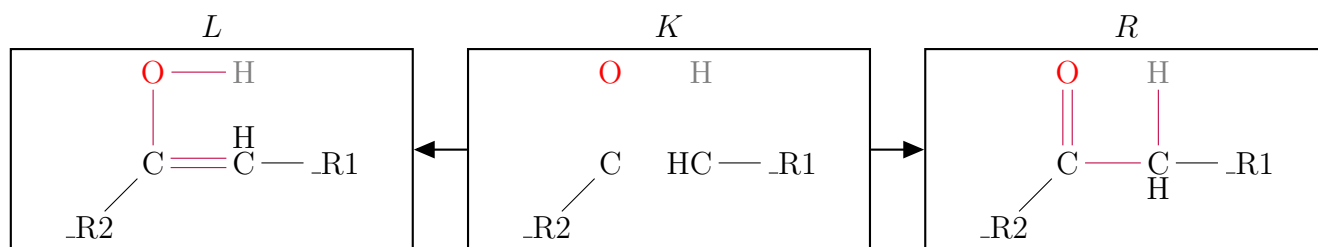


File: out/016_r_0_combined

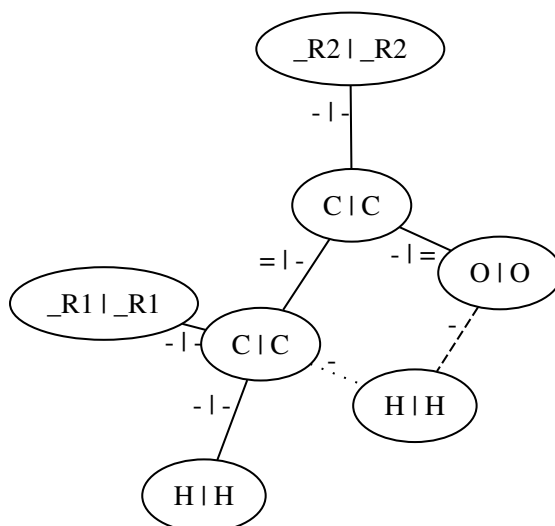
0.2.2 2.2.1 Aldol-Reaktion (saeurekatalytisch) Keto-Enol-Tautomerisation



Files: out/019_r_1.10100000.{L, K, R}

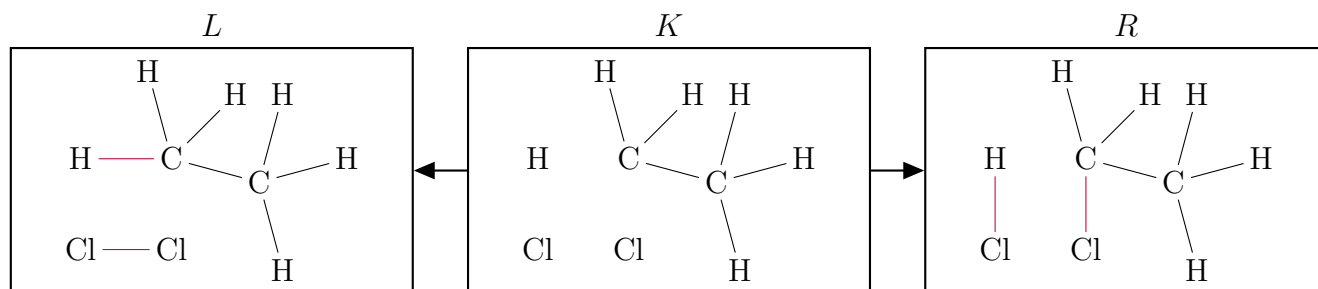


Files: out/020_r_1.11100100.{L, K, R}

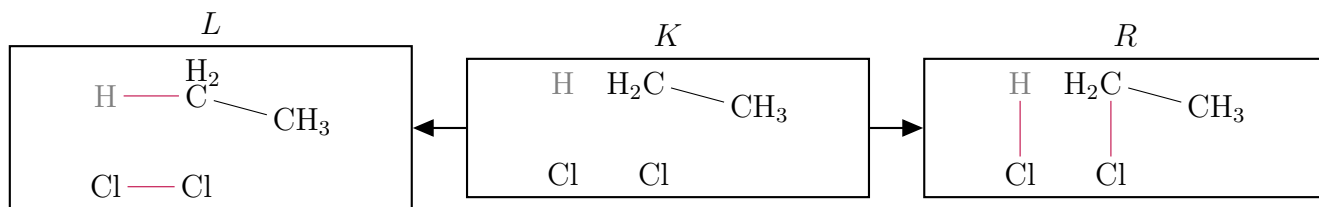


File: out/021_r_1_combined

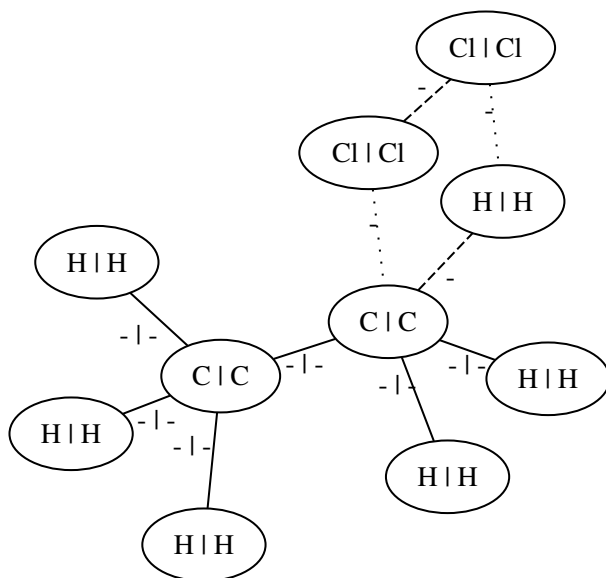
0.2.3 1.1. Chlorierung Alkane



Files: out/024_r_2.10100000.{L, K, R}

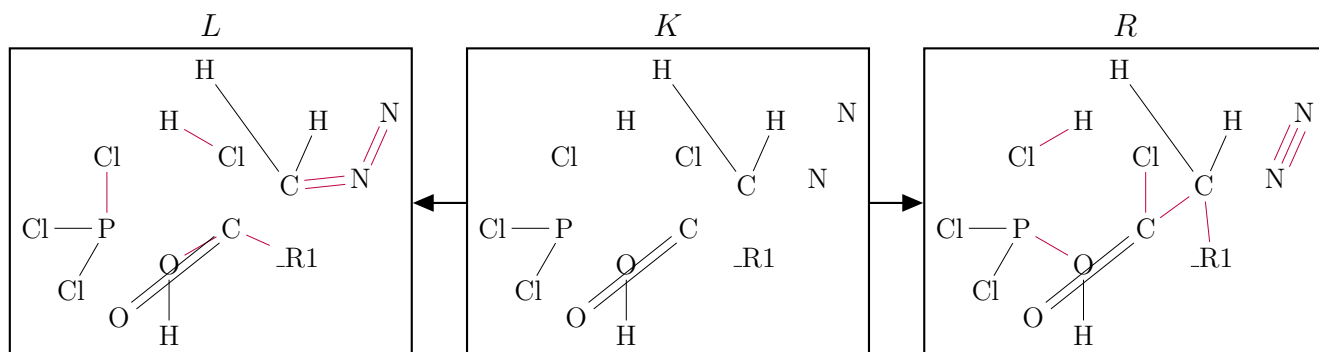


Files: out/025_r_2.11100100.{L, K, R}

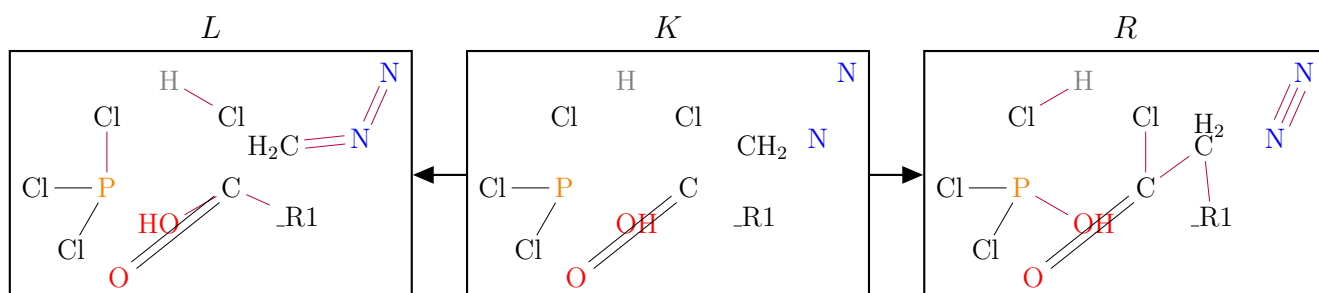


File: out/026_r_2_combined

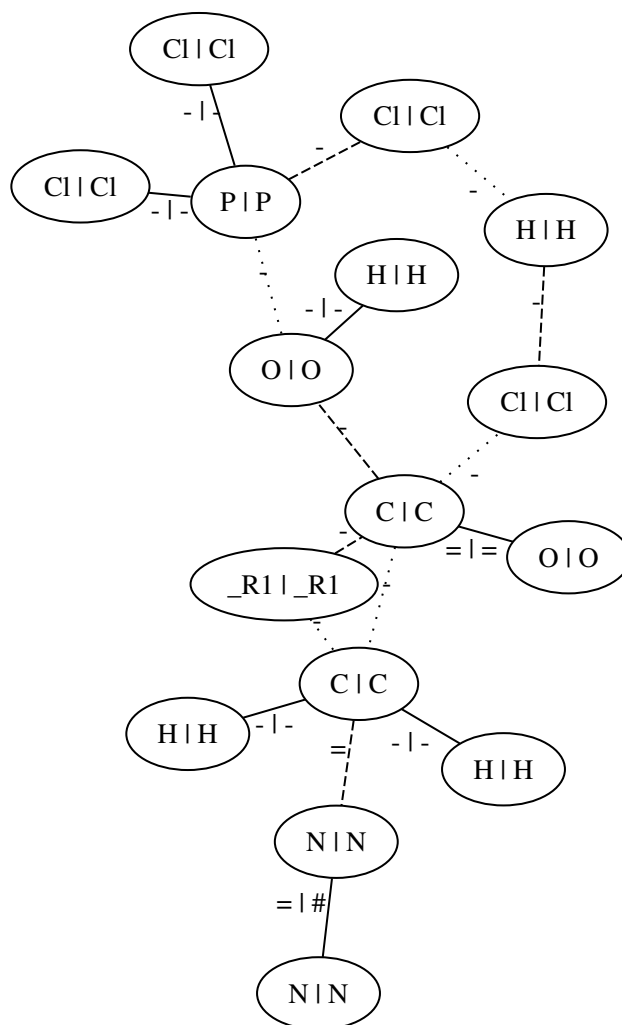
0.2.4 1.2.1 Arndt-Eistert-Synthese



Files: out/029_r_3.10100000.{L, K, R}

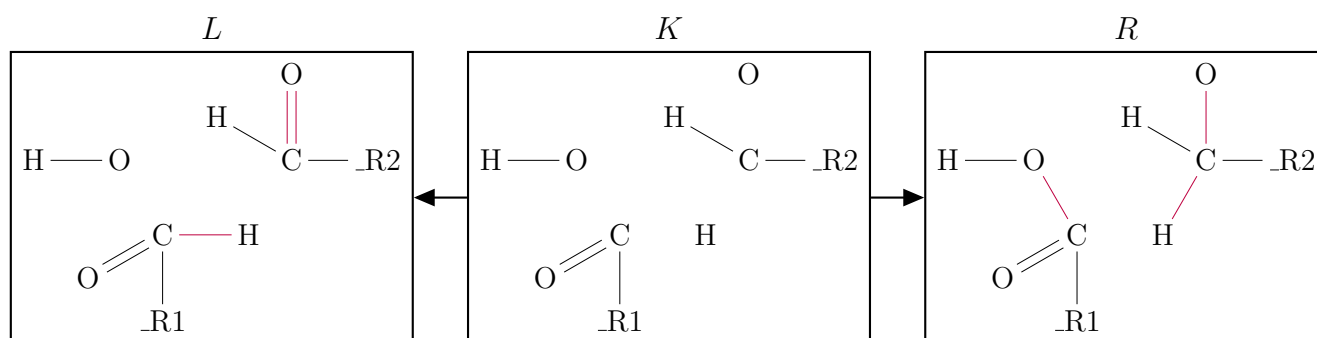


Files: out/030_r_3.11100100.{L, K, R}

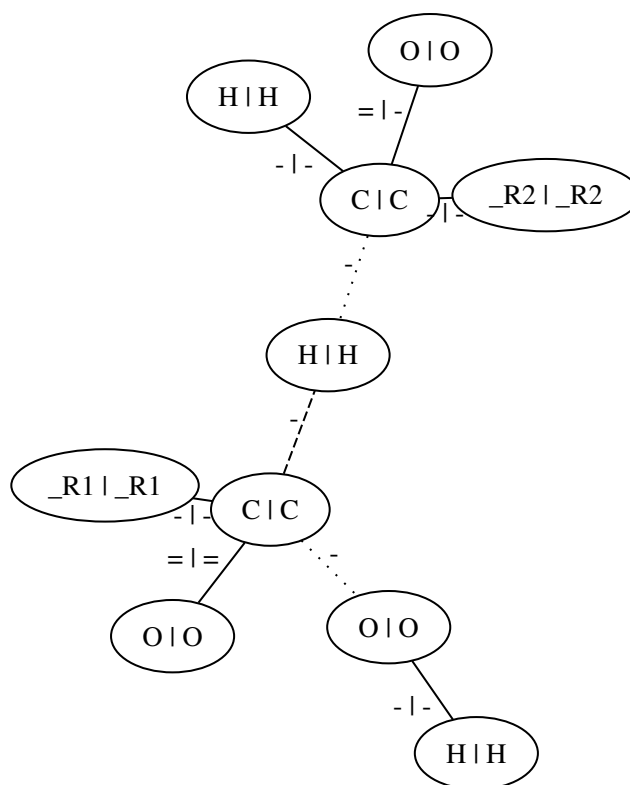
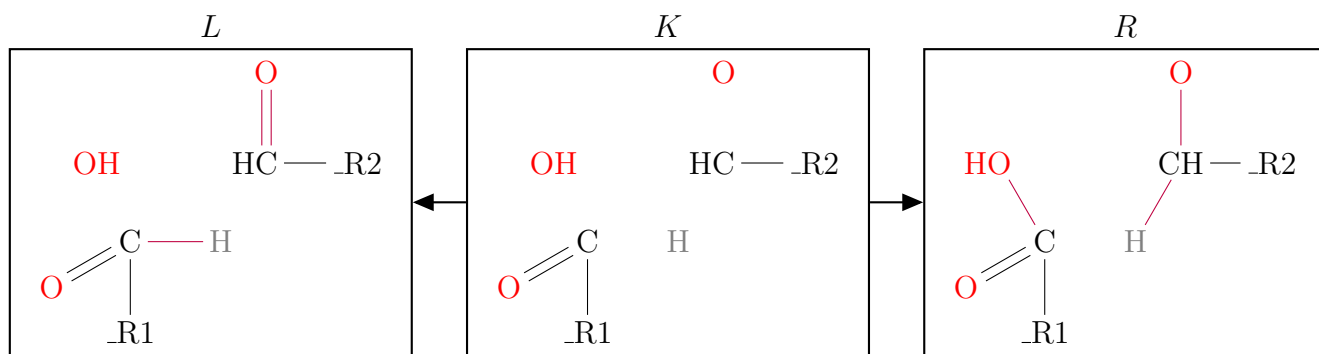


File: out/031_r_3_combined

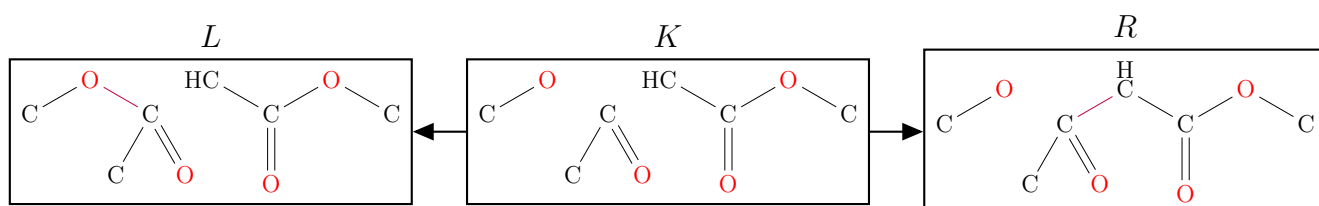
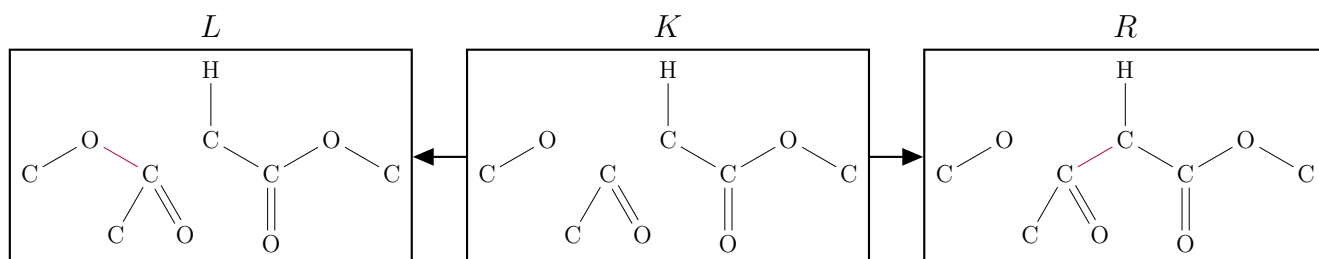
0.2.5 1.2.2 cannizzaro-Reaktion



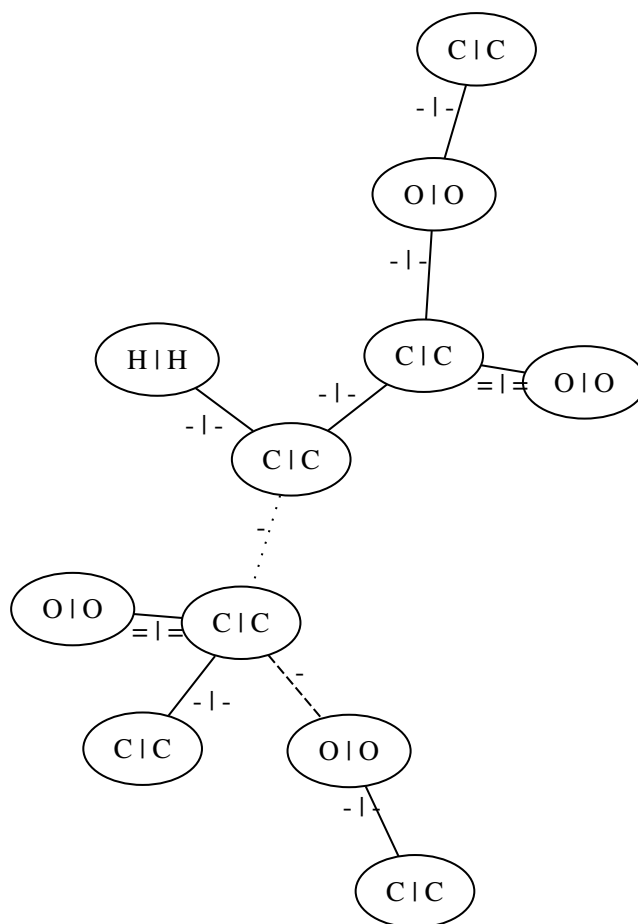
Files: out/034_r_4.10100000.{L, K, R}



0.2.6 1.2.3. Claisen-Kondensation

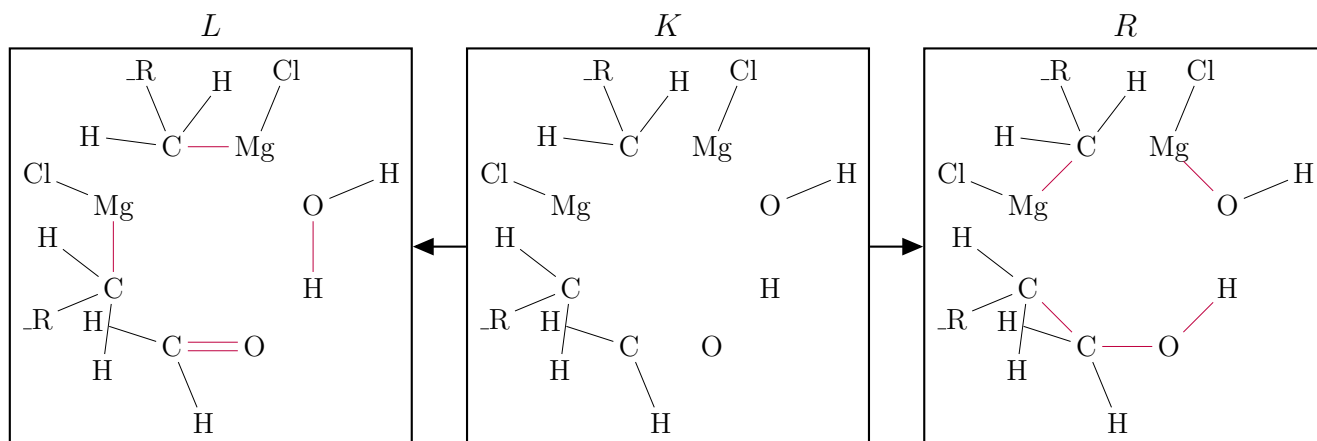


Files: out/040_r_5.11100100.{L, K, R}

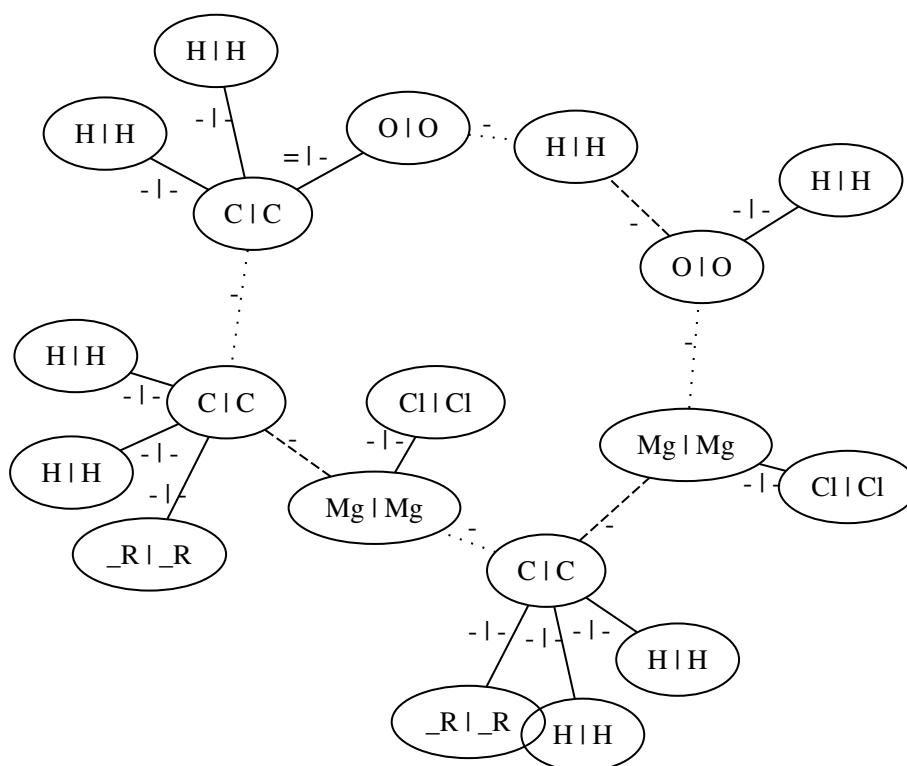
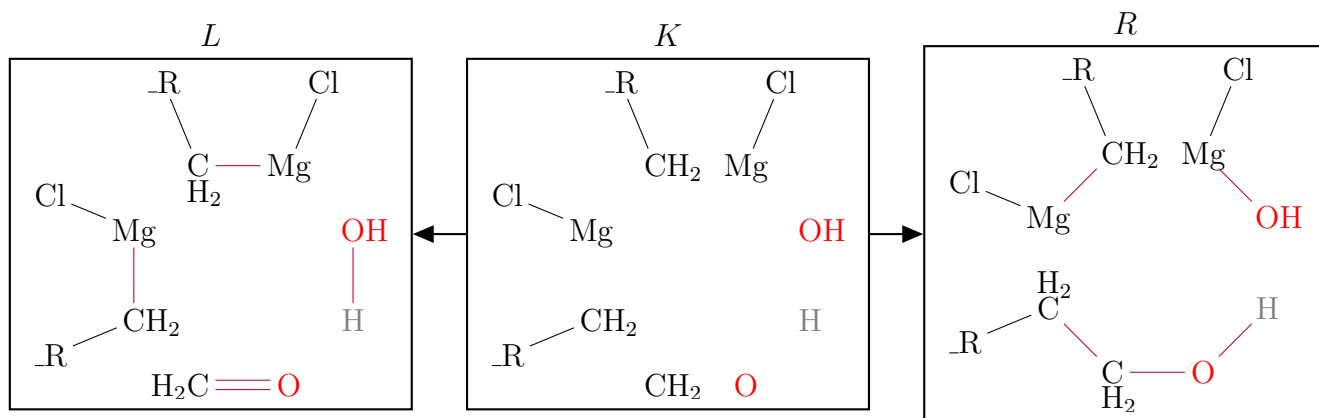


File: out/041_r_5_combined

0.2.7 1.2.4. Grignard-Reaktion 1

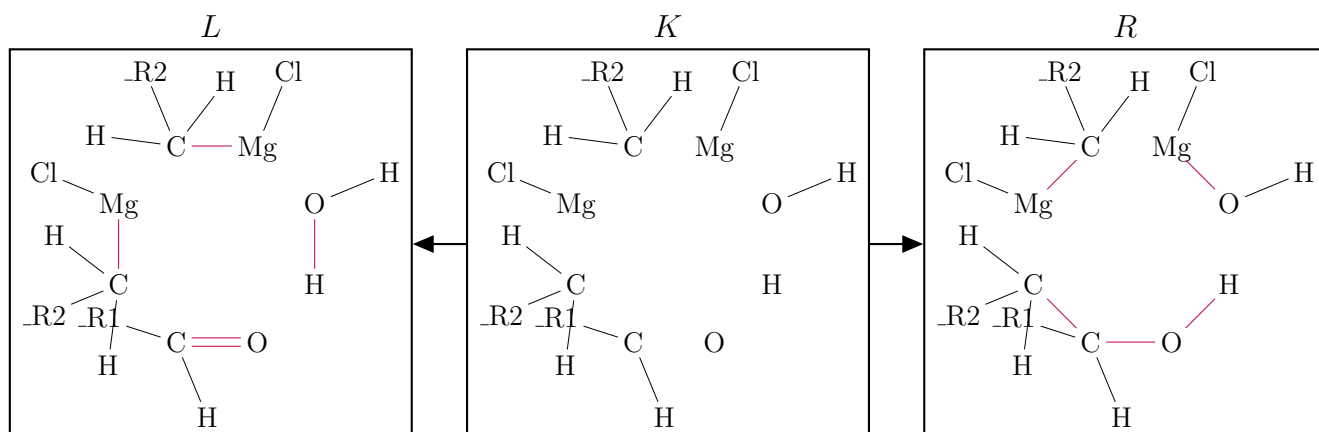


Files: out/044_r_6.10100000.{L, K, R}

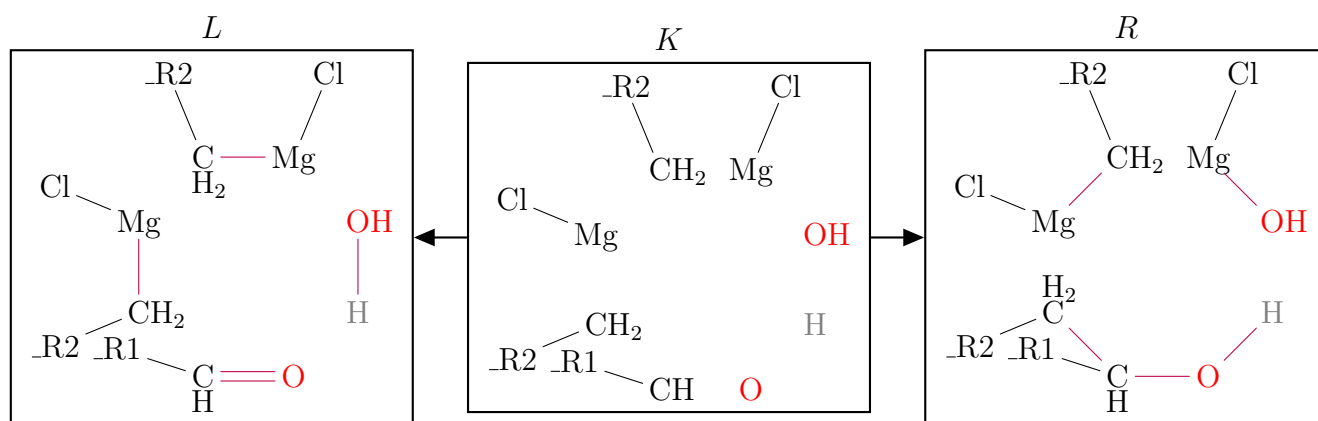


File: out/046_r_6_combined

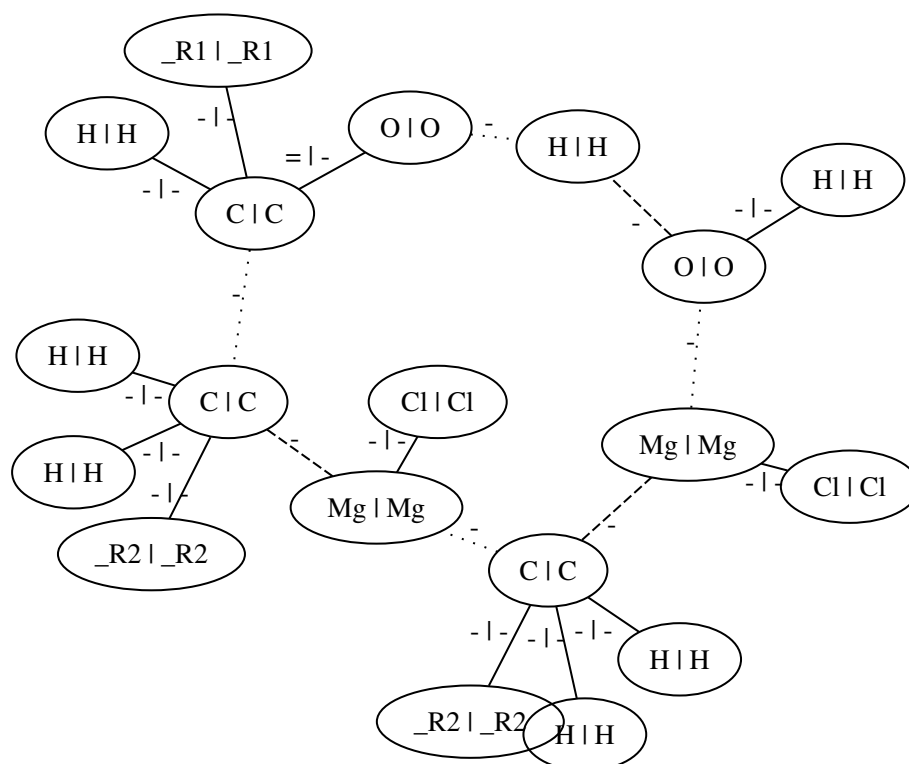
0.2.8 1.2.4. Grignard-Reaktion 2



Files: out/049_r_7.10100000.{L, K, R}

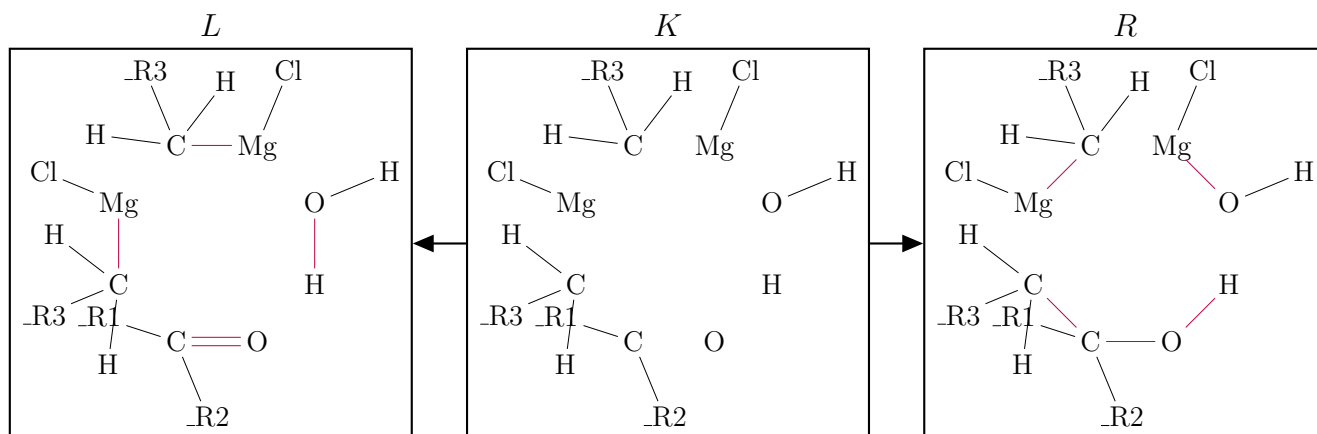


Files: out/050_r_7.11100100.{L, K, R}

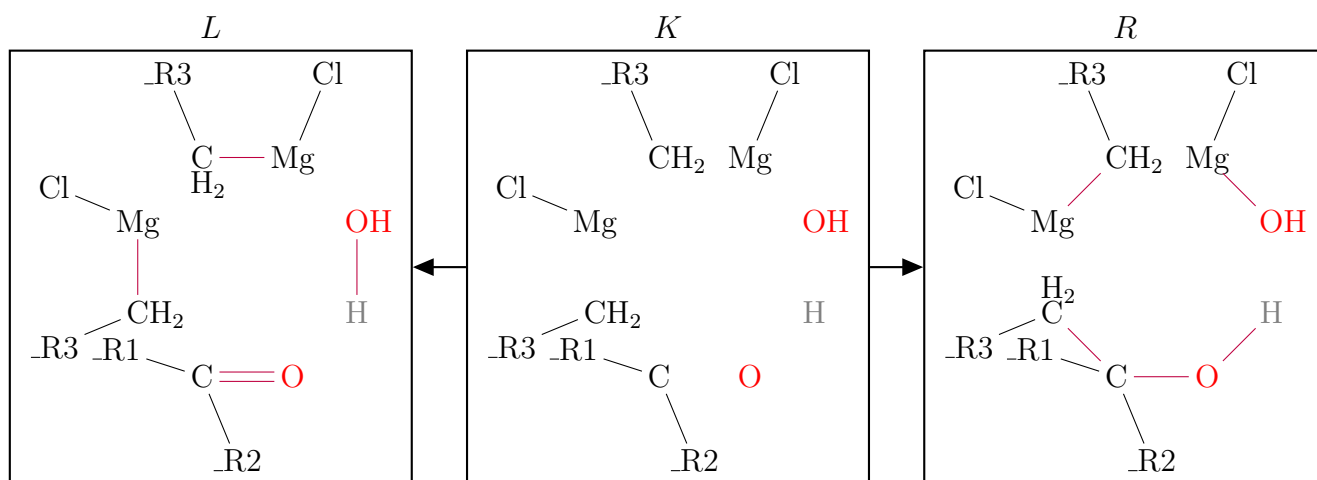


File: out/051_r_7_combined

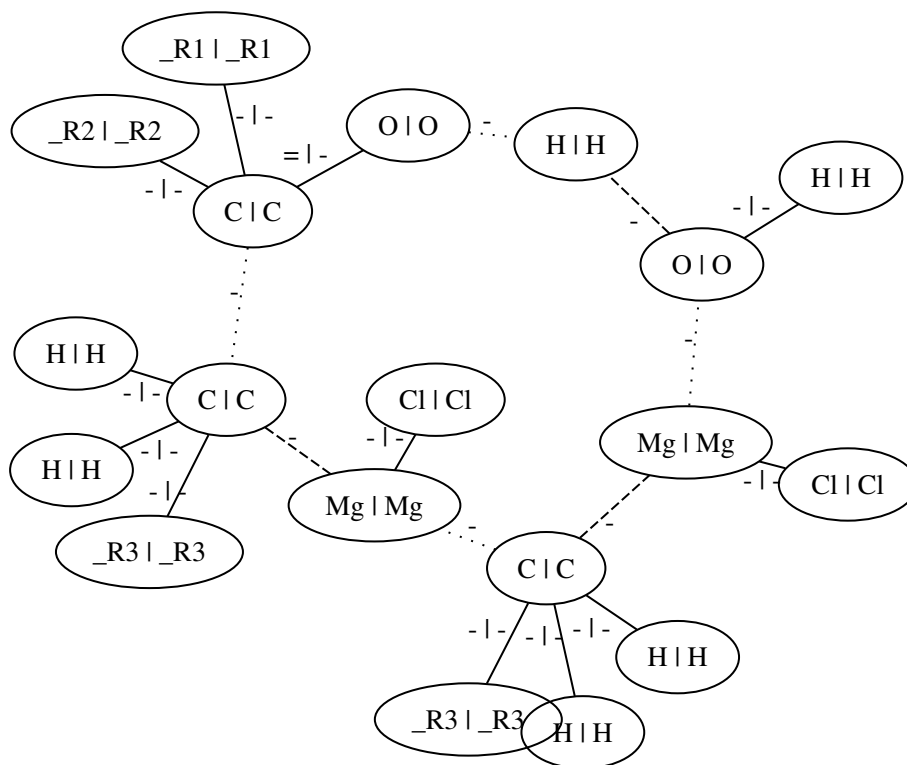
0.2.9 1.2.4. Grignard-Reaktion 1



Files: out/054_r_8.10100000.{L, K, R}

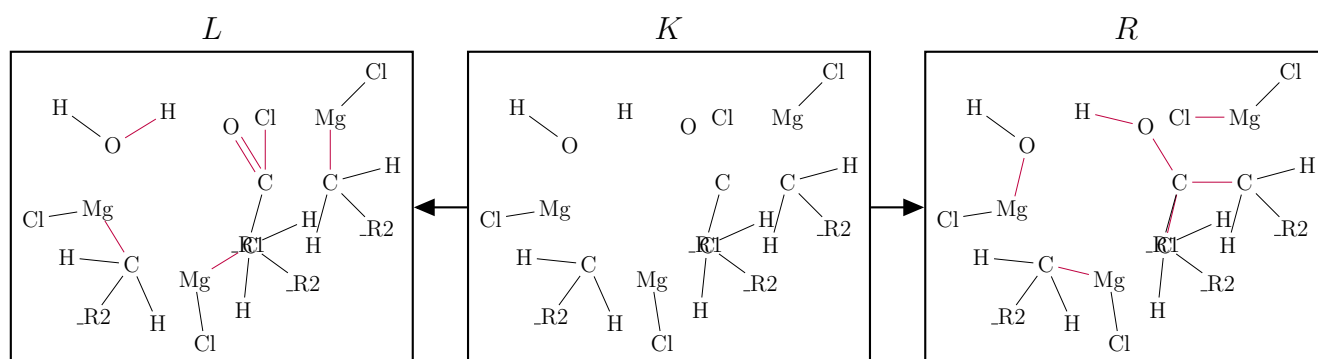


Files: out/055_r_8.11100100.{L, K, R}

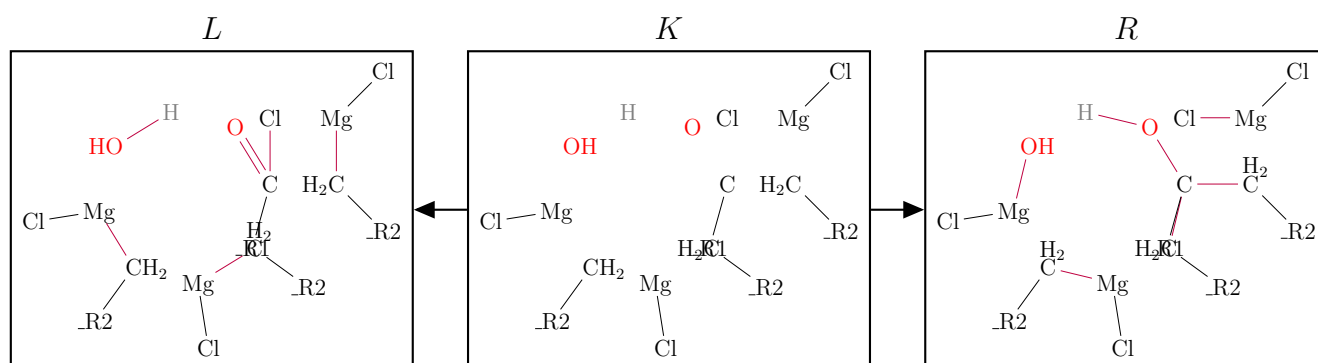


File: out/056_r_8_combined

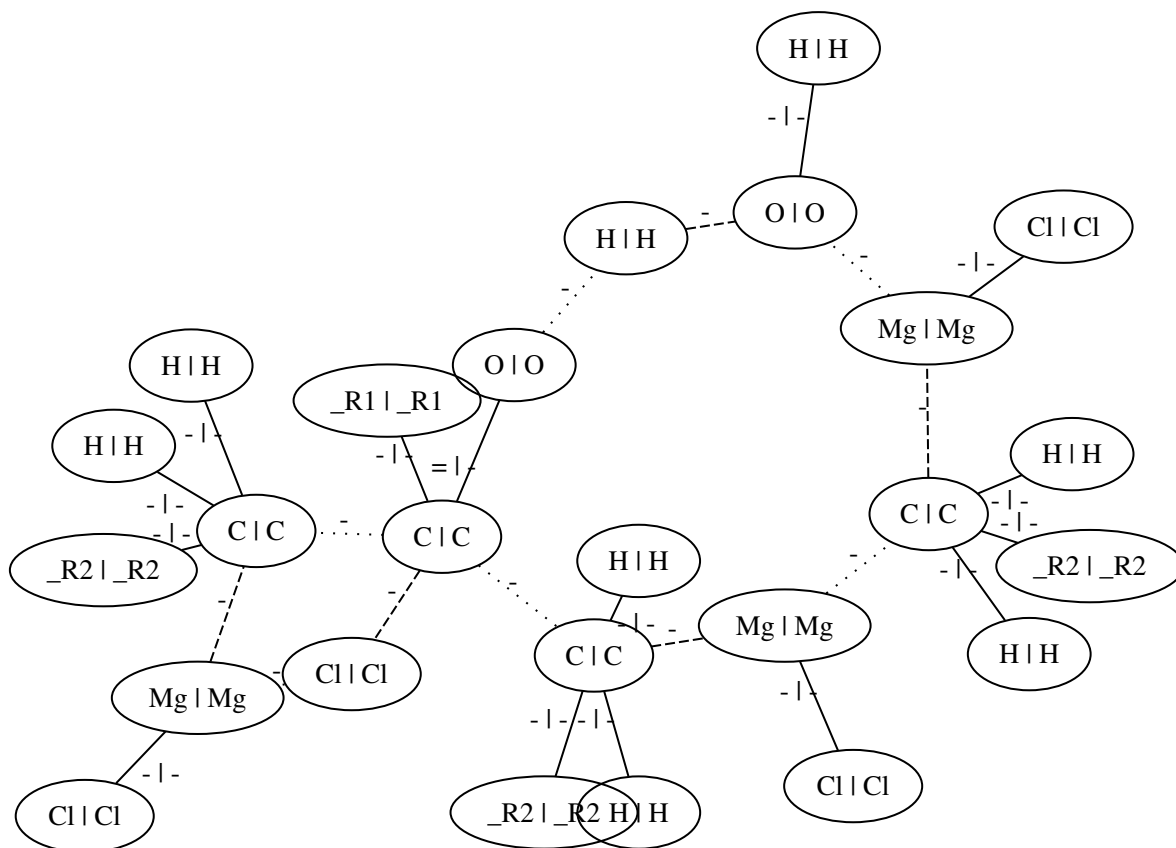
0.2.10 1.2.4. Grignard-Reaktion 4



Files: out/059_r_9.10100000.{L, K, R}

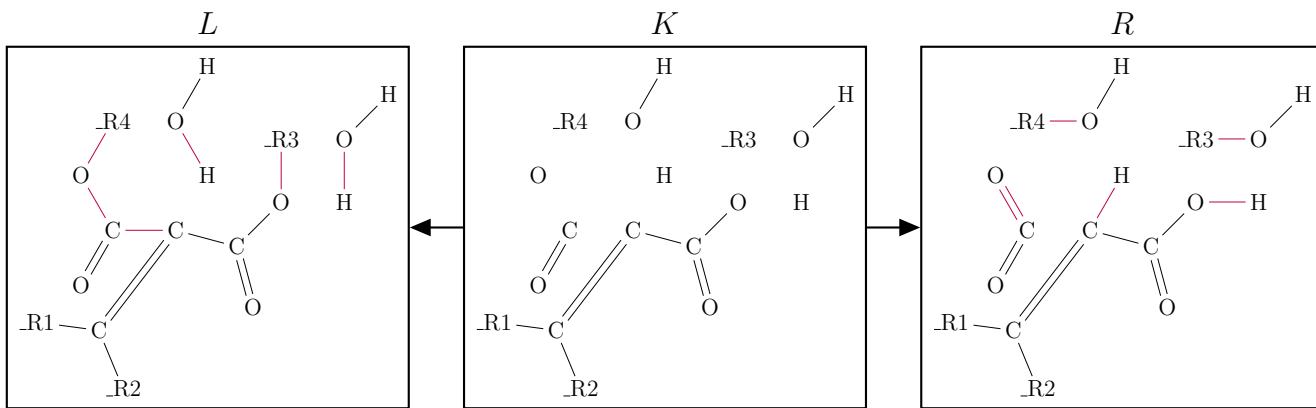


Files: out/060_r_9.11100100.{L, K, R}

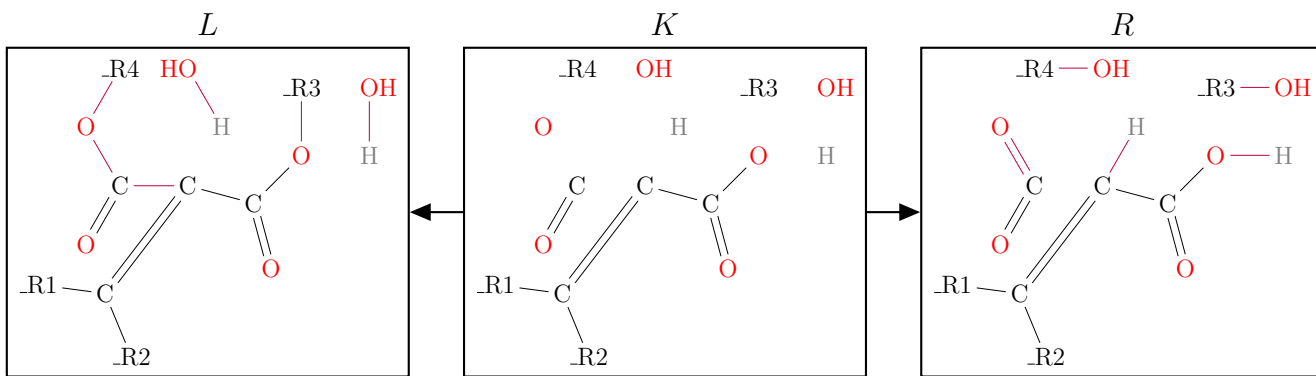


File: out/061_r_9_combined

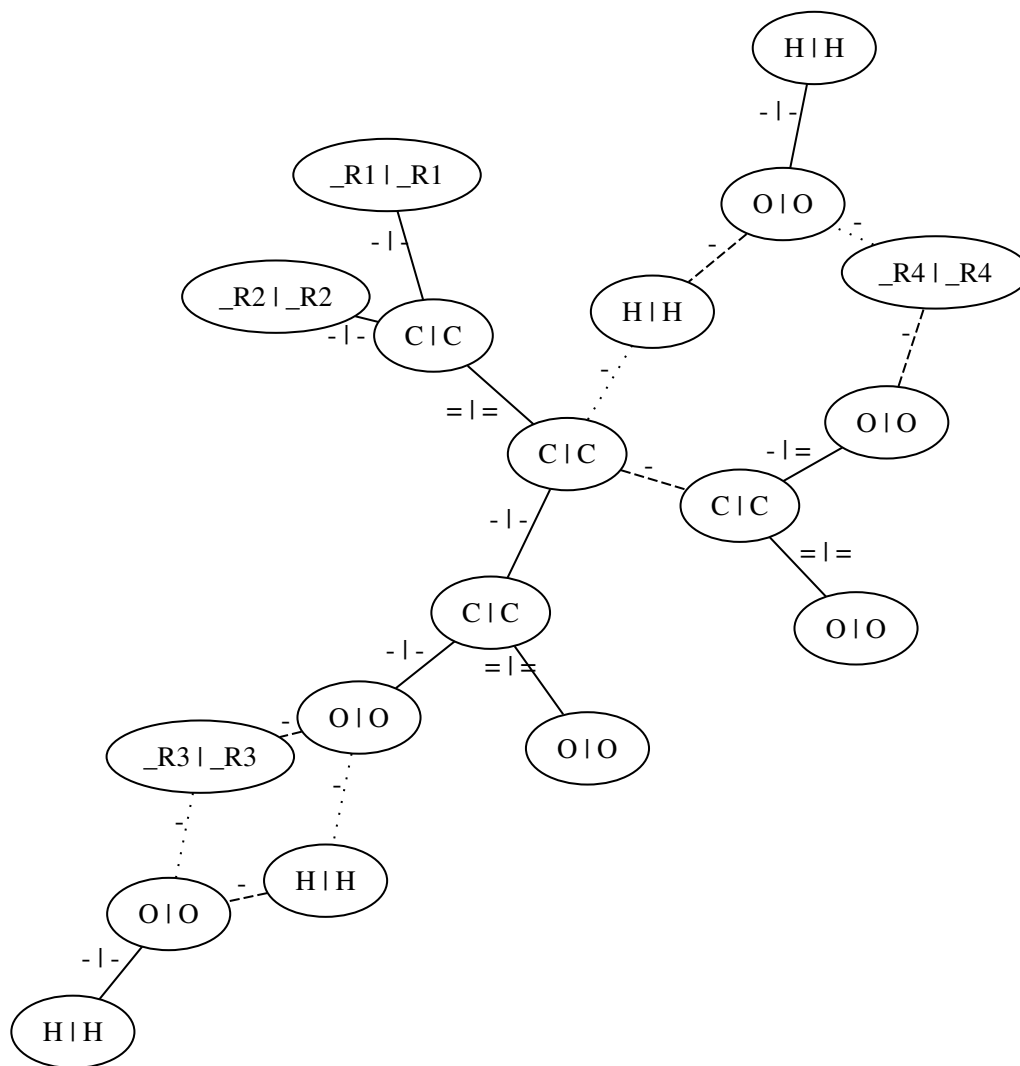
0.2.11 1.2.5 Knoevenagel-Reaktion Esterspaltung



Files: out/064_r_10.10100000.{L, K, R}

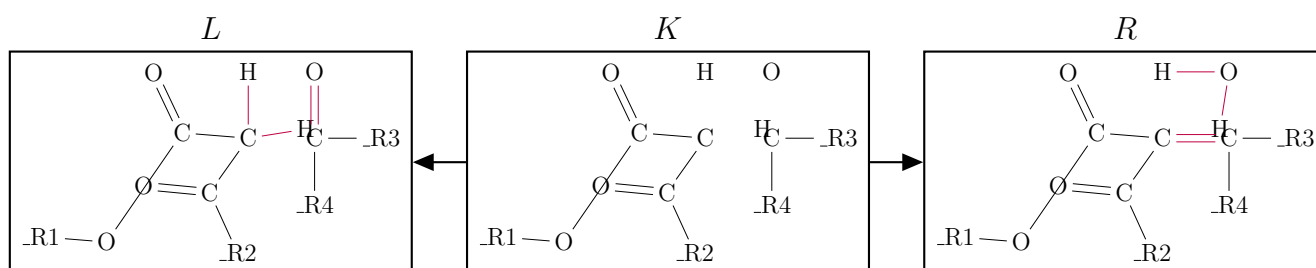


Files: out/065_r_10.11100100.{L, K, R}

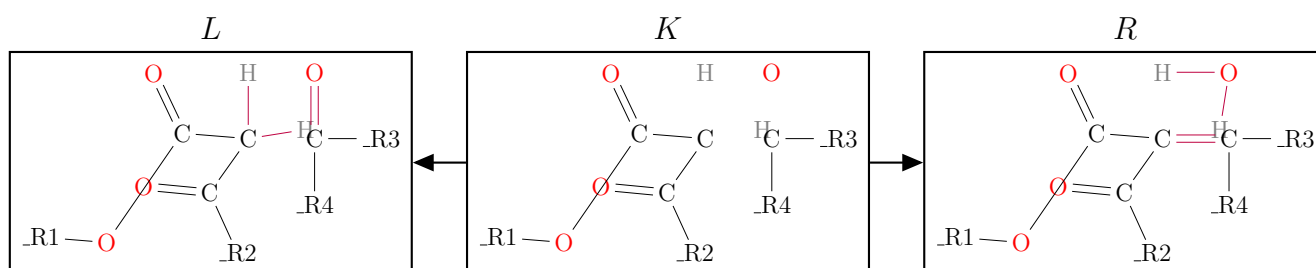


File: out/066_r_10_combined

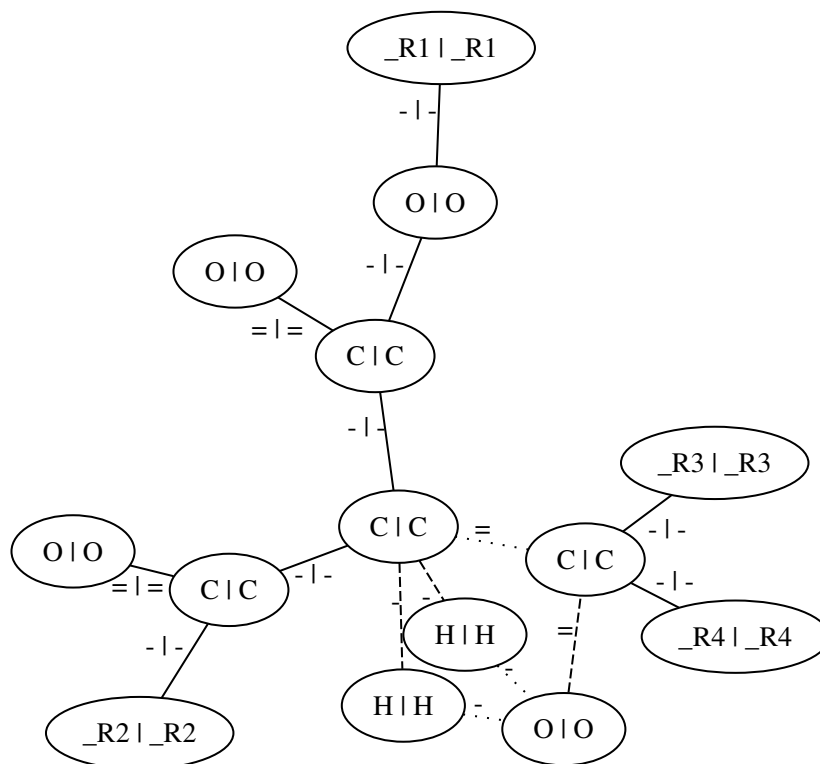
0.2.12 1.2.5 Knoevenagel-Reaktion hin



Files: out/069_r_11.10100000.{L, K, R}

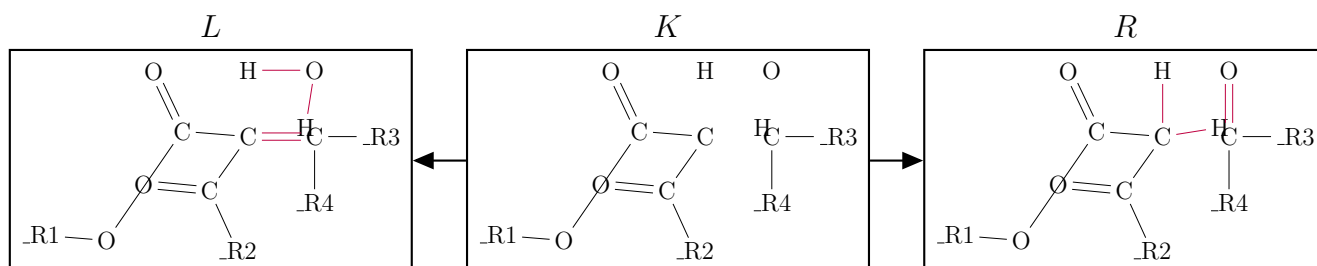


Files: out/070_r_11.11100100.{L, K, R}

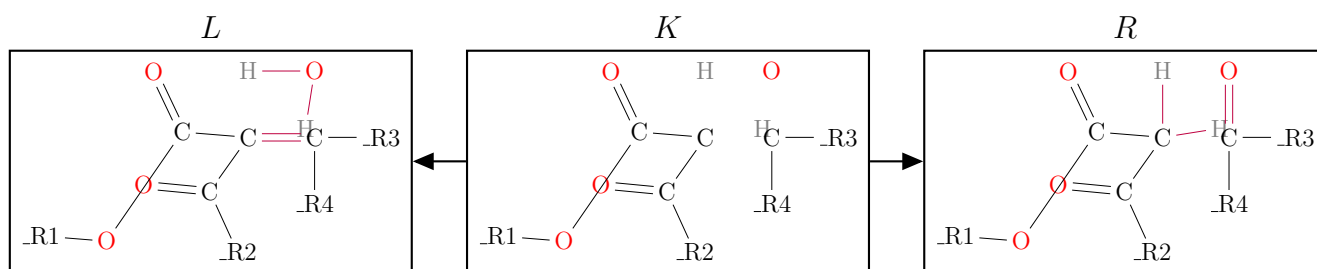


File: out/071_r_11_combined

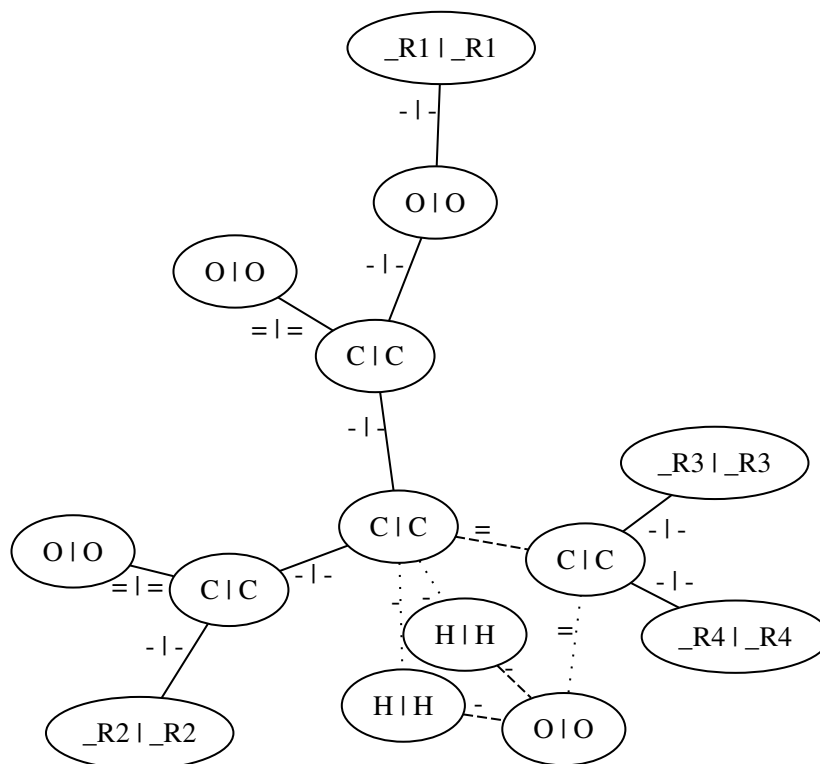
0.2.13 1.2.5 Knoevenagel-Reaktion rueck



Files: out/074_r_12.10100000.{L, K, R}

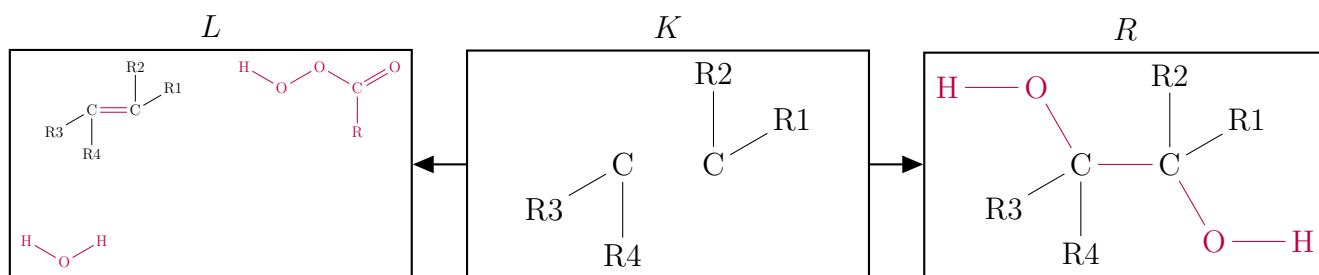


Files: out/075_r_12.11100100.{L, K, R}

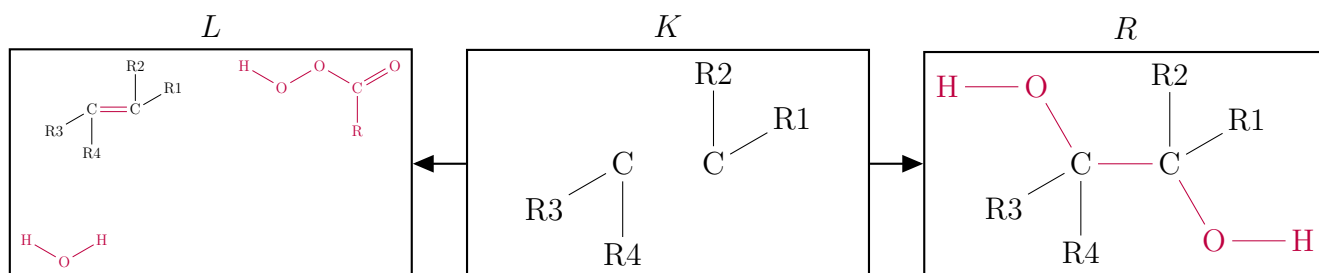


File: out/076_r_12_combined

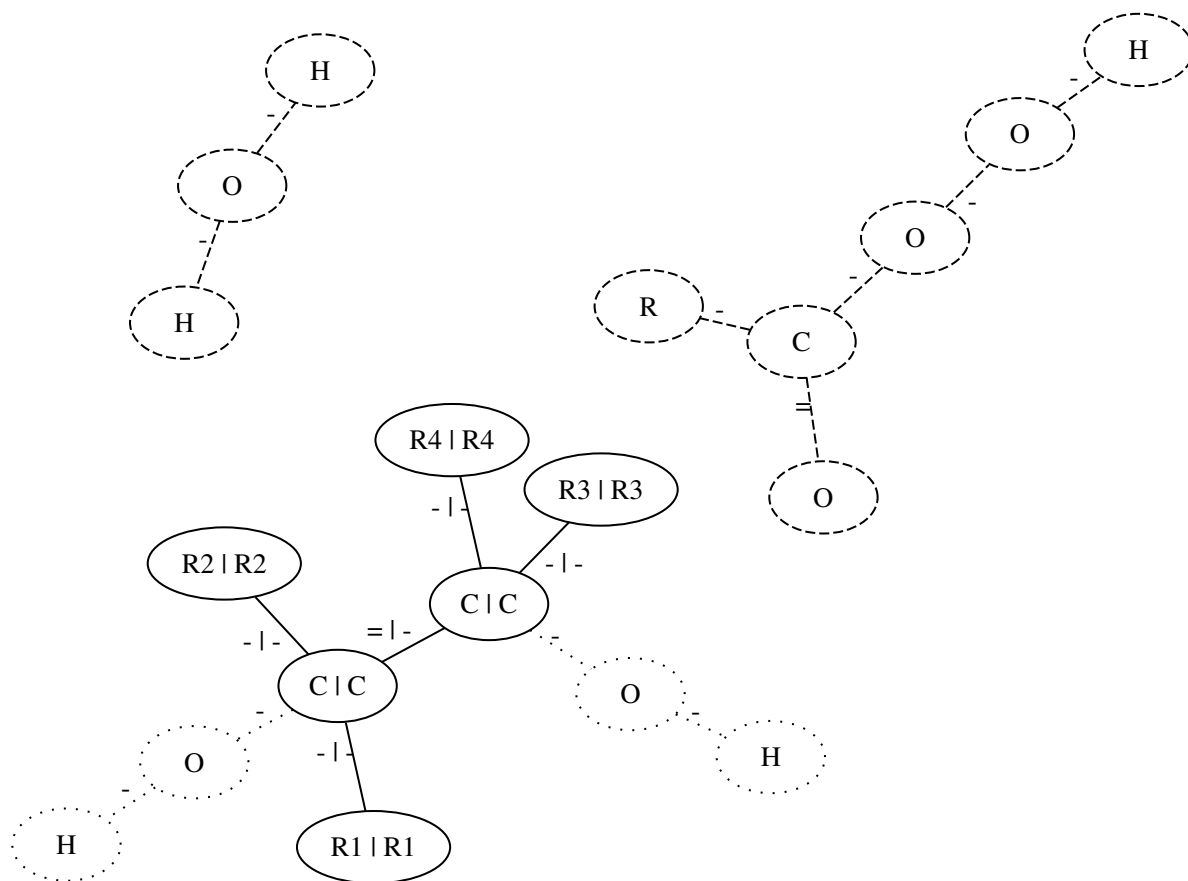
0.2.14 1.2.6 Prileschajew-Oxidation 1



Files: out/079_r_13.10100000.{L, K, R}

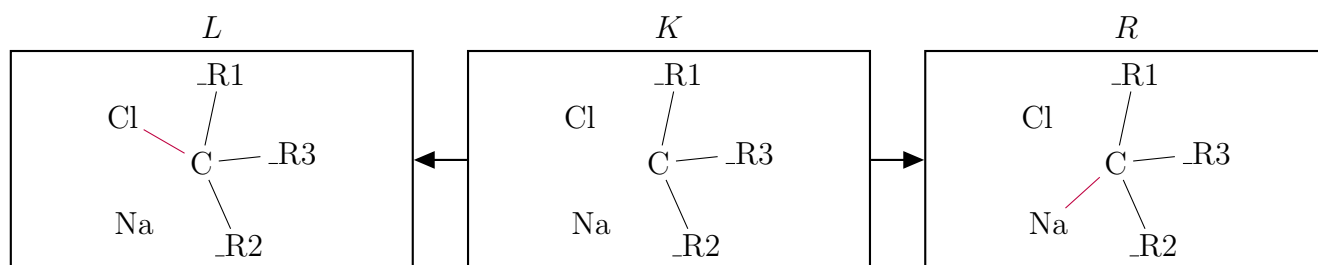


Files: out/080_r_13.11100100.{L, K, R}

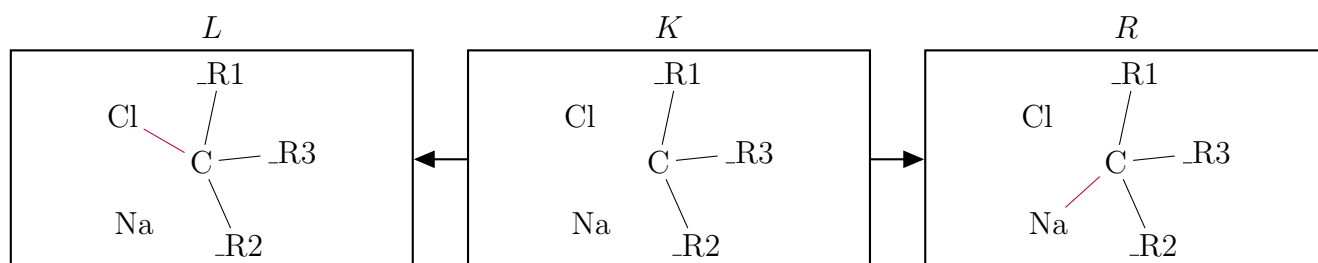


File: out/081_r_13_combined

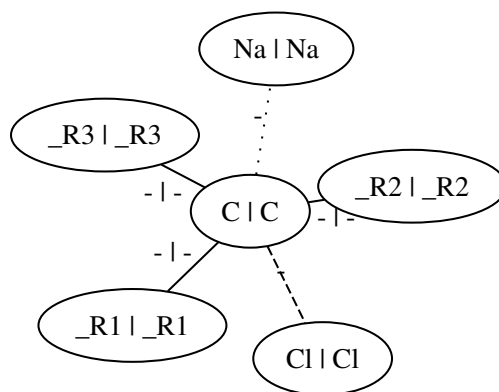
0.2.15 br-naexchange



Files: out/084_r_14.10100000.{L, K, R}

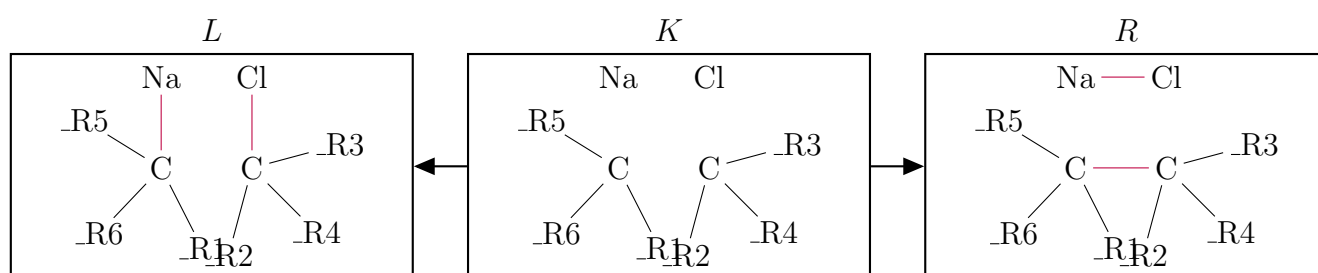


Files: out/085_r_14.11100100.{L, K, R}

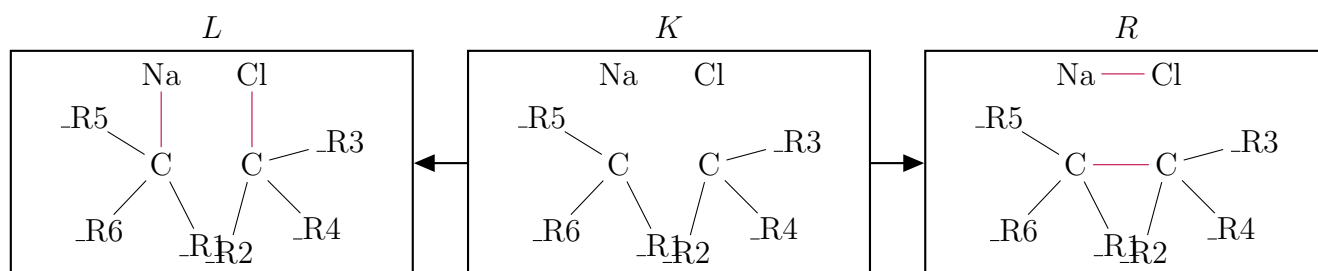


File: out/086_r_14_combined

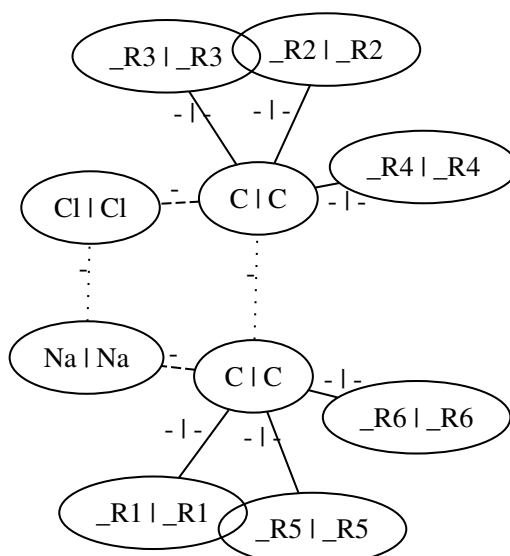
0.2.16 1.2.7 Wurz-Reaktion c-bondformation



Files: out/089_r_15.10100000.{L, K, R}

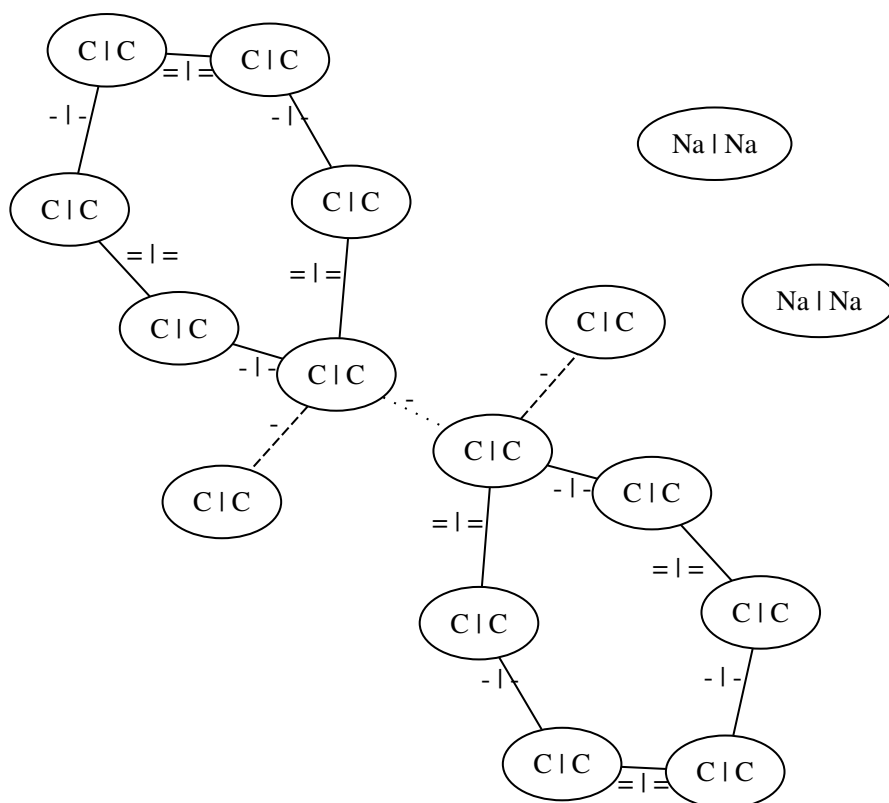
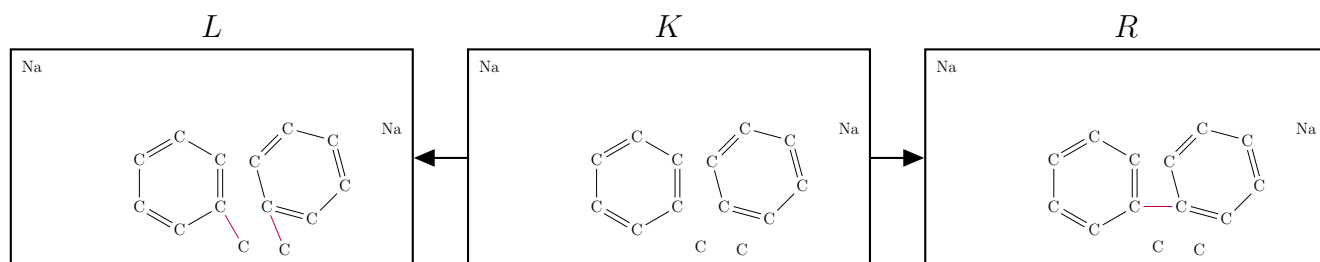
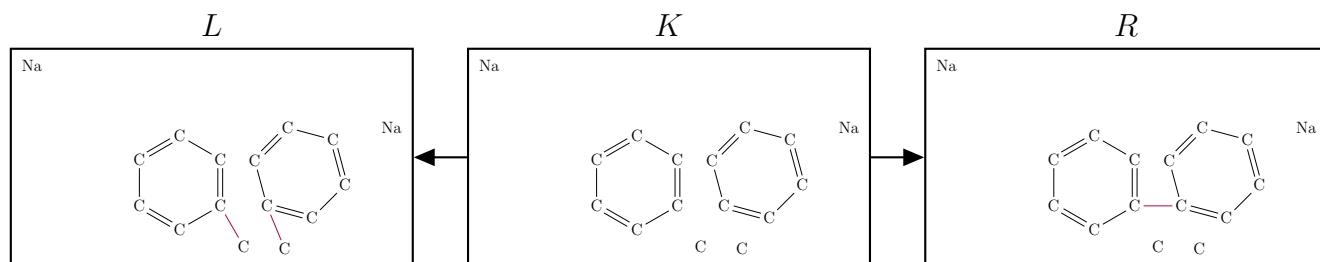


Files: out/090_r_15.11100100.{L, K, R}



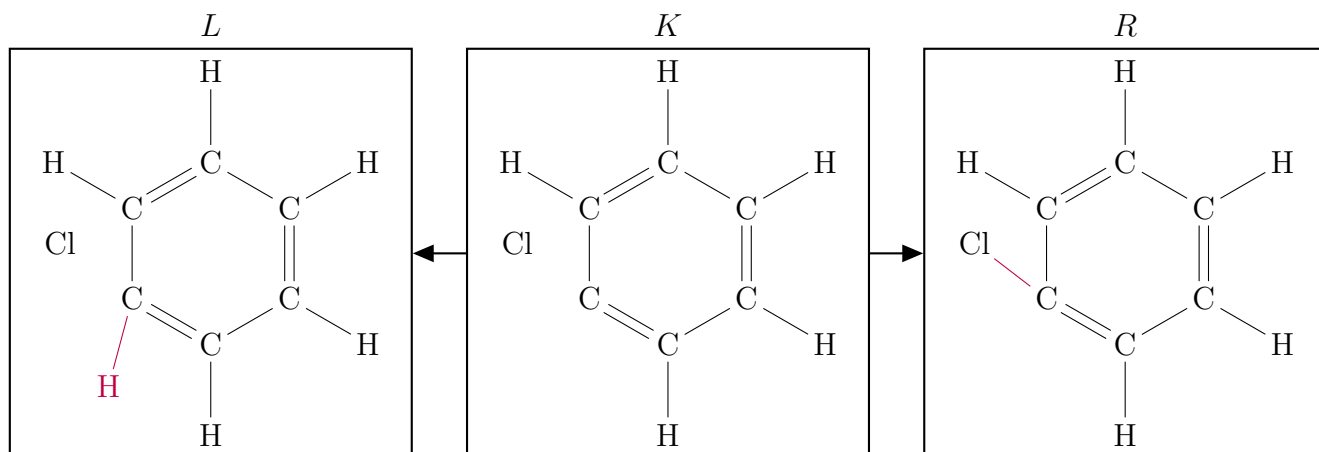
File: out/091_r_15_combined

0.2.17 1.2.8 Wurz-Fittig-Synthese

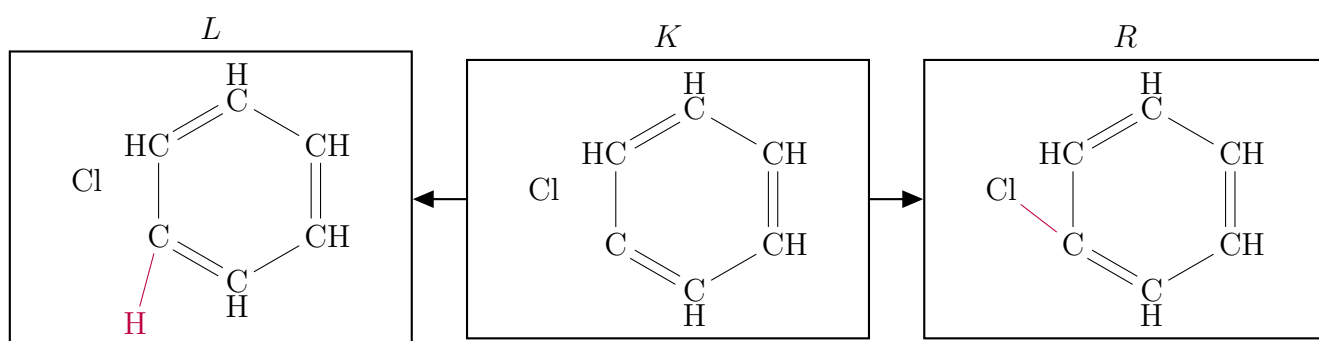


File: out/096_r_16_combined

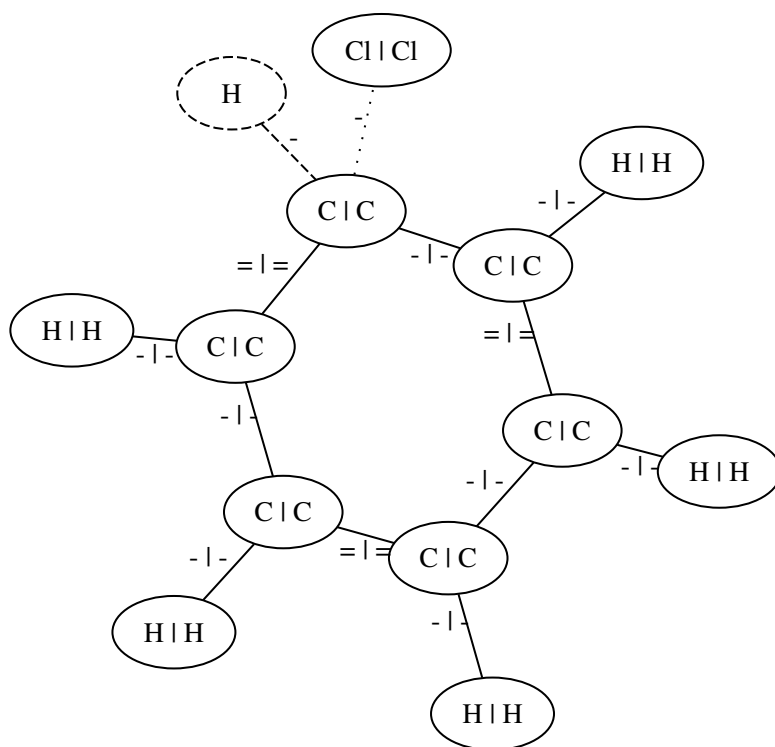
0.2.18 1.3.1 Kerhalogenierung von Aromaten



Files: out/099_r_17.10100000.{L, K, R}

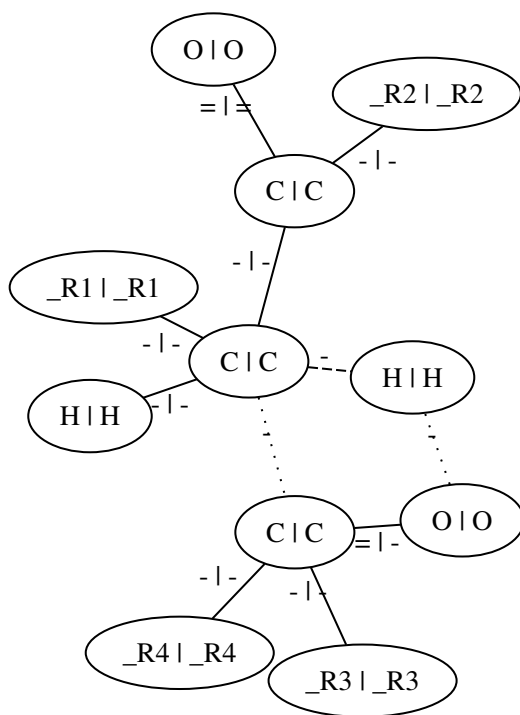
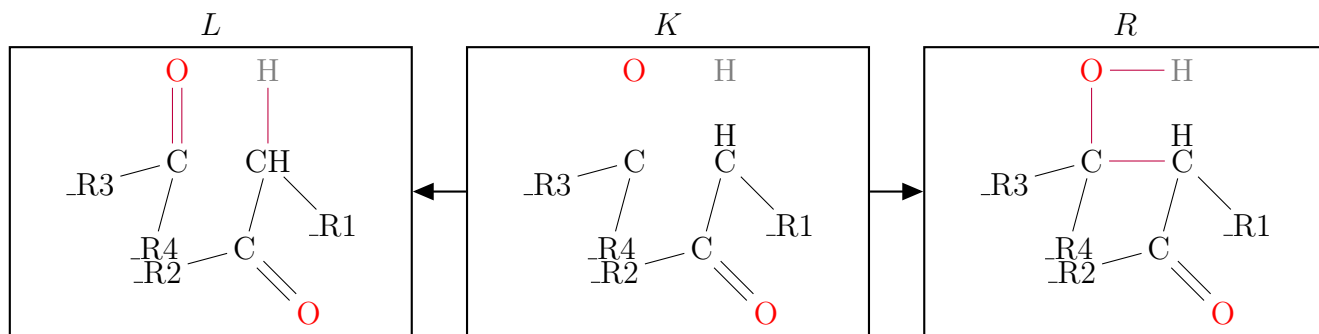
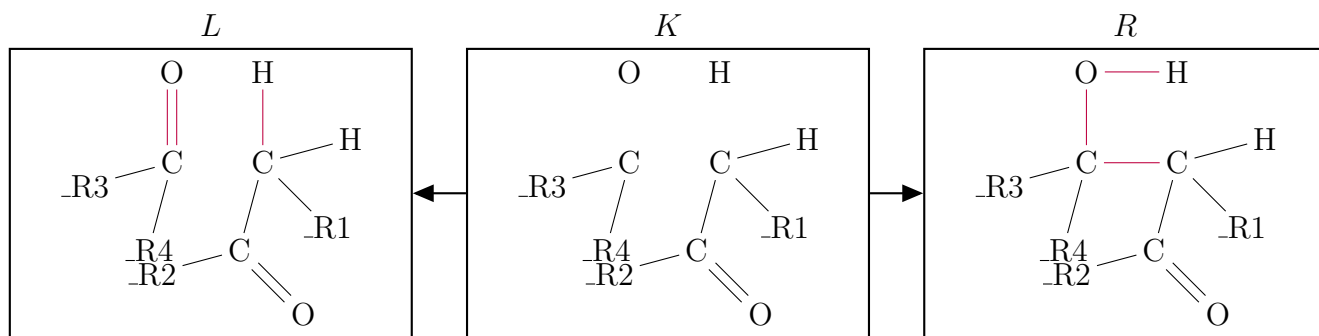


Files: out/100_r_17.11100100.{L, K, R}

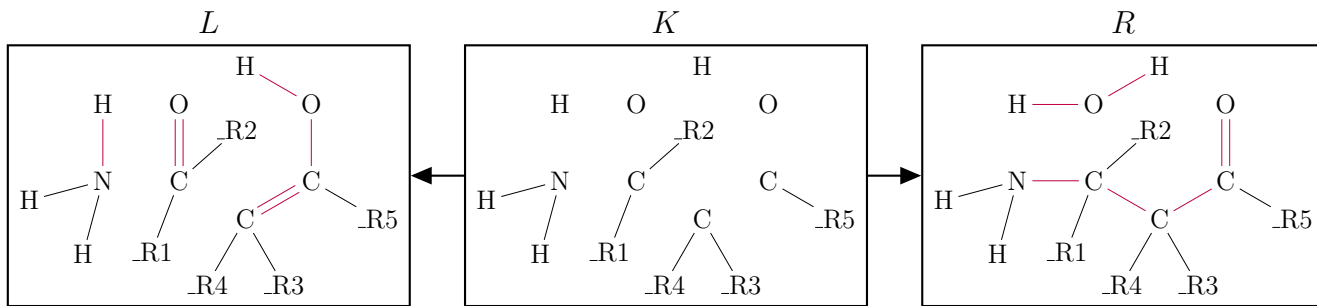


File: out/101_r_17_combined

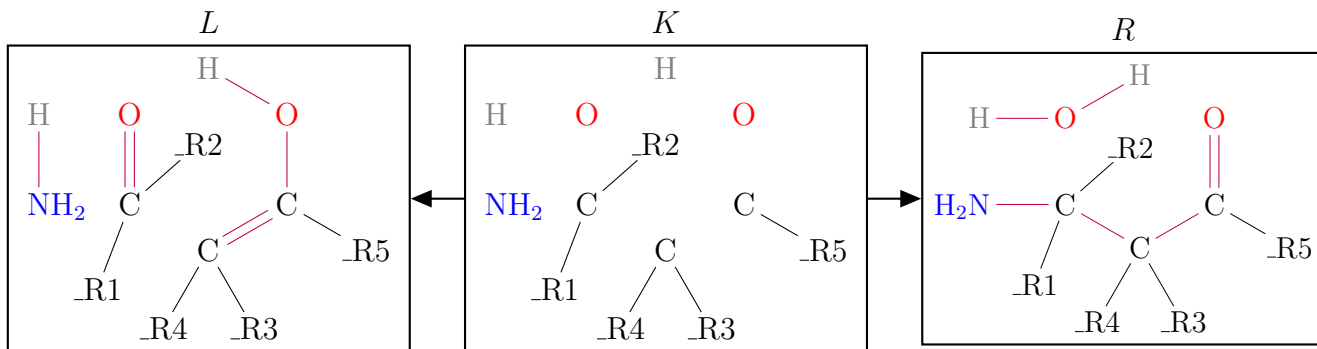
0.2.19 2.1.1 Aldol-Reaktion (basekatalysiert)



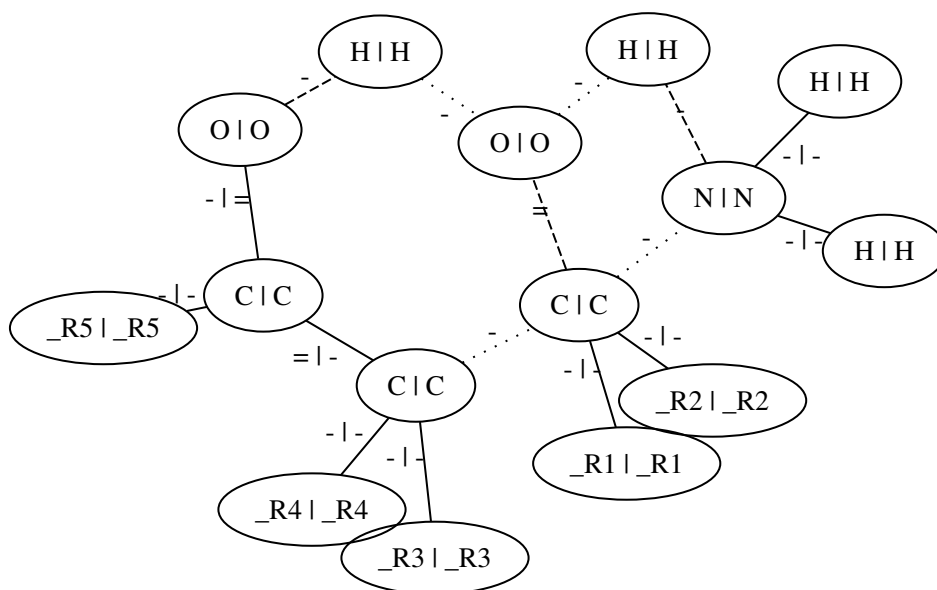
0.2.20 2.1.2 Mannich Reaktion



Files: out/109_r_19.10100000.{L, K, R}

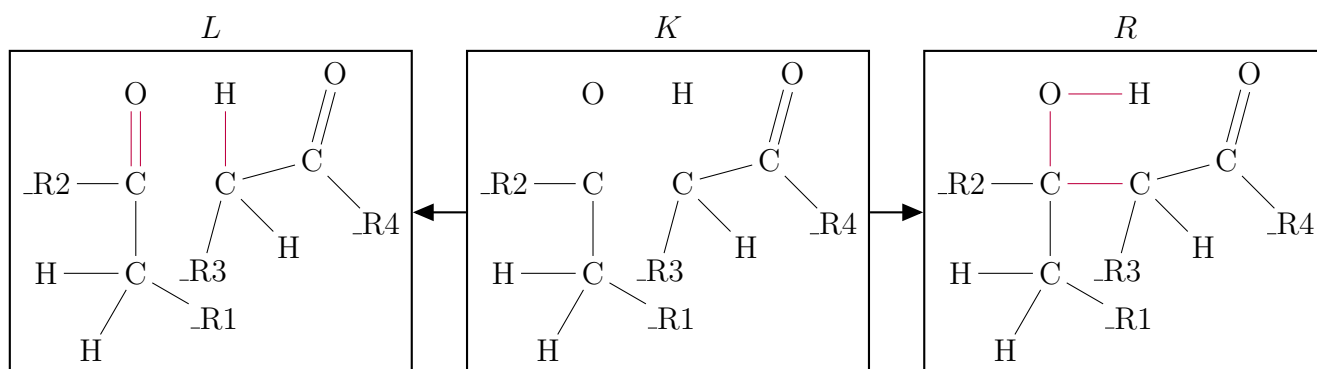


Files: out/110_r_19.11100100.{L, K, R}

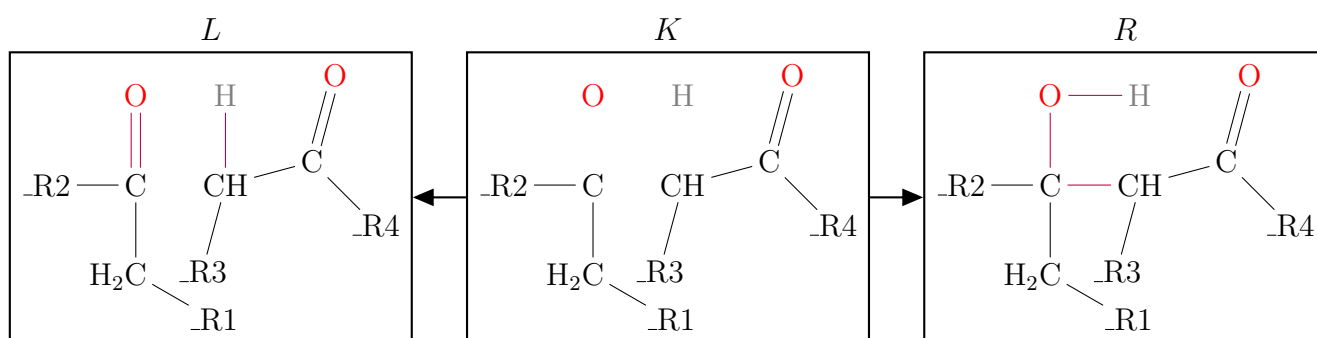


File: out/111_r_19_combined

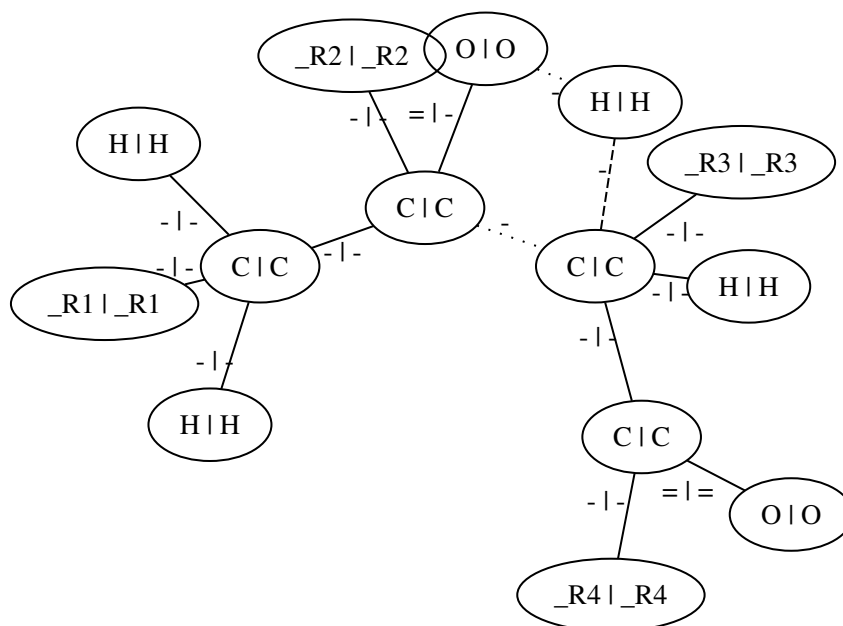
0.2.21 2.2.1 Aldol-Reaktion (saeurekatalytisch) main



Files: out/114_r_20.10100000.{L, K, R}

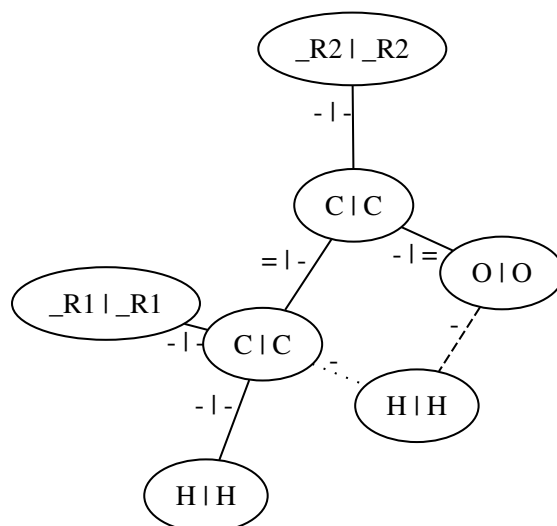
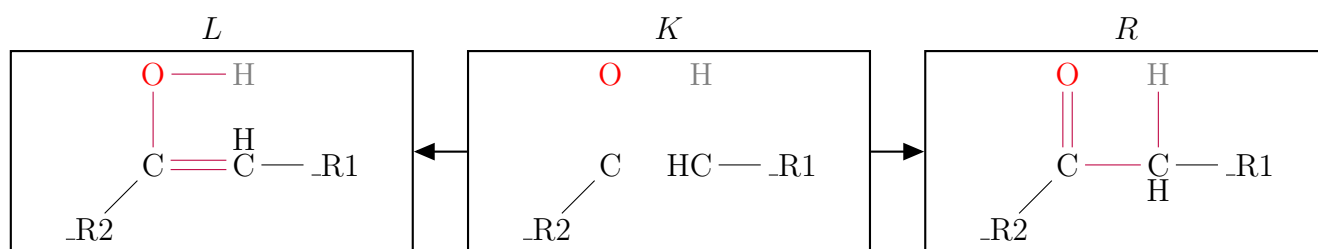
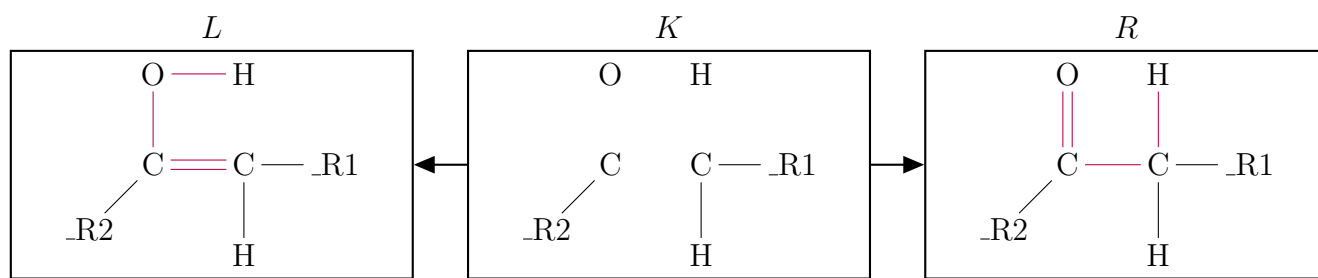


Files: out/115_r_20.11100100.{L, K, R}

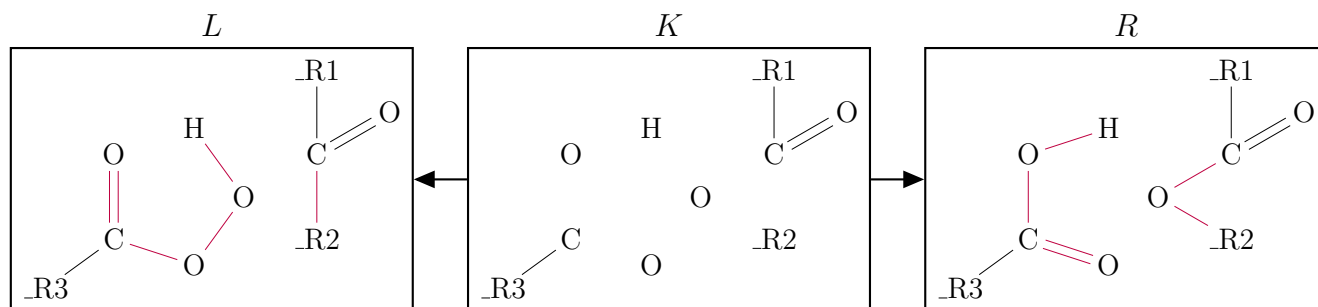


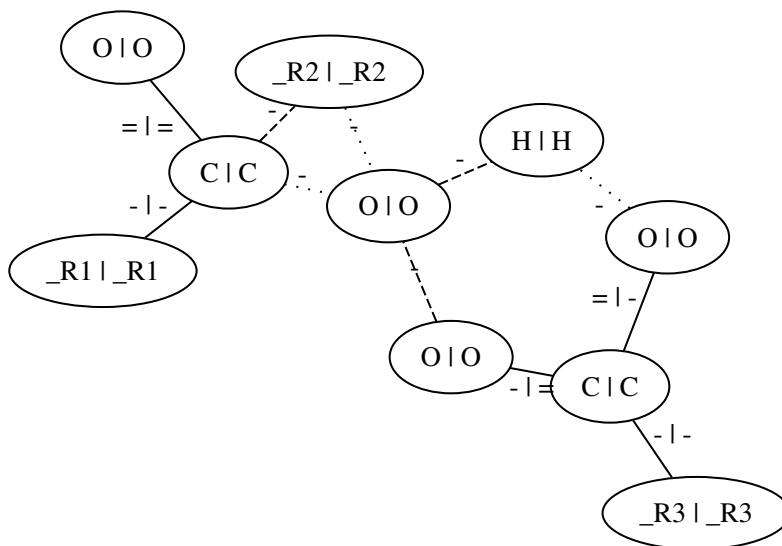
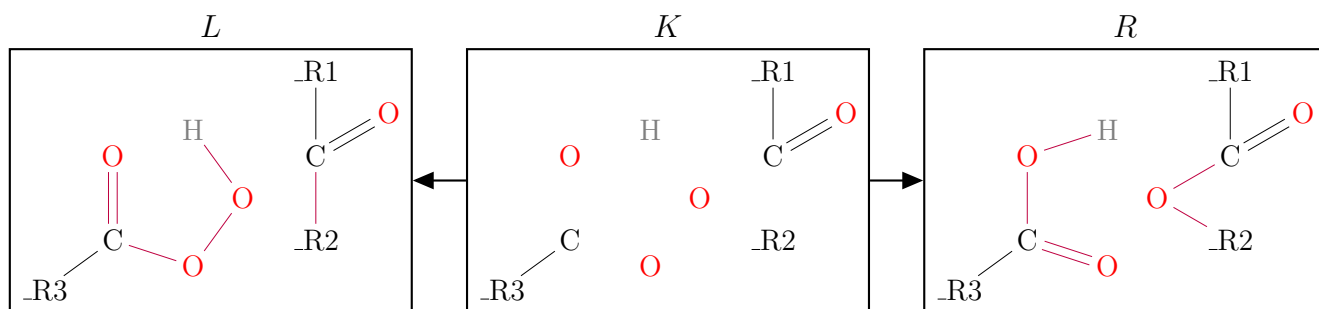
File: out/116_r_20_combined

0.2.22 2.2.1 Aldol-Reaktion (saeurekatalytisch) Keto-Enol-Tautomerisation

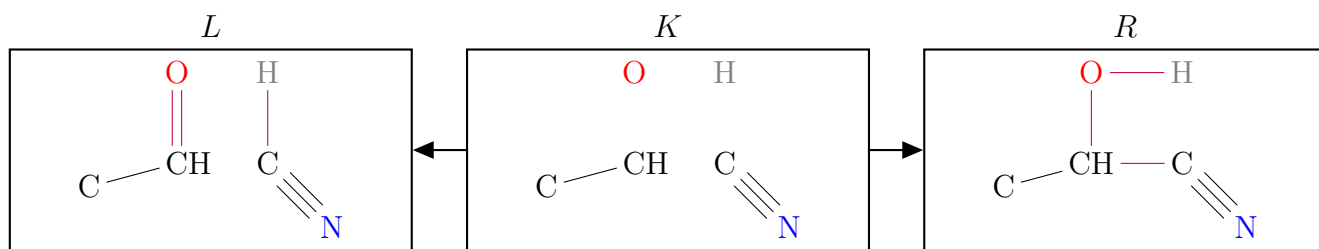
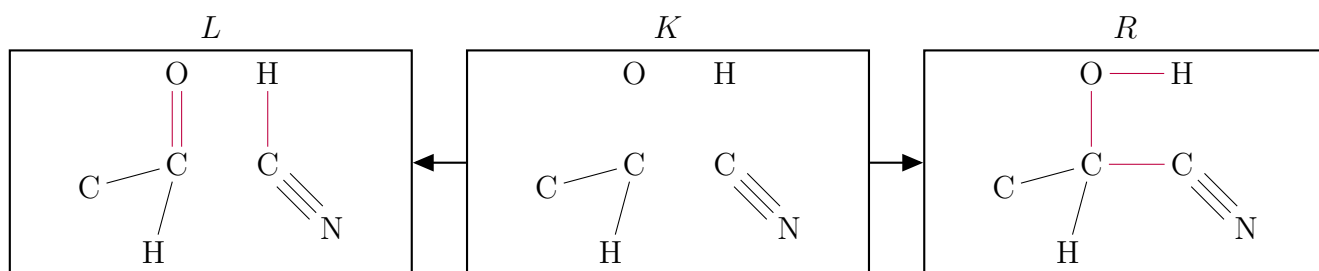


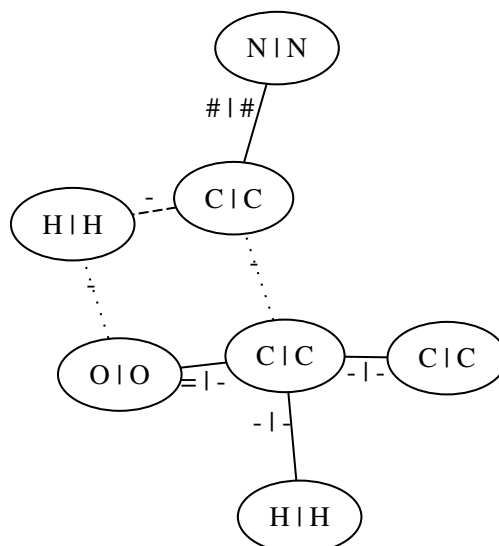
0.2.23 2.2.2 Baeyer-Villiger-Oxidation





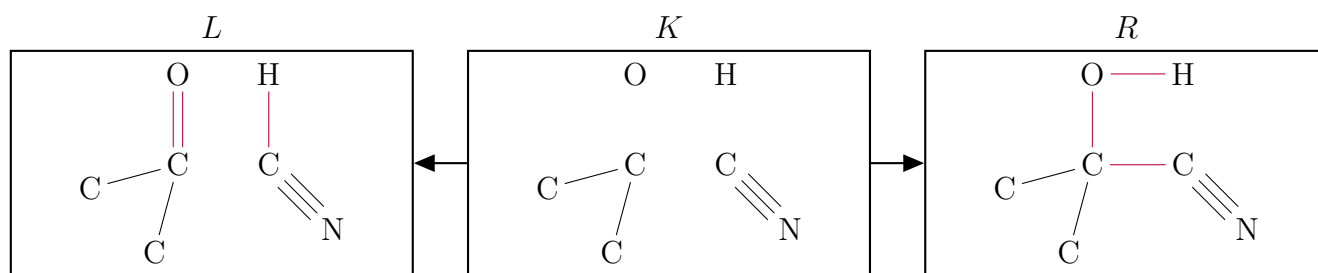
0.2.24 2.2.3 cyanhydrinbildung aldehyd



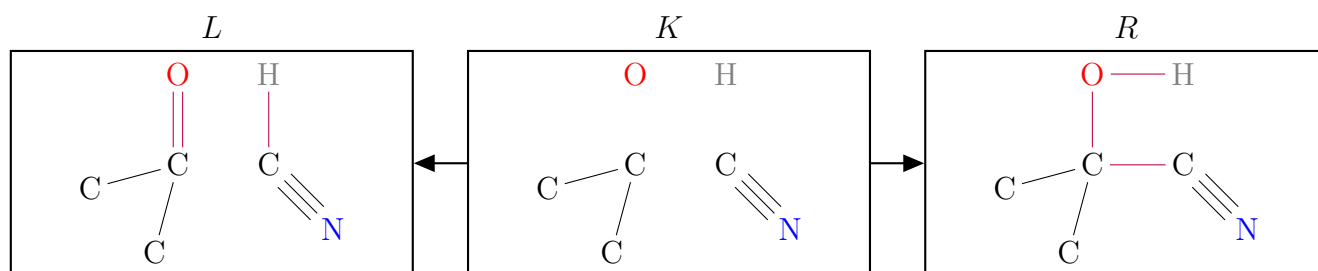


File: out/131_r_23_combined

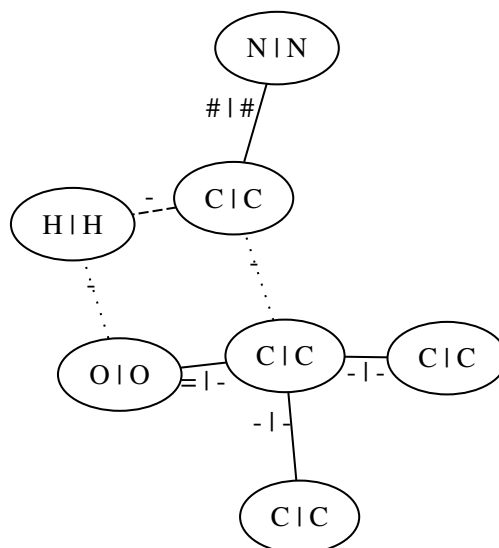
0.2.25 2.2.3 cyanhydrinbildung ketone



Files: out/134_r_24.10100000.{L, K, R}

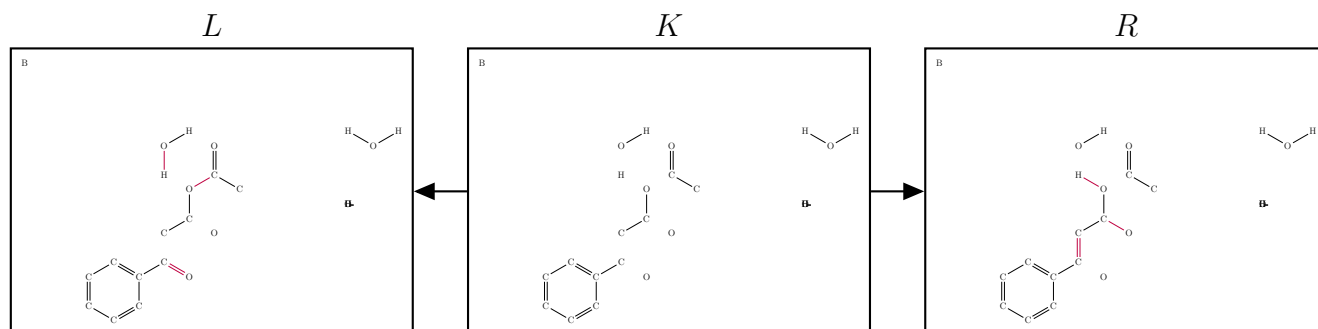


Files: out/135_r_24.11100100.{L, K, R}

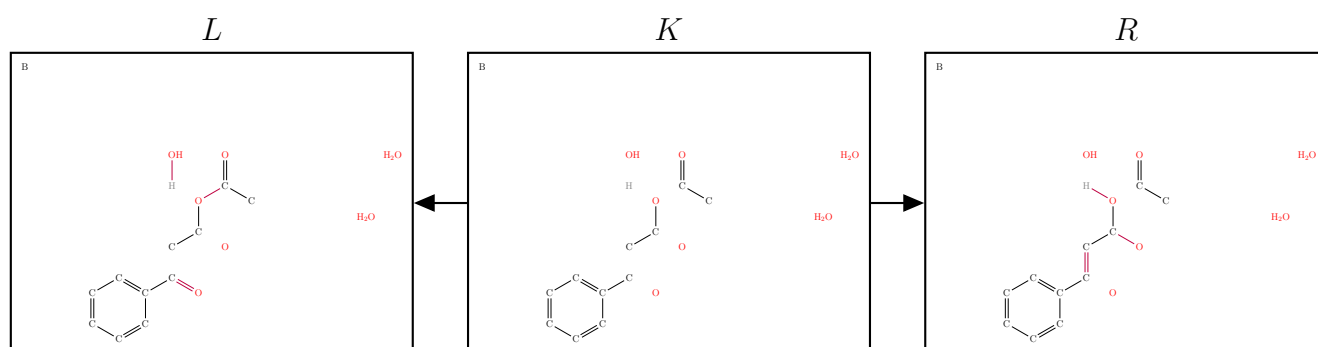


File: out/136_r_24_combined

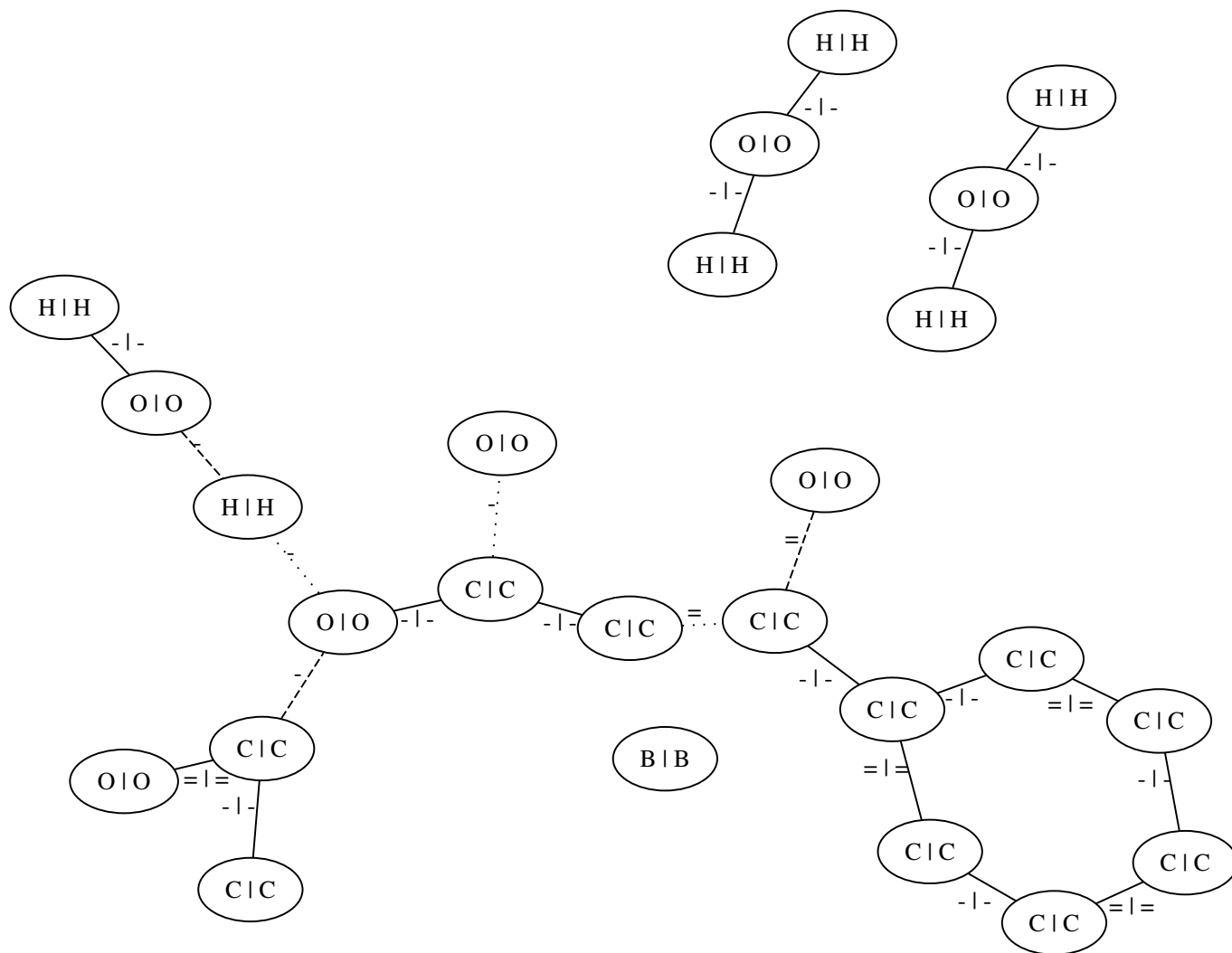
0.2.26 2.2.4 Perkin-Reaktion



Files: out/139_r_25.10100000.{L, K, R}

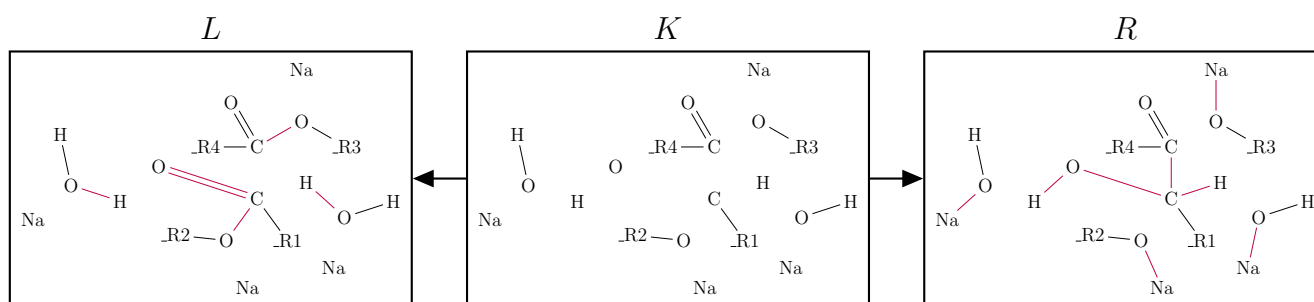


Files: out/140_r_25.11100100.{L, K, R}

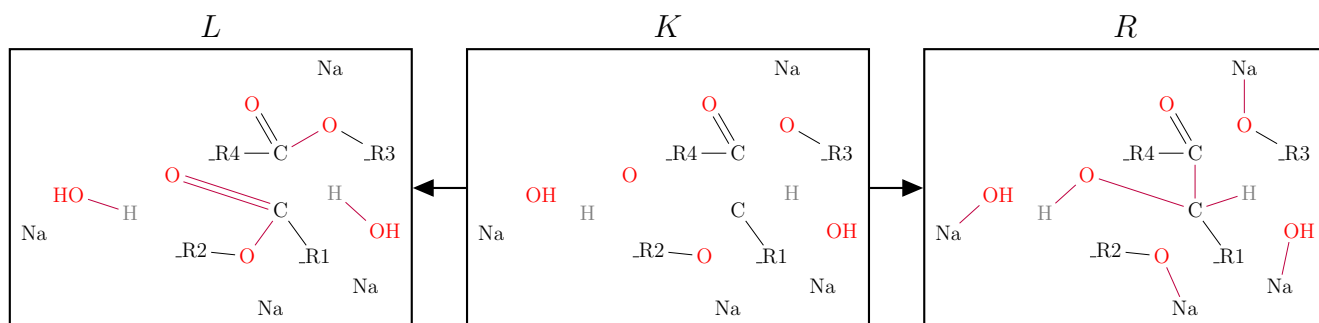


File: out/141_r_25_combined

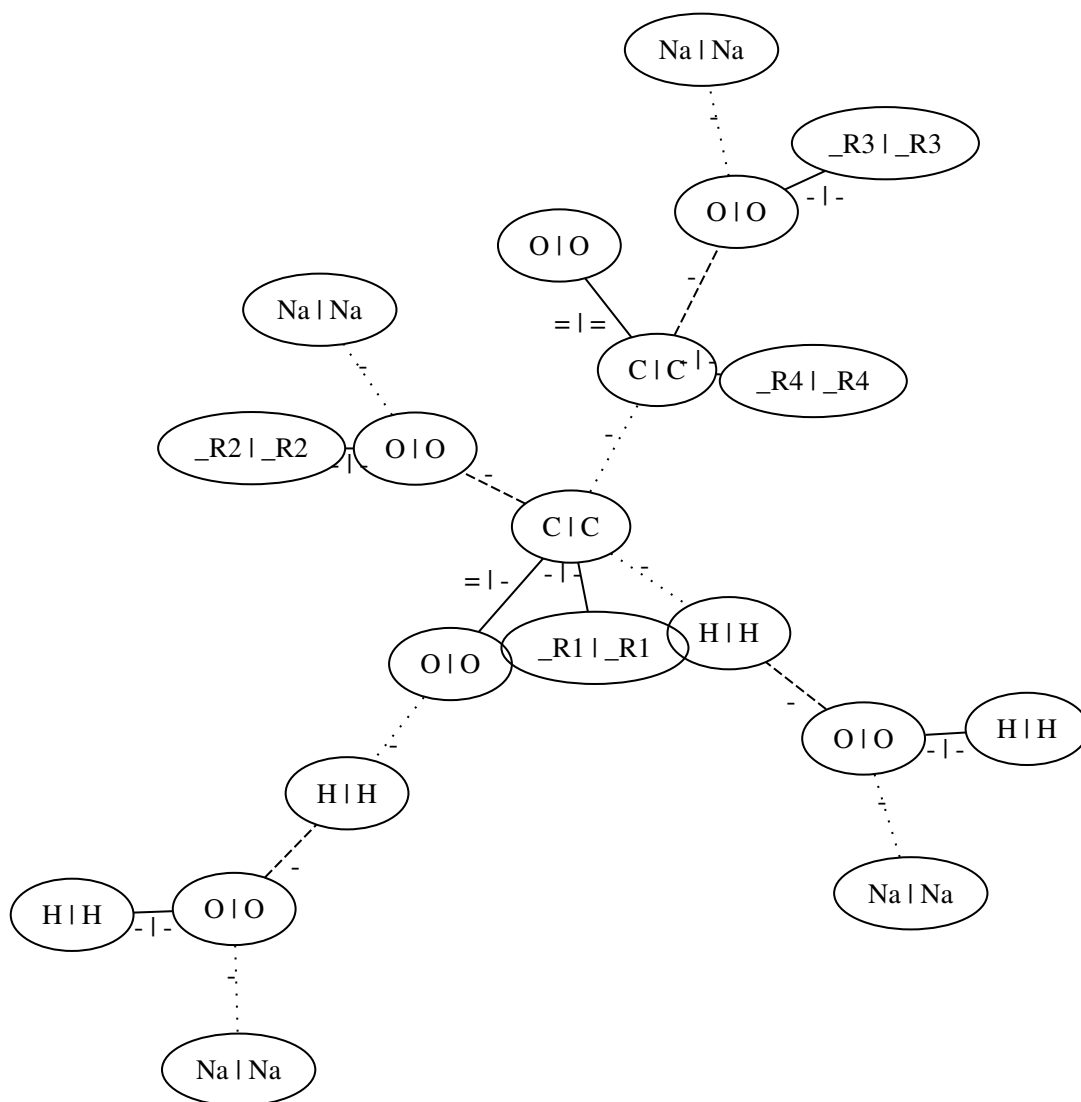
0.2.27 2.3.1 AcyloinKondensation



Files: out/144_r_26.10100000.{L, K, R}

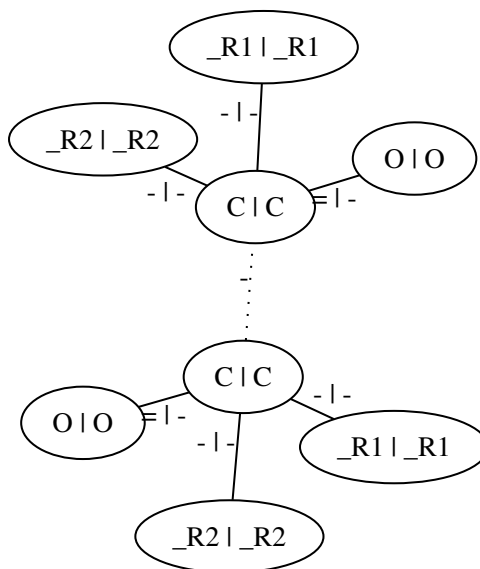
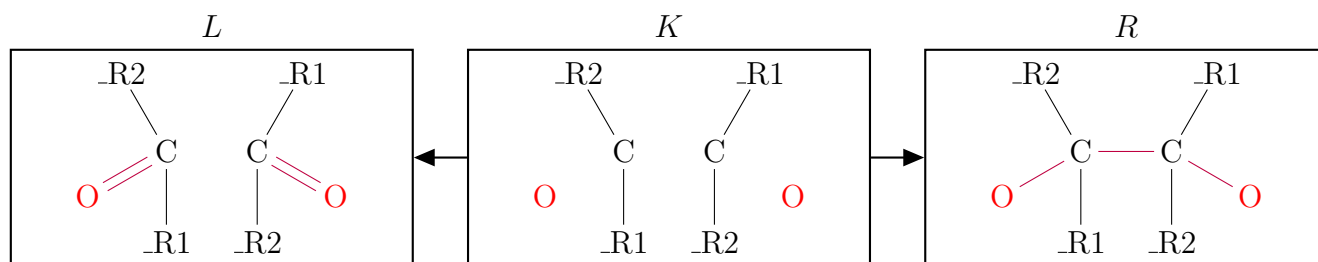
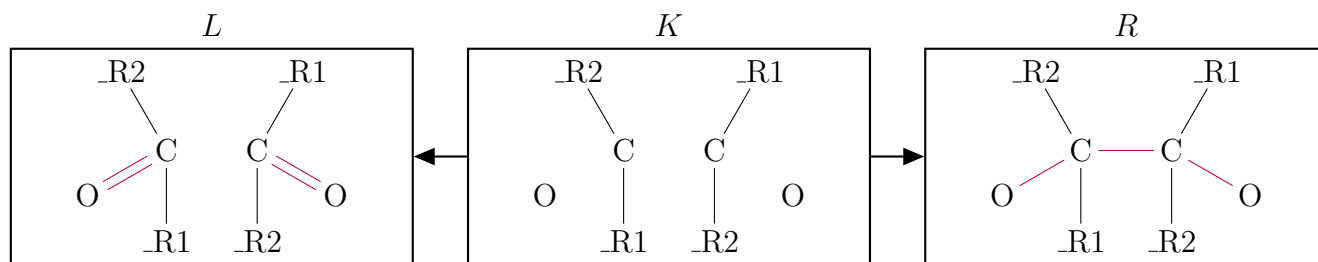


Files: out/145_r_26.11100100.{L, K, R}

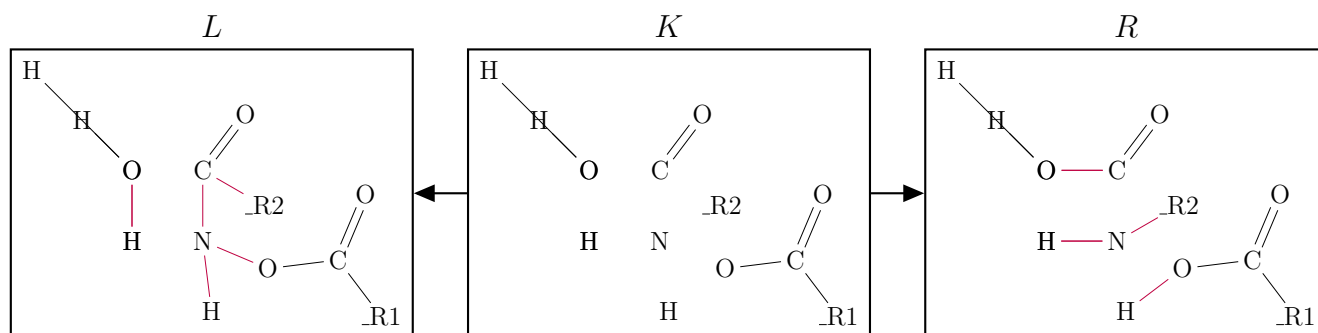


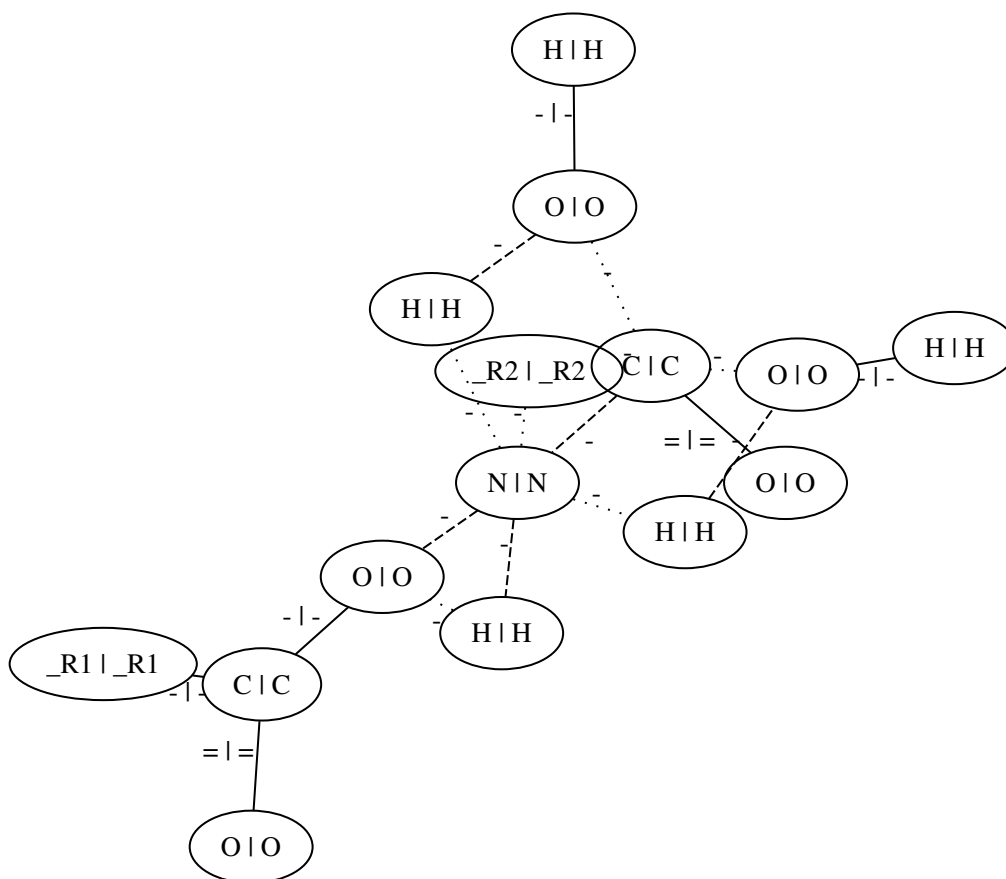
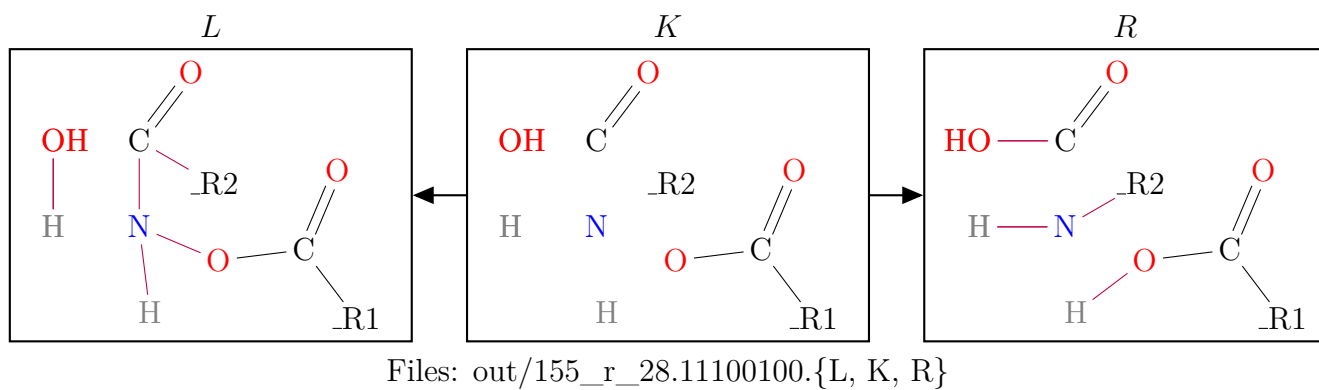
File: out/146_r_26_combined

0.2.28 2.3.2. Pinakol-Kopplung

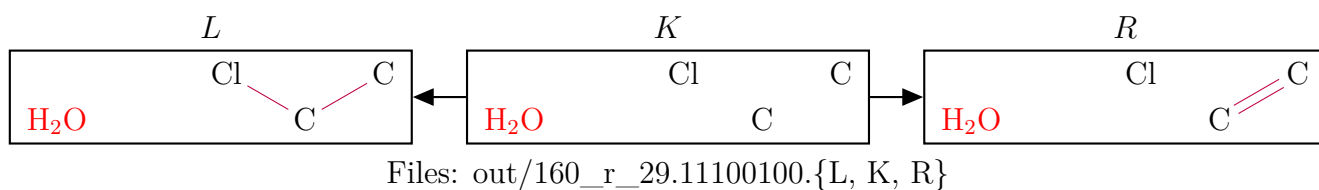
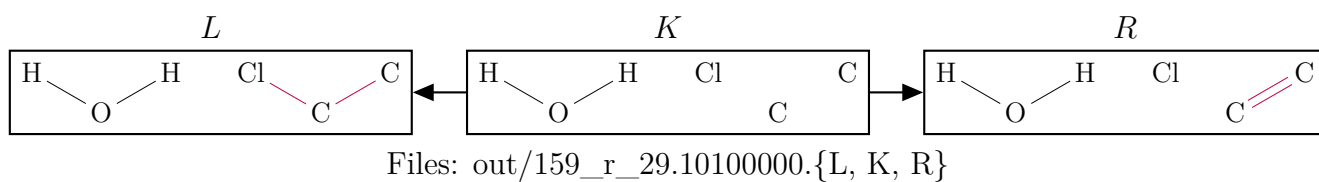


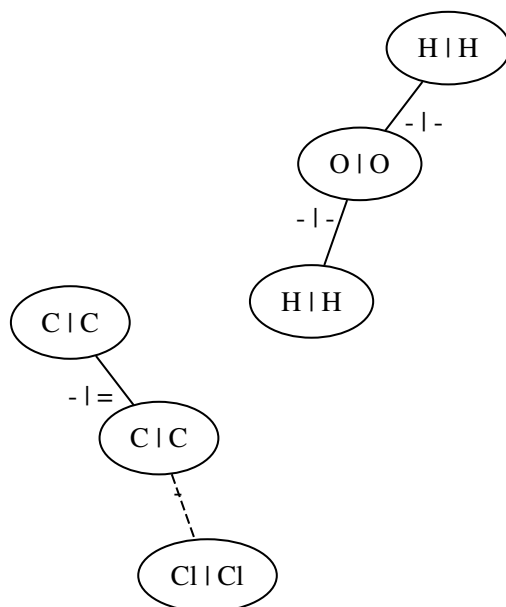
0.2.29 3.1.1 Lossen-Abbau





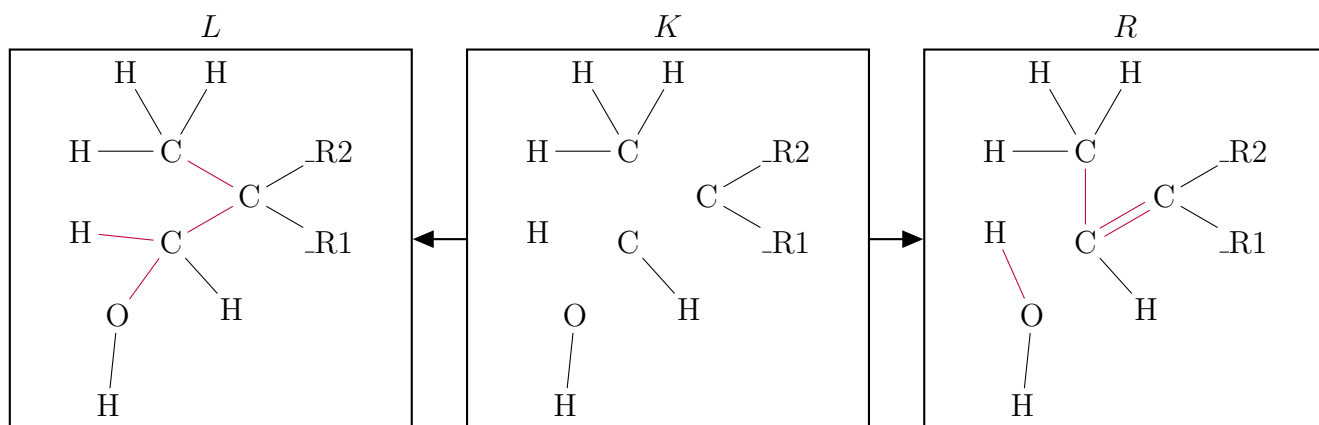
0.2.30 3.2 Bimolekulare Eliminierung, E2



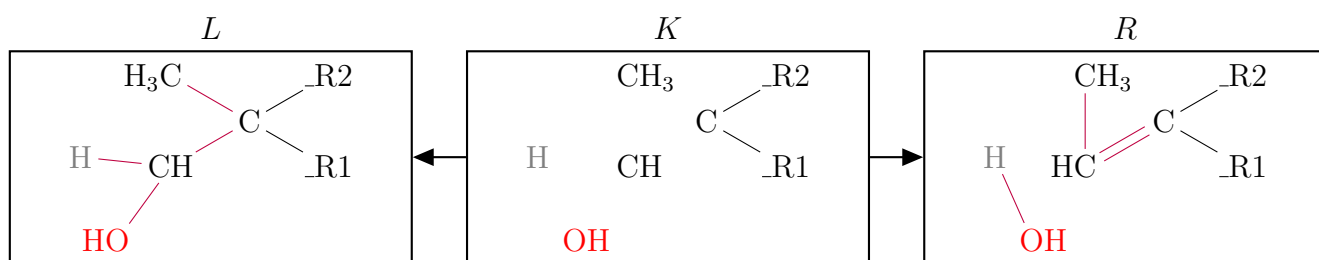


File: out/161_r_29_combined

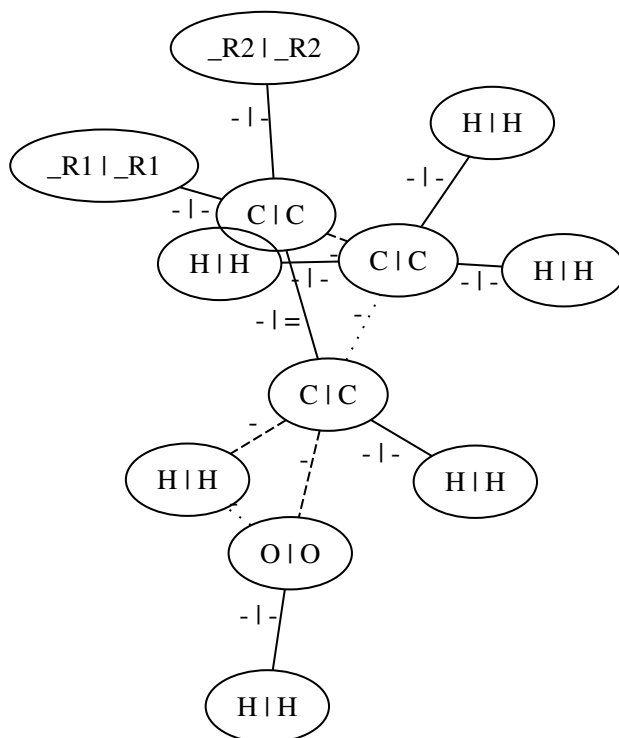
0.2.31 4.1 Wagner-Meerwein-Umlagerung



Files: out/164_r_30.10100000.{L, K, R}

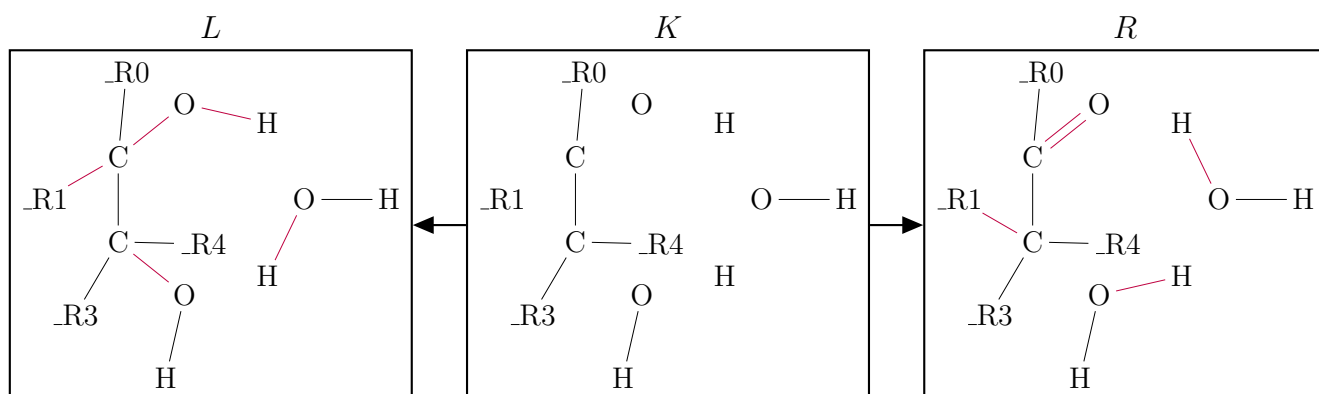


Files: out/165_r_30.11100100.{L, K, R}

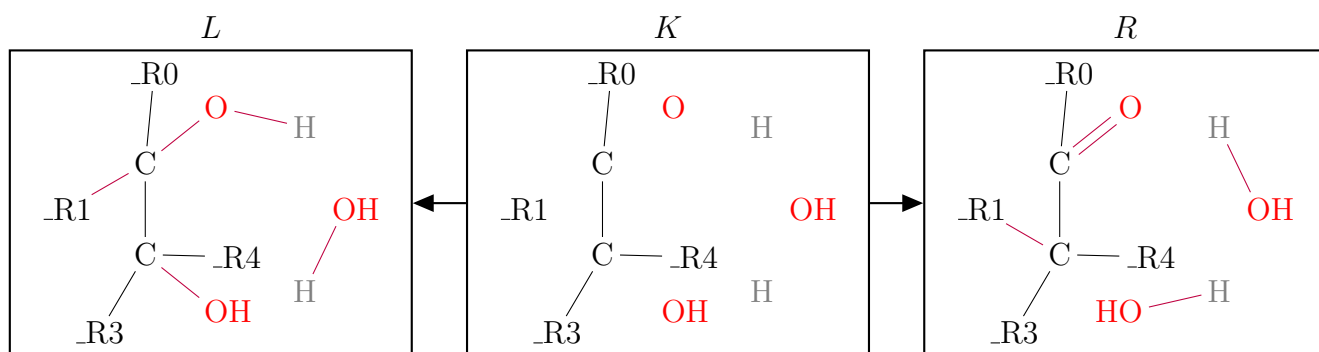


File: out/166_r_30_combined

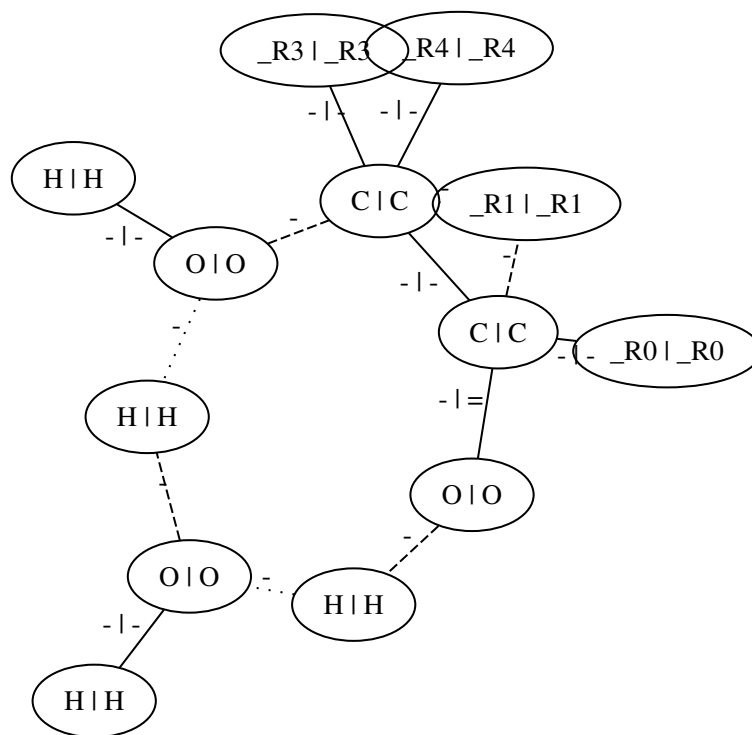
0.2.32 4.2. Pinakol Umlagerung 1



Files: out/169_r_31.10100000.{L, K, R}

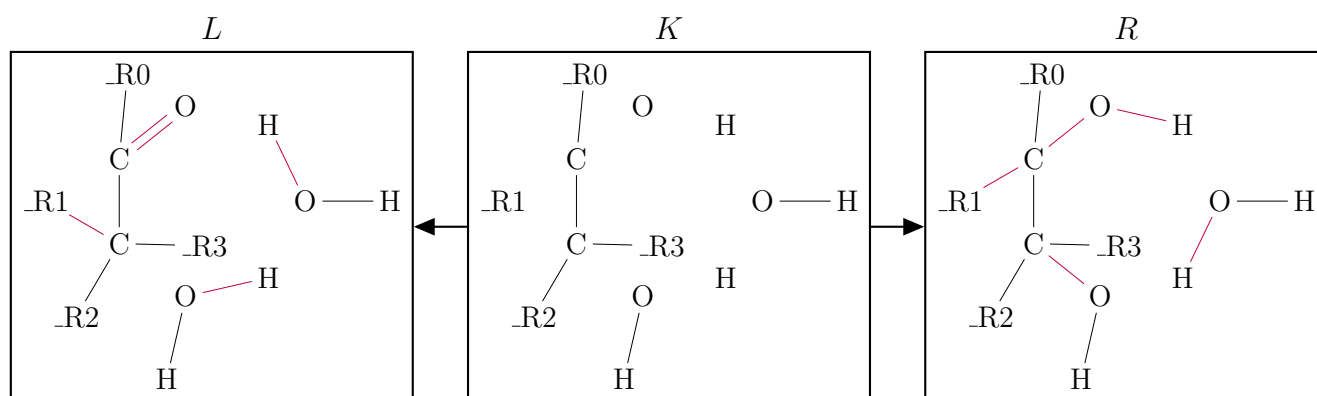


Files: out/170_r_31.11100100.{L, K, R}

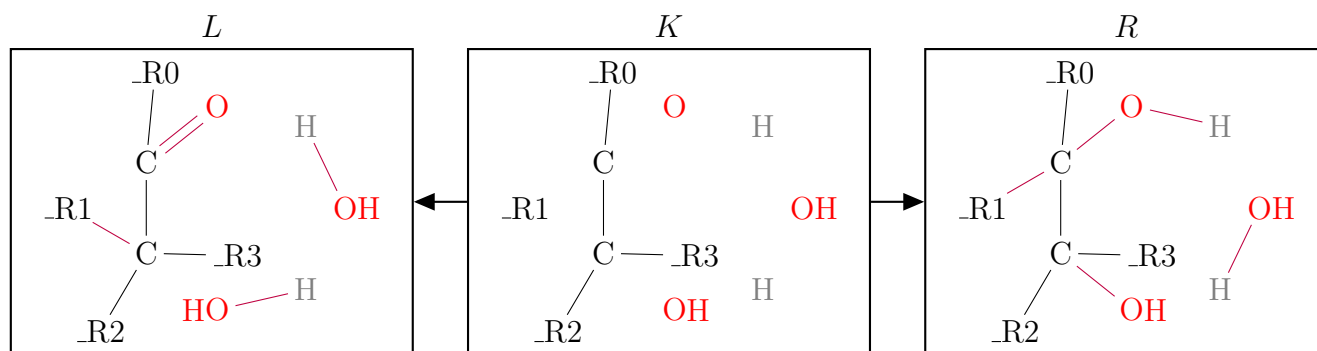


File: out/171_r_31_combined

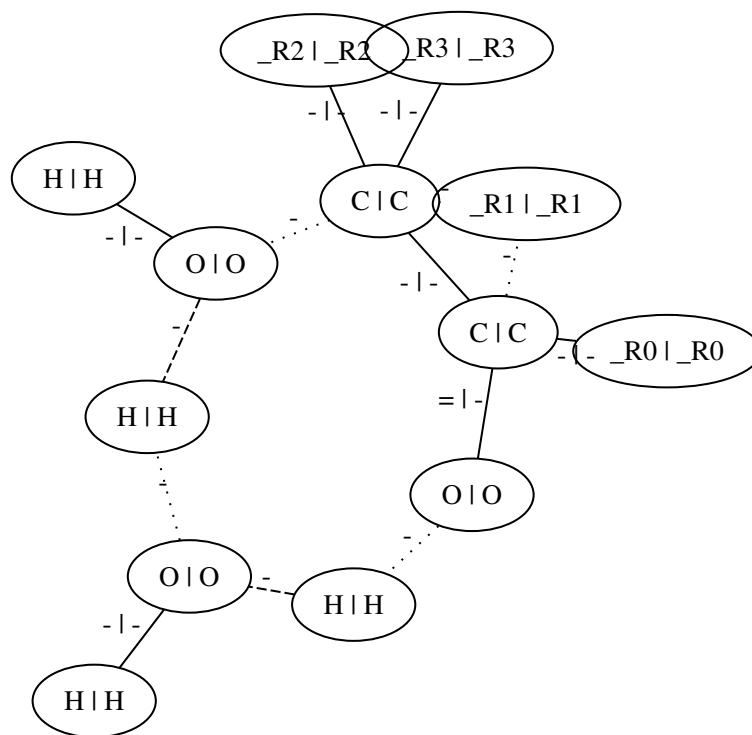
0.2.33 4.2. Pinakol Umlagerung 2



Files: out/174_r_32.10100000.{L, K, R}

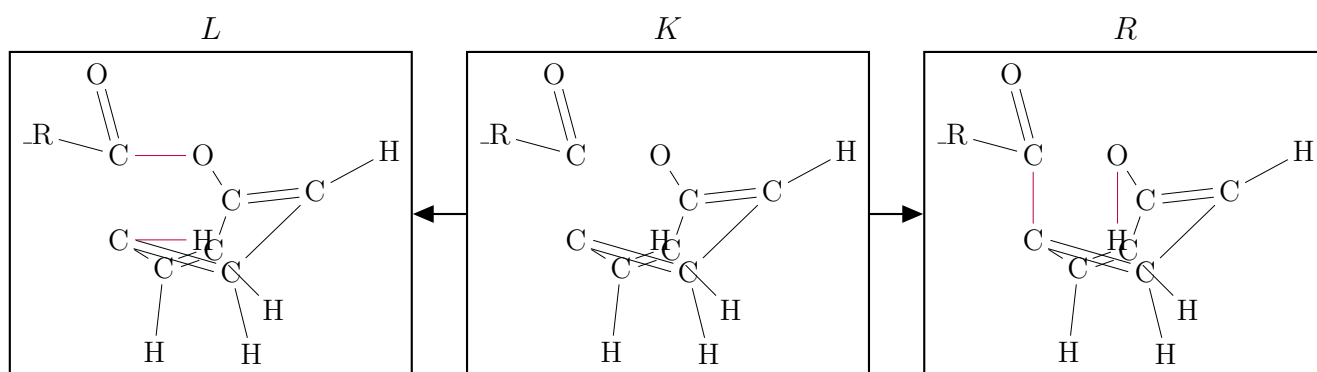


Files: out/175_r_32.11100100.{L, K, R}

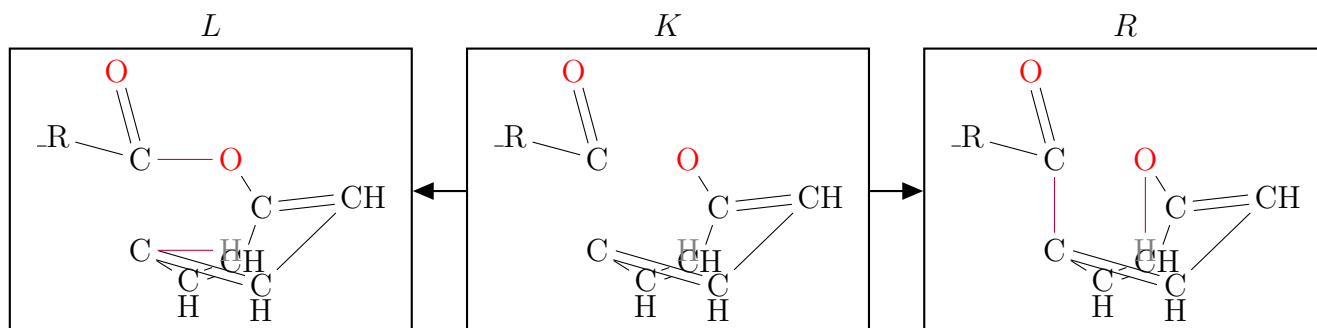


File: out/176_r_32_combined

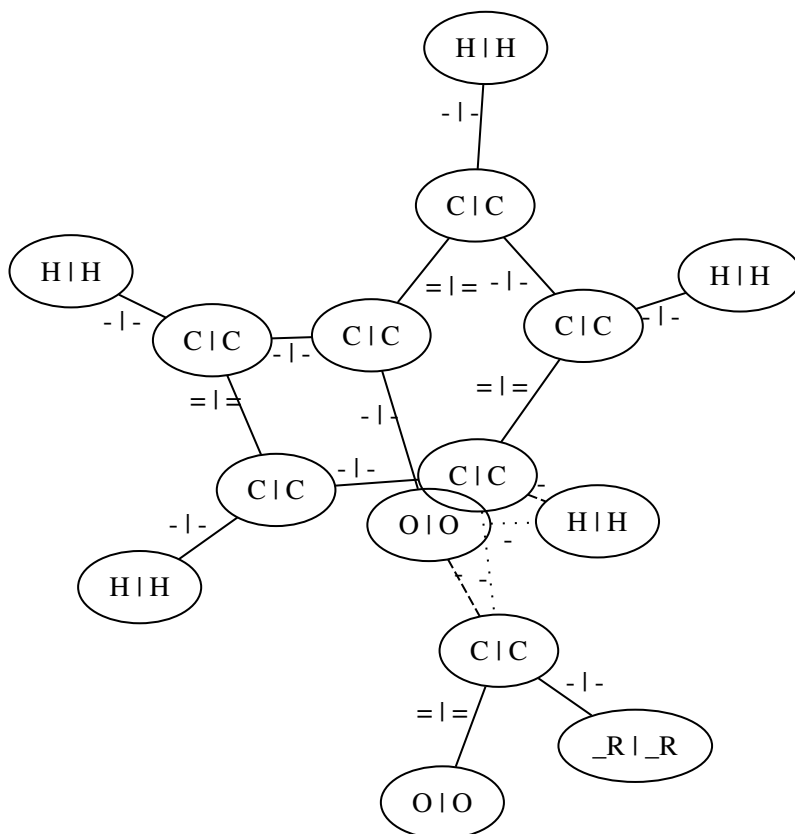
0.2.34 4.3. Fries-Umlagerung Para 1



Files: out/179_r_33.10100000.{L, K, R}

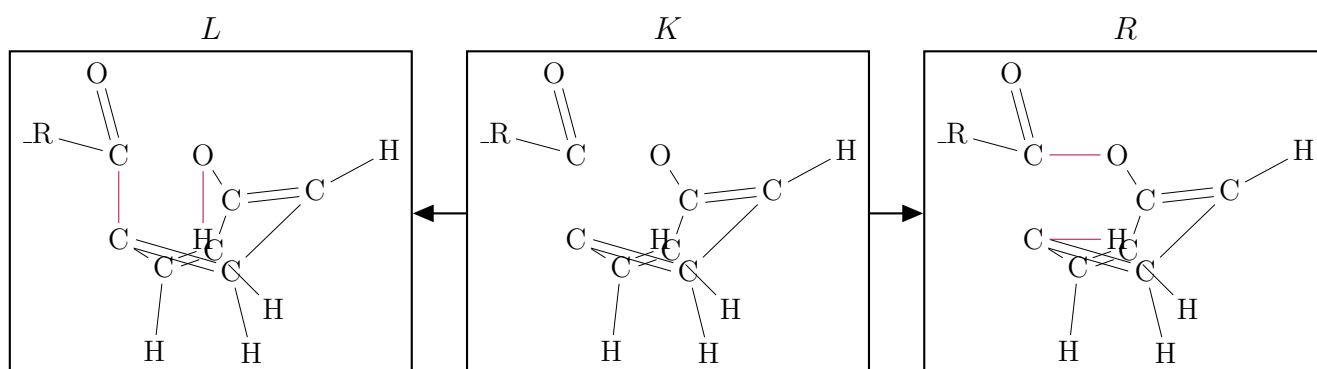


Files: out/180_r_33.11100100.{L, K, R}

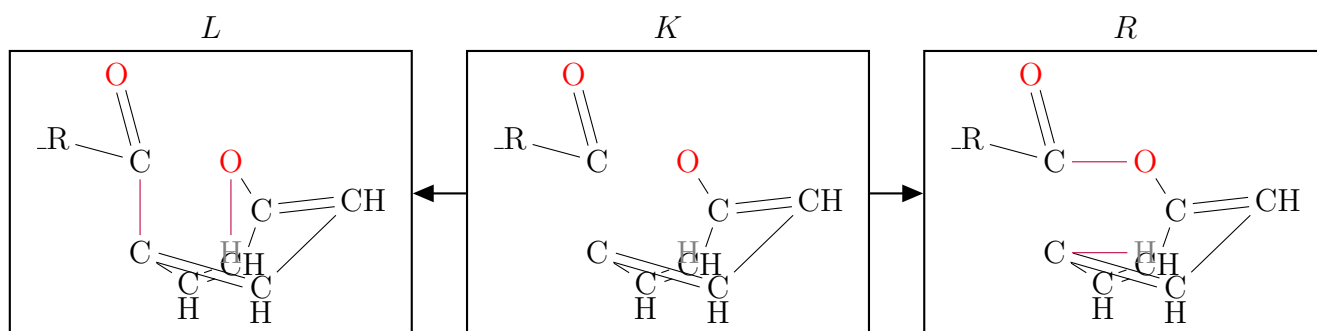


File: out/181_r_33_combined

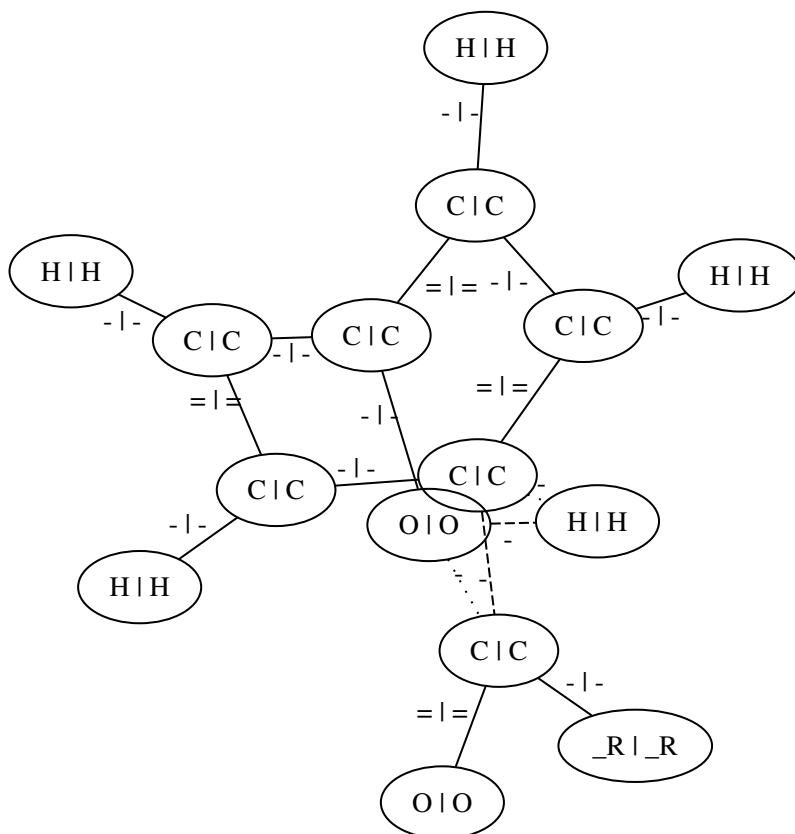
0.2.35 4.3. Fries-Umlagerung Para 2



Files: out/184_r_34.10100000.{L, K, R}

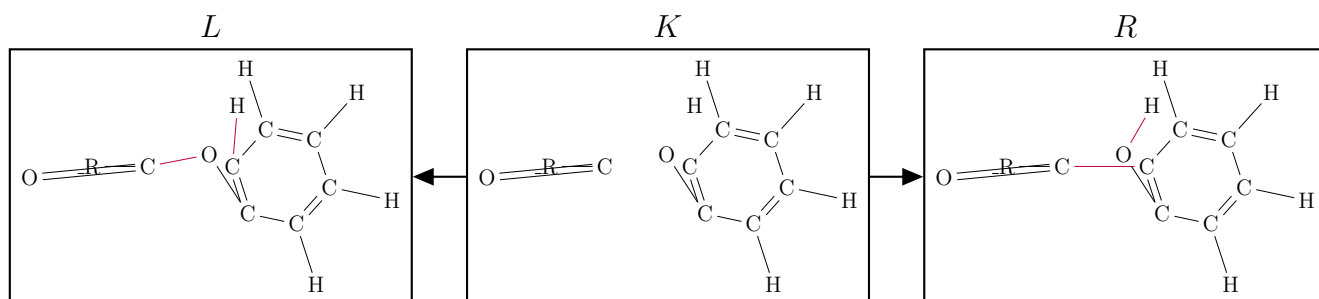


Files: out/185_r_34.11100100.{L, K, R}

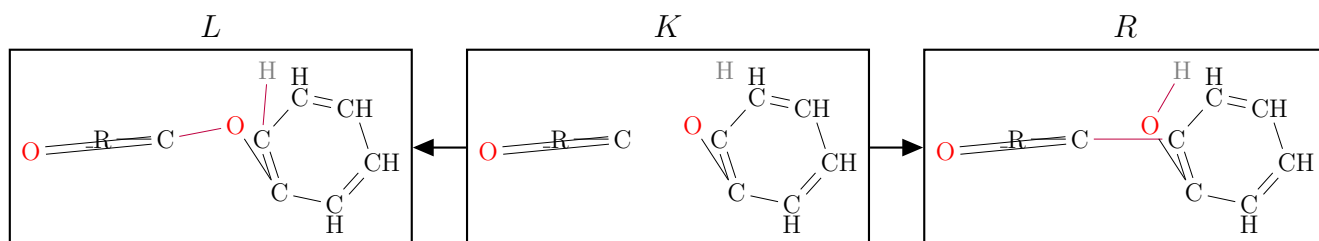


File: out/186_r_34_combined

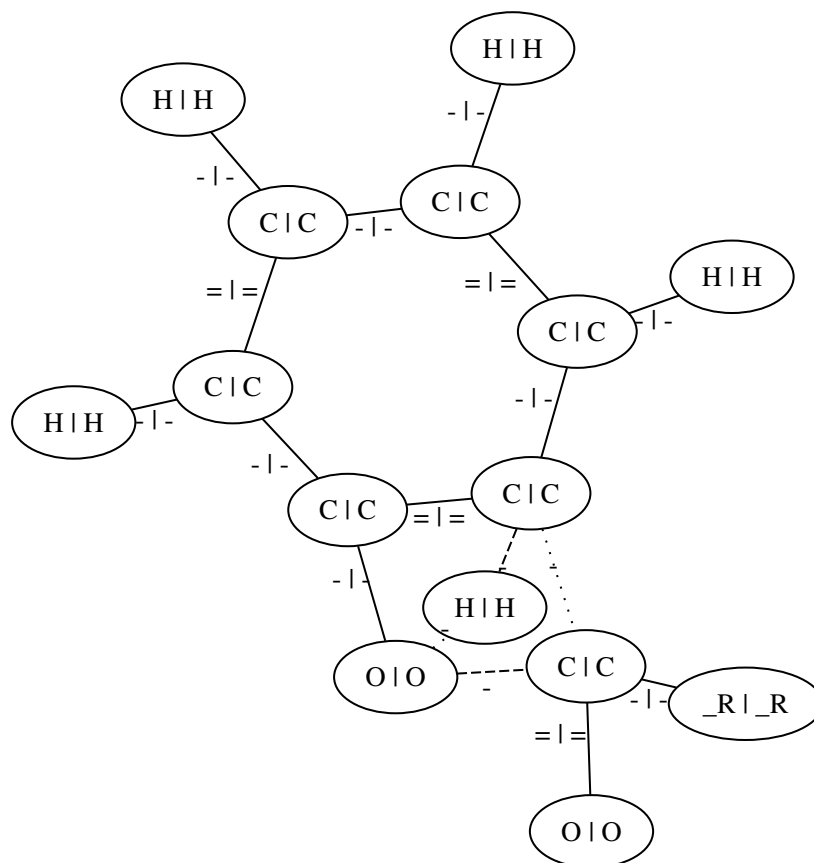
0.2.36 4.3. Fries-Umlagerung Ortho 3



Files: out/189_r_35.10100000.{L, K, R}

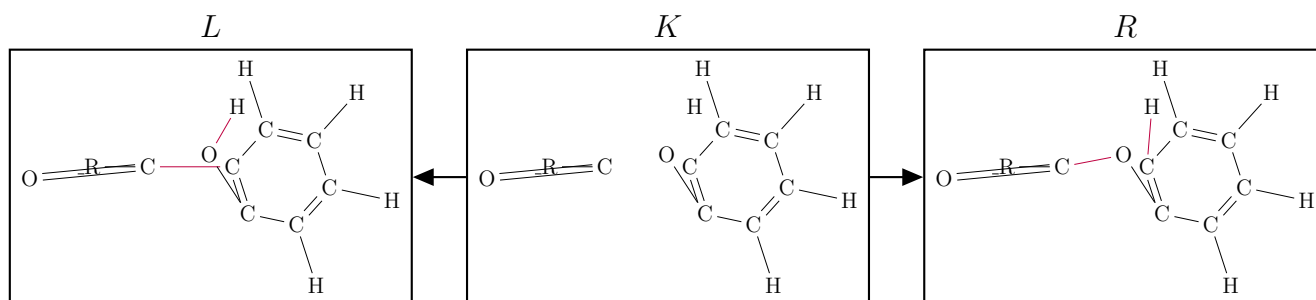


Files: out/190_r_35.11100100.{L, K, R}

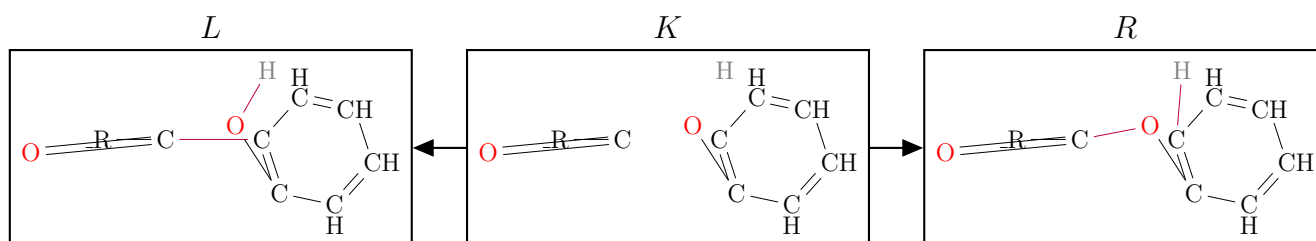


File: out/191_r_35_combined

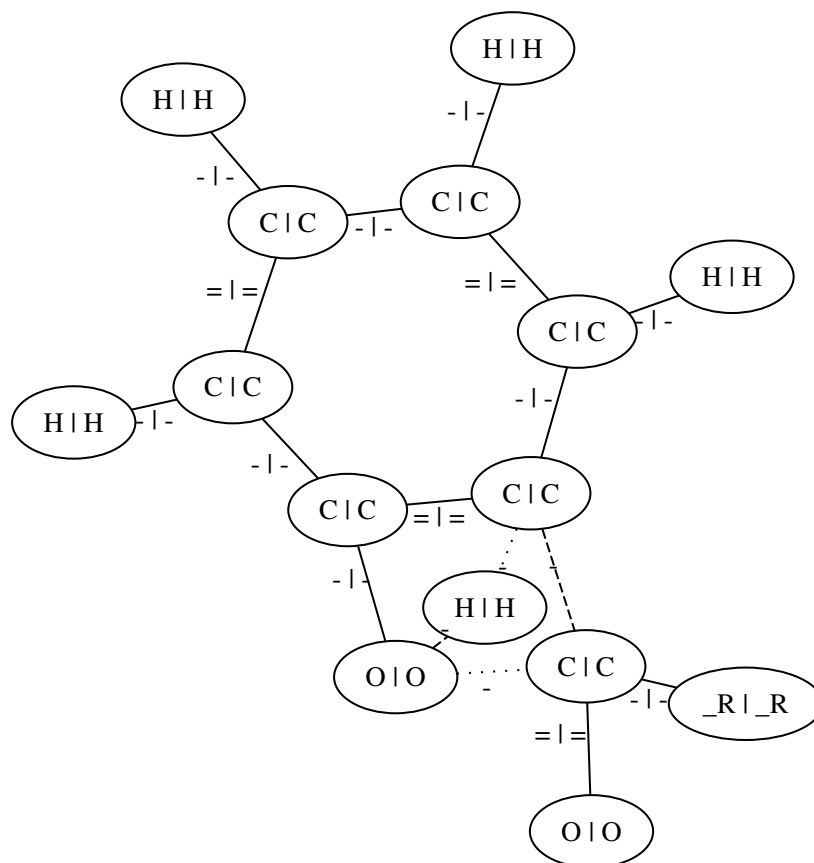
0.2.37 4.3. Fries-Umlagerung Ortho 4



Files: out/194_r_36.10100000.{L, K, R}

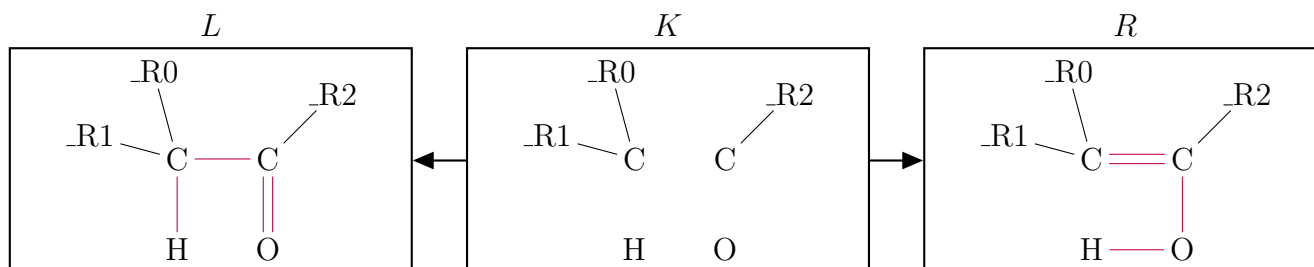


Files: out/195_r_36.11100100.{L, K, R}

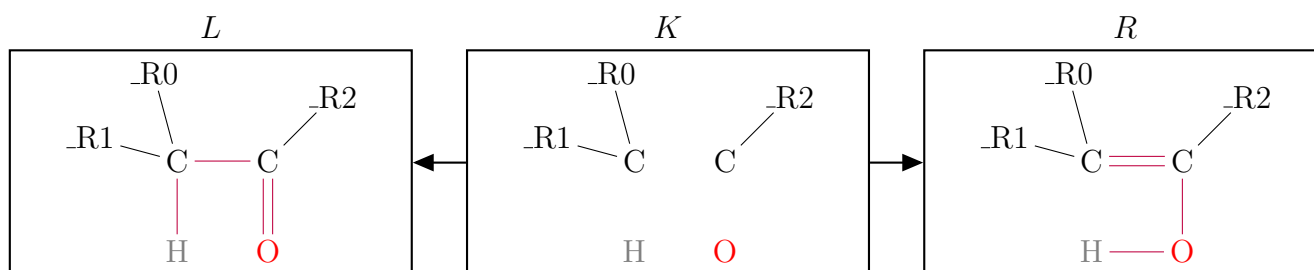


File: out/196_r_36_combined

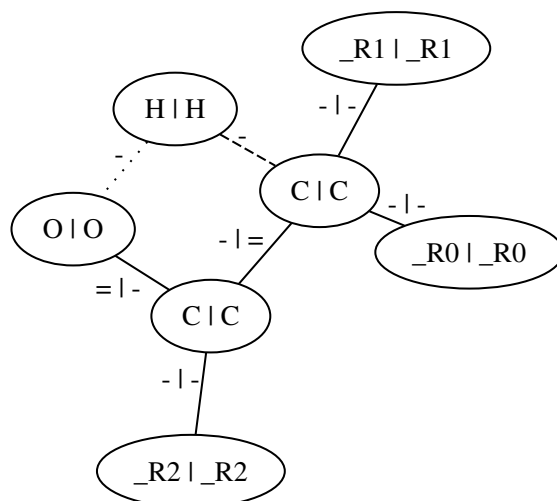
0.2.38 4.4. Keto-Enol-Tautomerie 1



Files: out/199_r_37.10100000.{L, K, R}

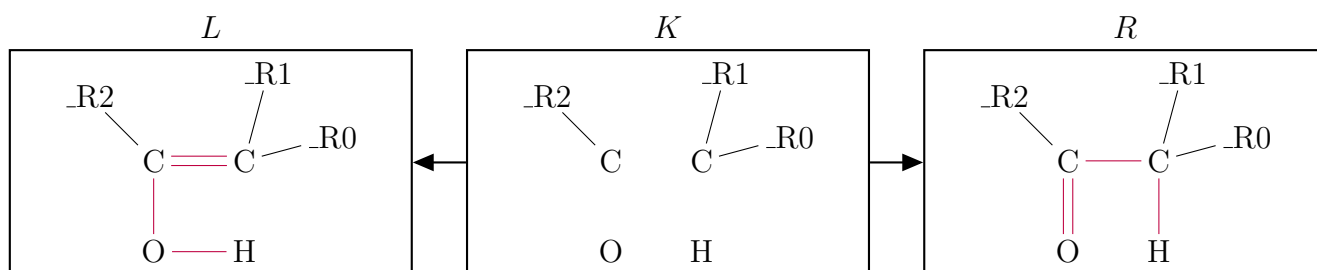


Files: out/200_r_37.11100100.{L, K, R}

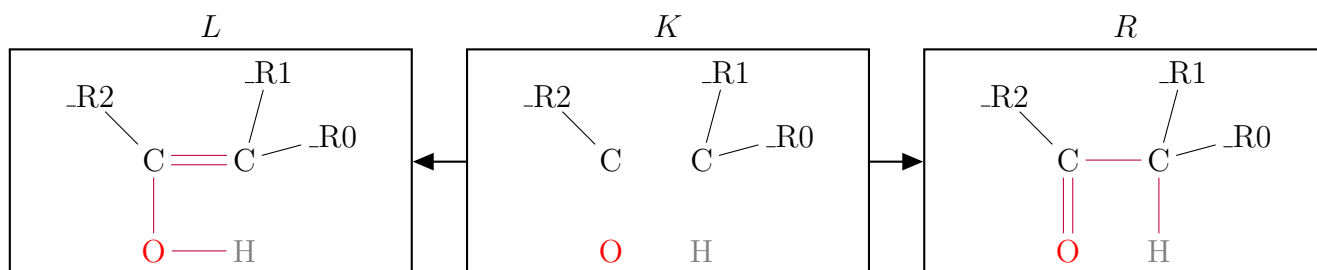


File: out/201_r_37_combined

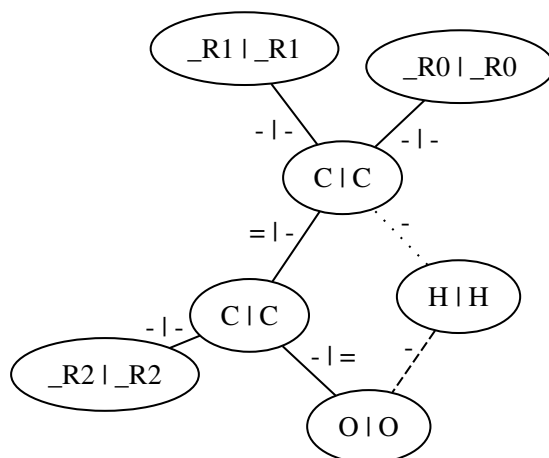
0.2.39 4.4. Keto-Enol-Tautomerie 2



Files: out/204_r_38.10100000.{L, K, R}

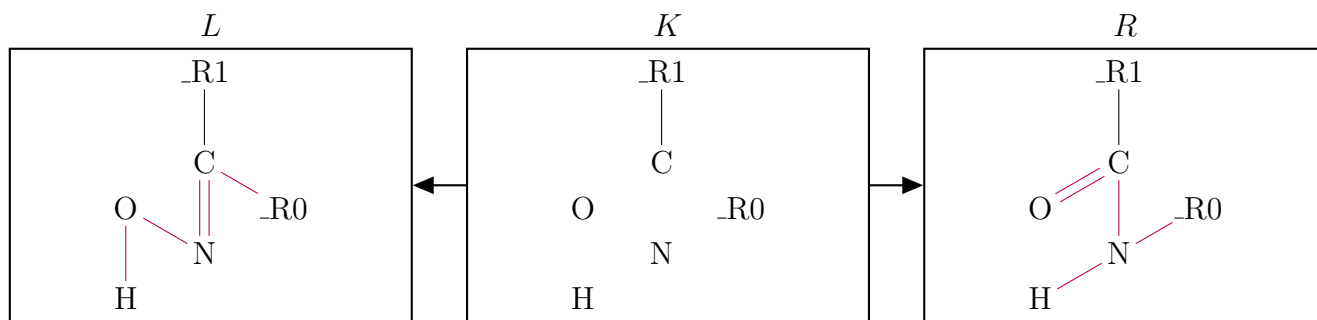


Files: out/205_r_38.11100100.{L, K, R}

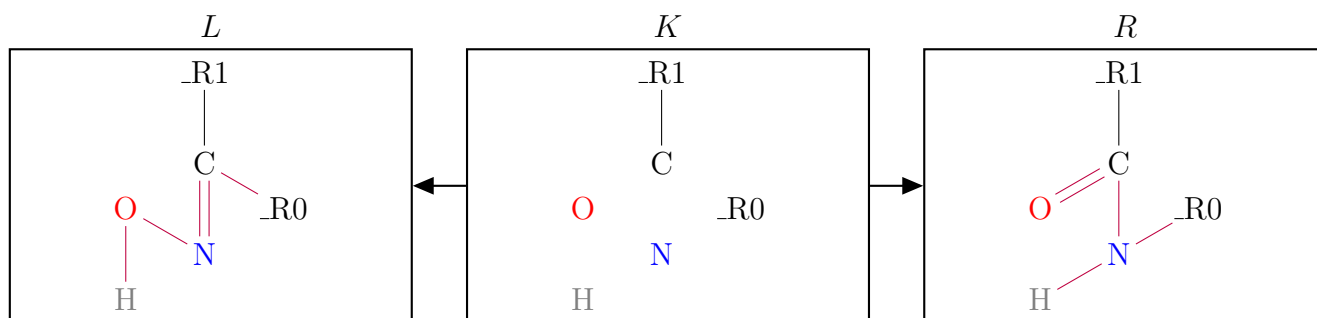


File: out/206_r_38_combined

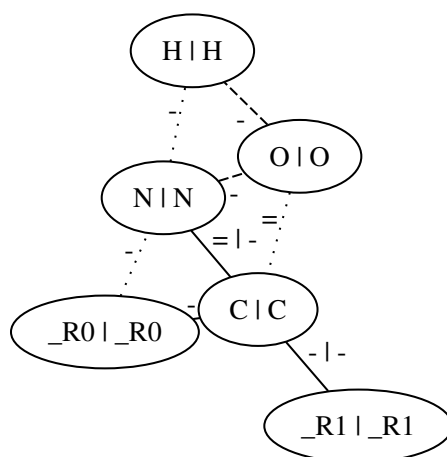
0.2.40 4.5. Beckmann-Umlagerung 1



Files: out/209_r_39.10100000.{L, K, R}

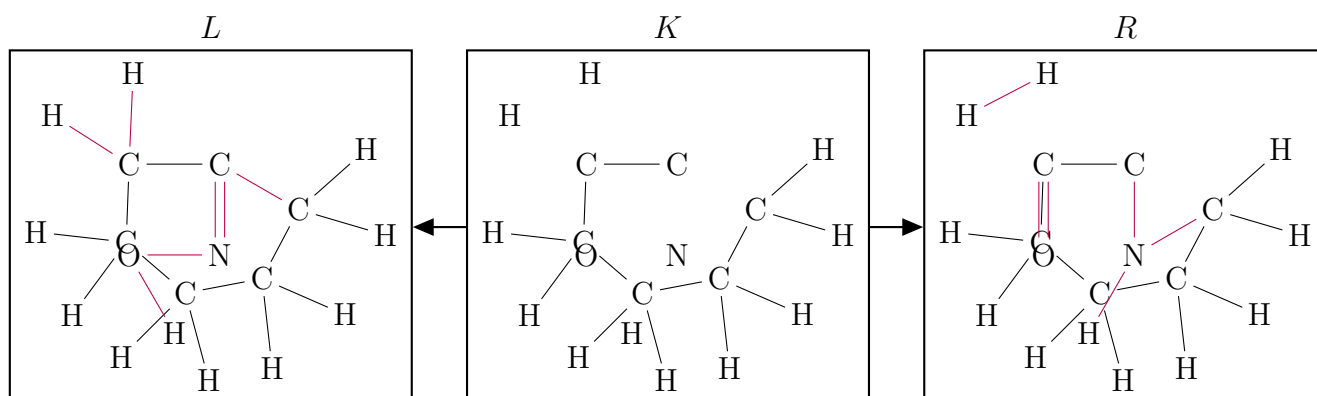


Files: out/210_r_39.11100100.{L, K, R}

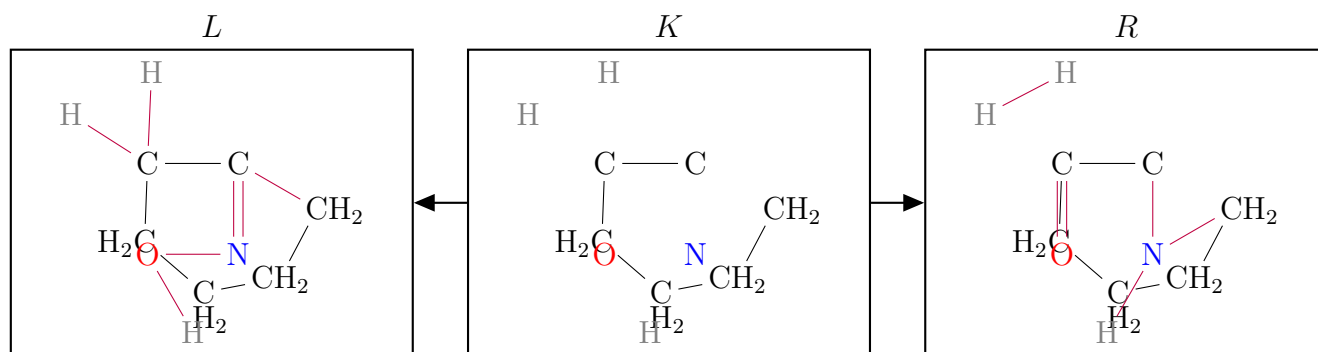


File: out/211_r_39_combined

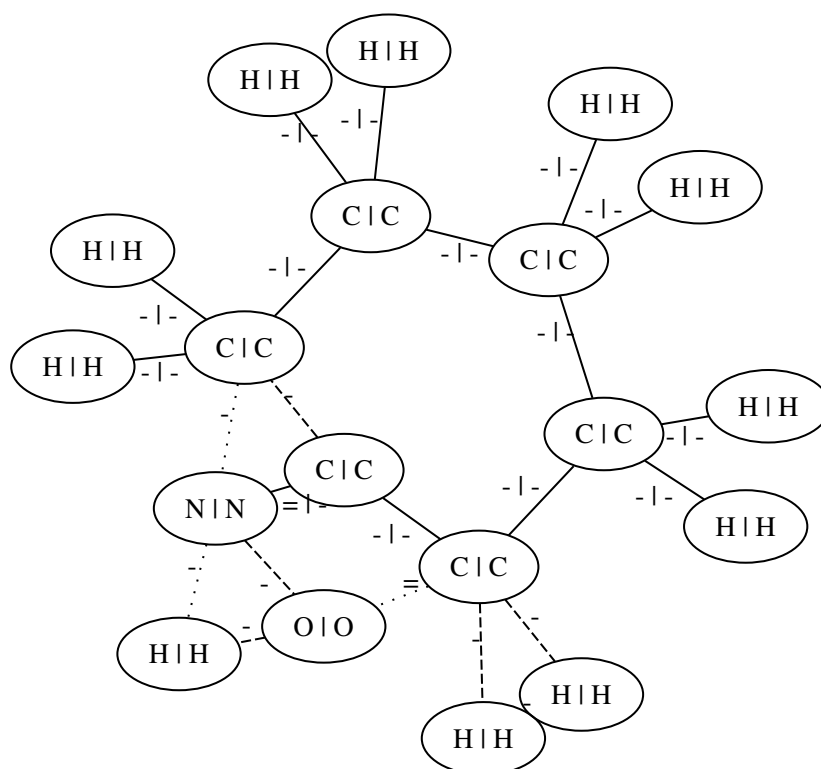
0.2.41 4.5. Beckmann-Umlagerung 2



Files: out/214_r_40.10100000.{L, K, R}

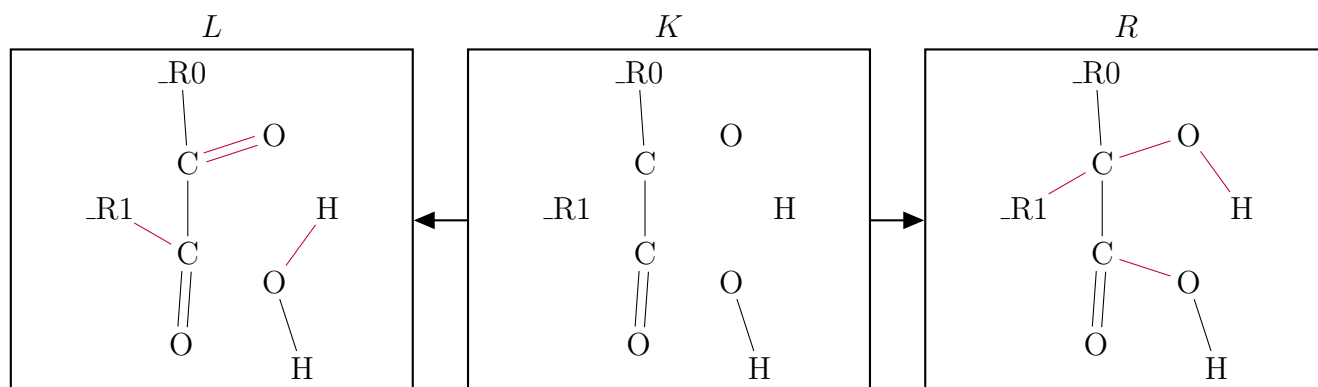


Files: out/215_r_40.11100100.{L, K, R}

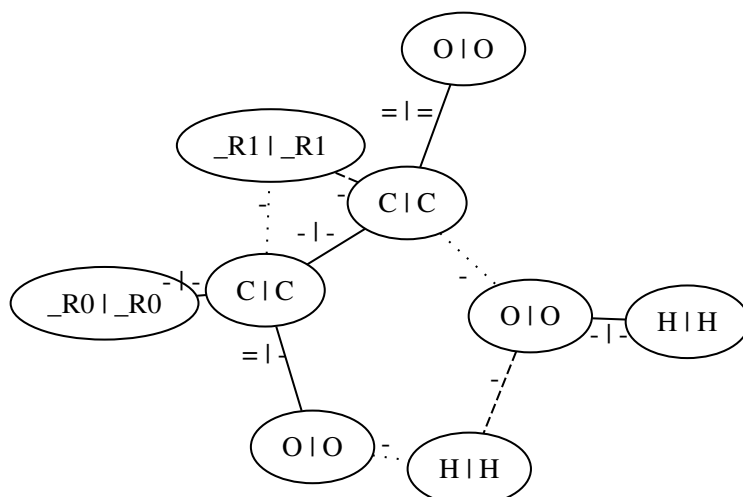
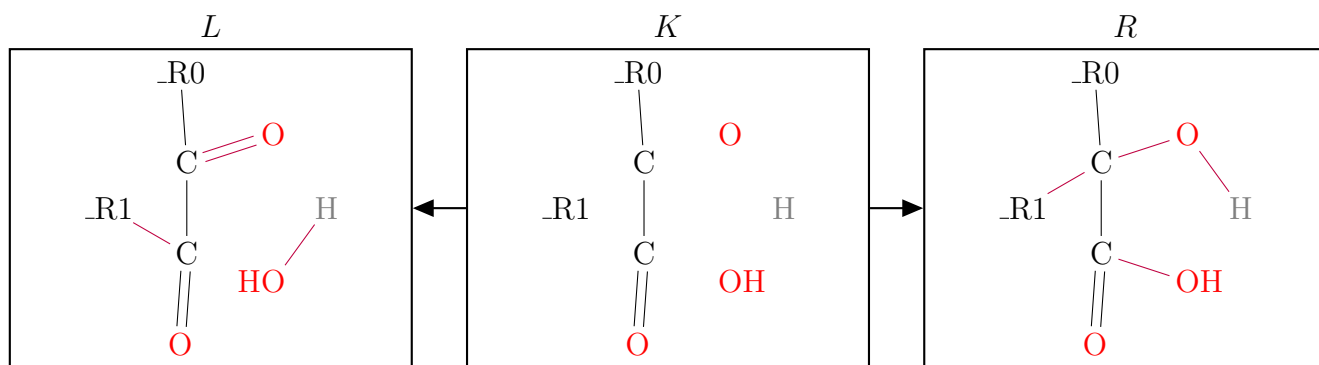


File: out/216_r_40_combined

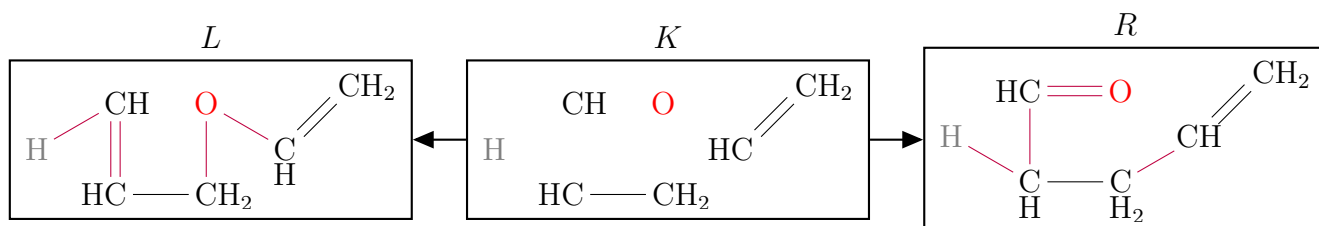
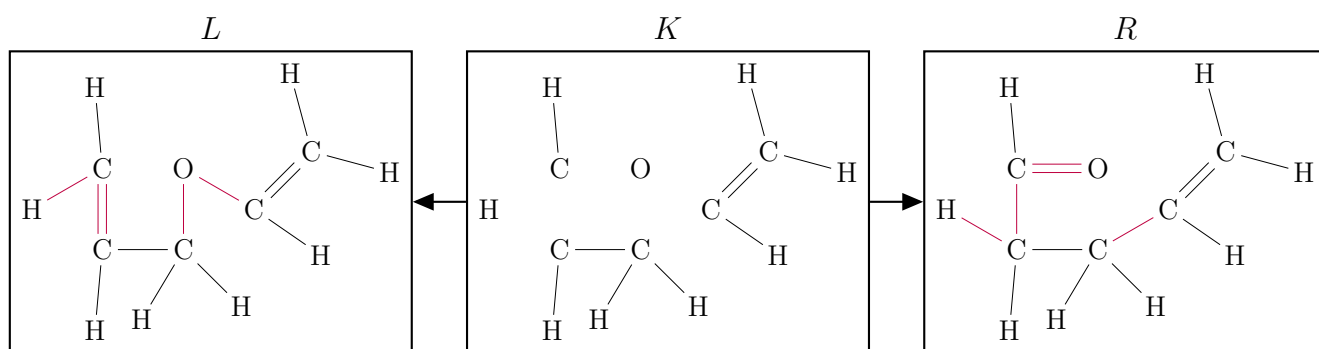
0.2.42 4.6 Benzilsaureumlagerung

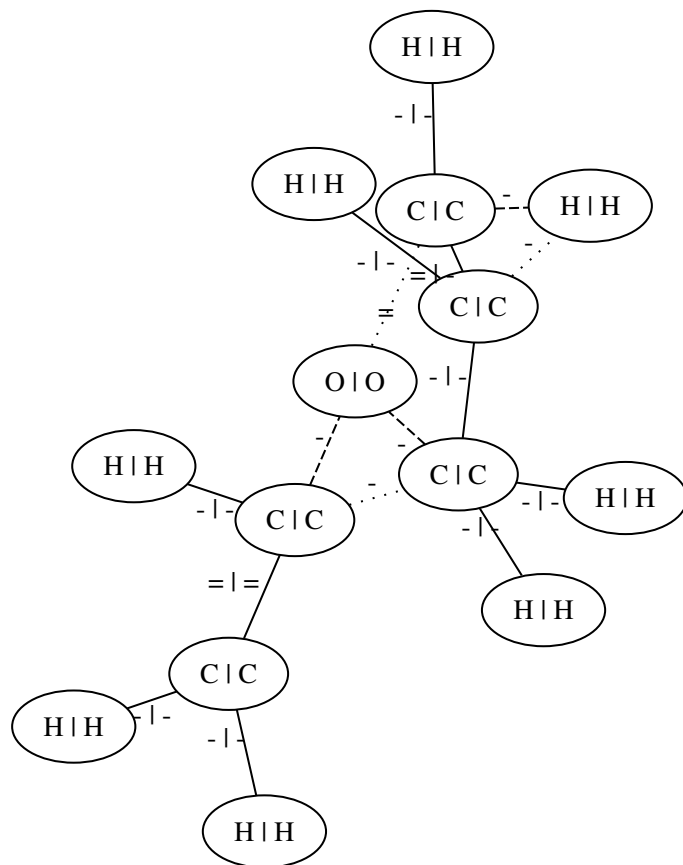


Files: out/219_r_41.10100000.{L, K, R}



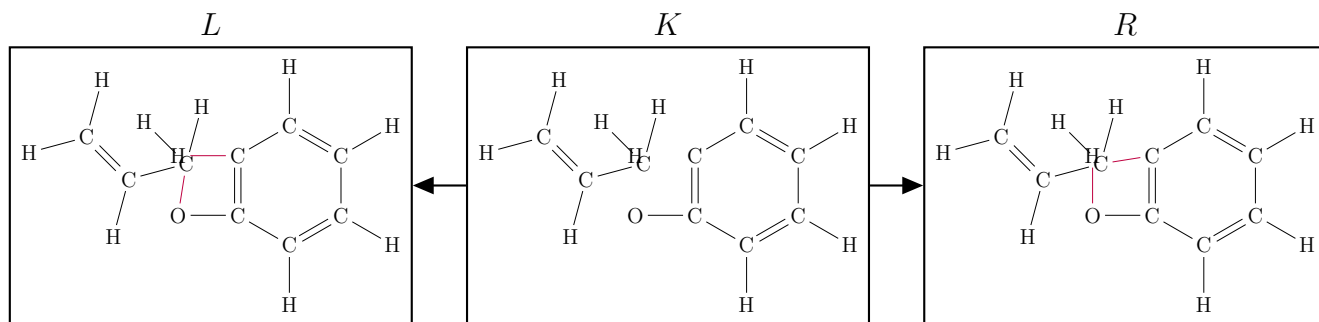
0.2.43 4.7. Claisen-Umlagerung 1



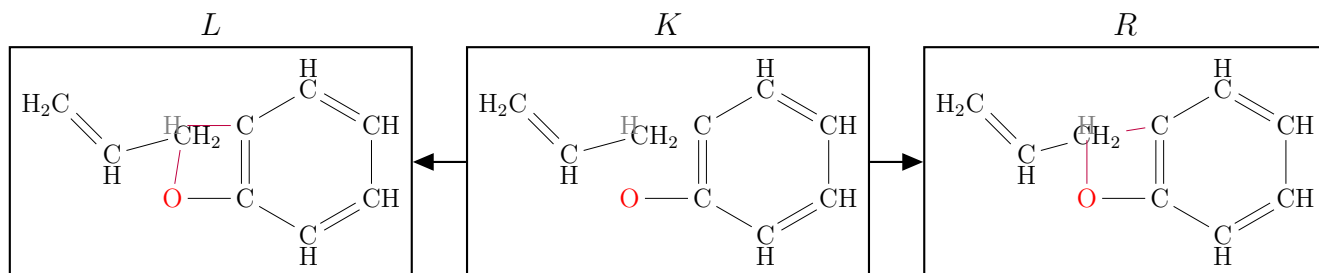


File: out/226_r_42_combined

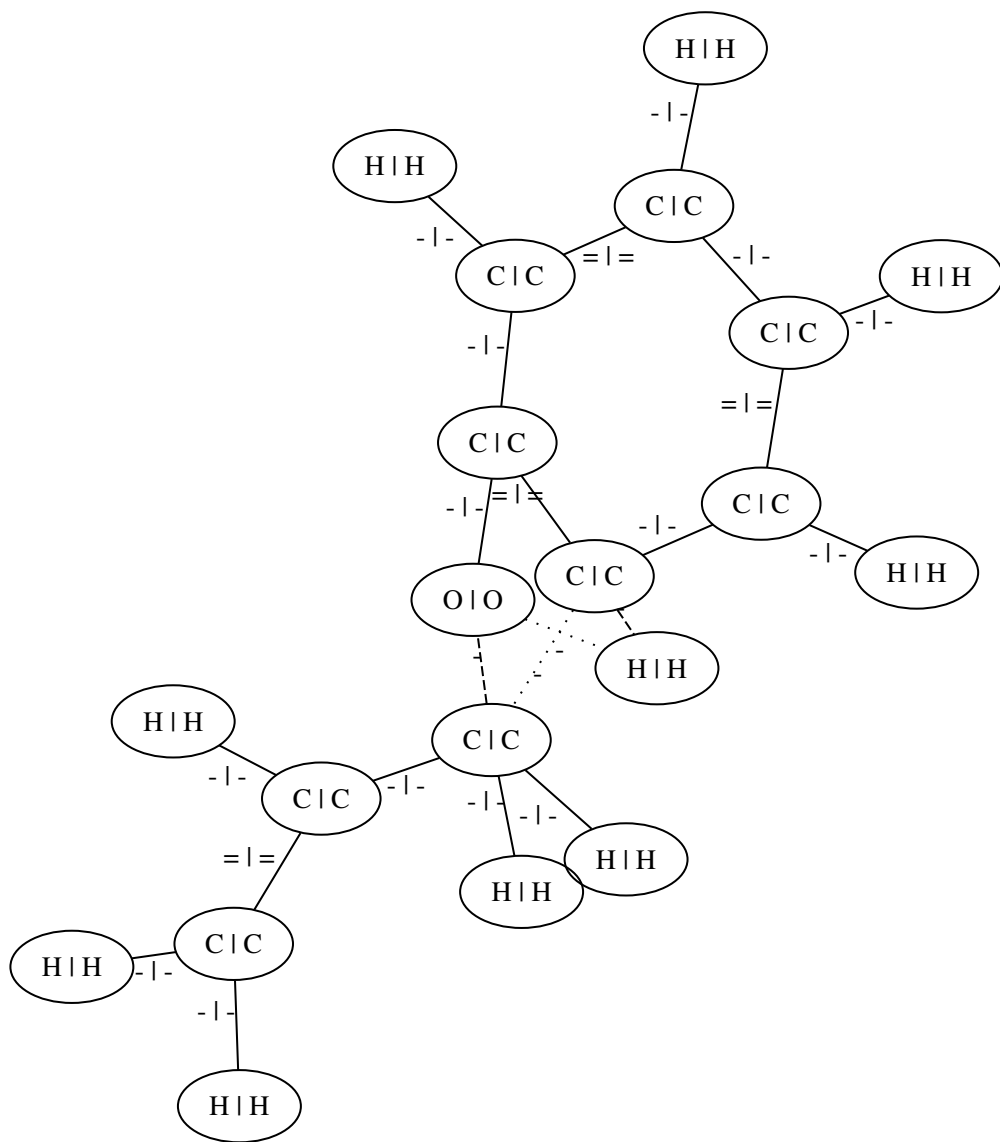
0.2.44 4.7. Claisen-Umlagerung 2



Files: out/229_r_43.10100000.{L, K, R}

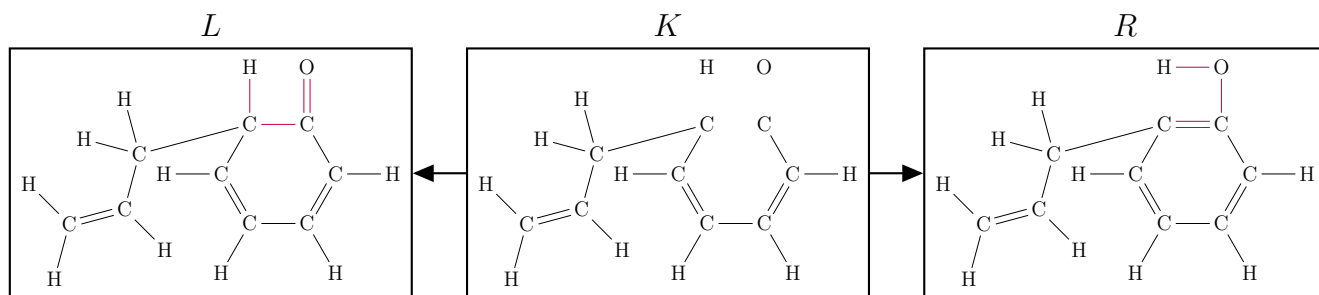


Files: out/230_r_43.11100100.{L, K, R}

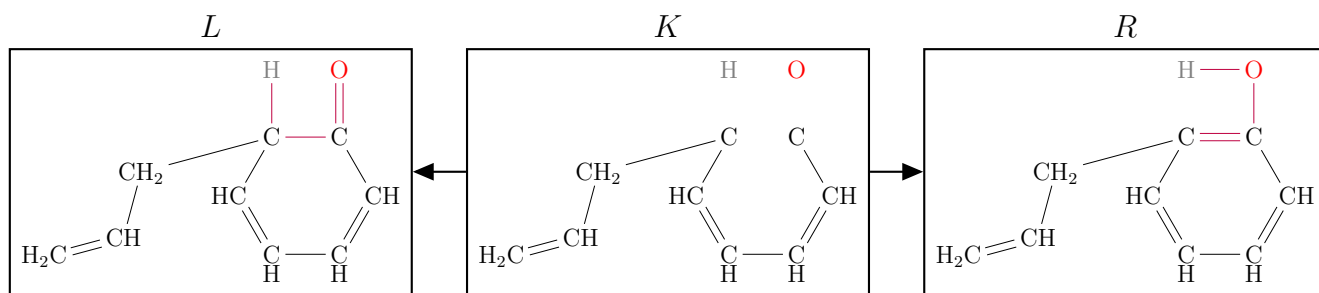


File: out/231_r_43_combined

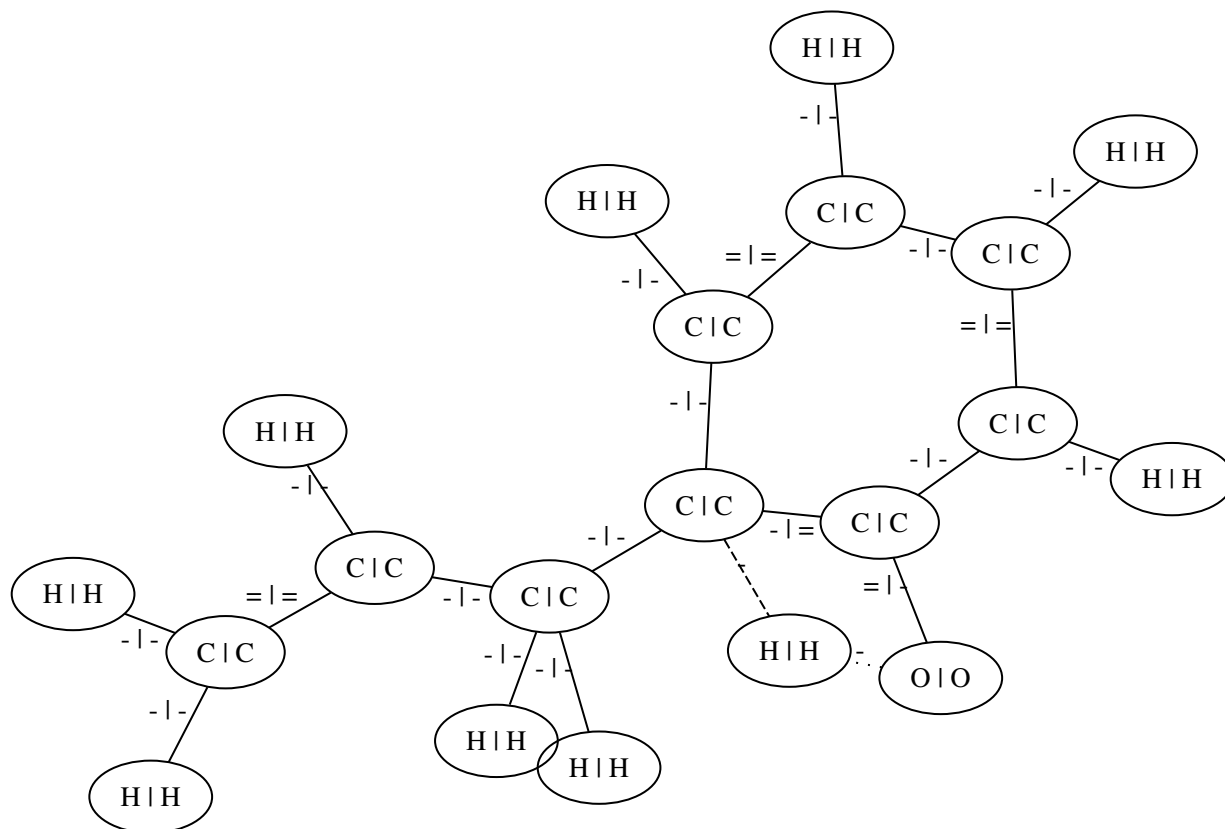
0.2.45 4.7. Claisen-Umlagerung 3



Files: out/234_r_44.10100000.{L, K, R}

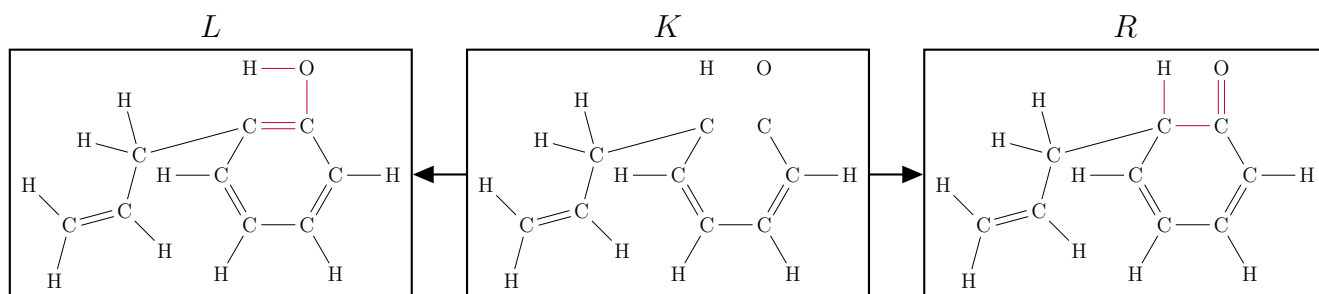


Files: out/235_r_44.11100100.{L, K, R}

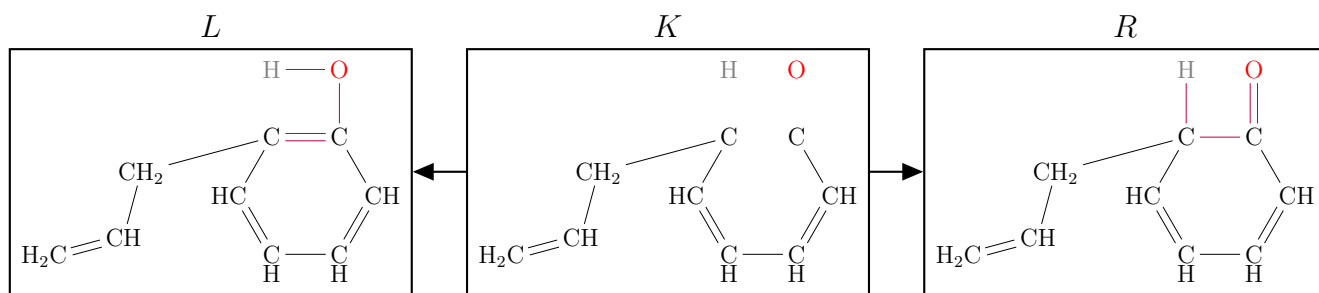


File: out/236_r_44_combined

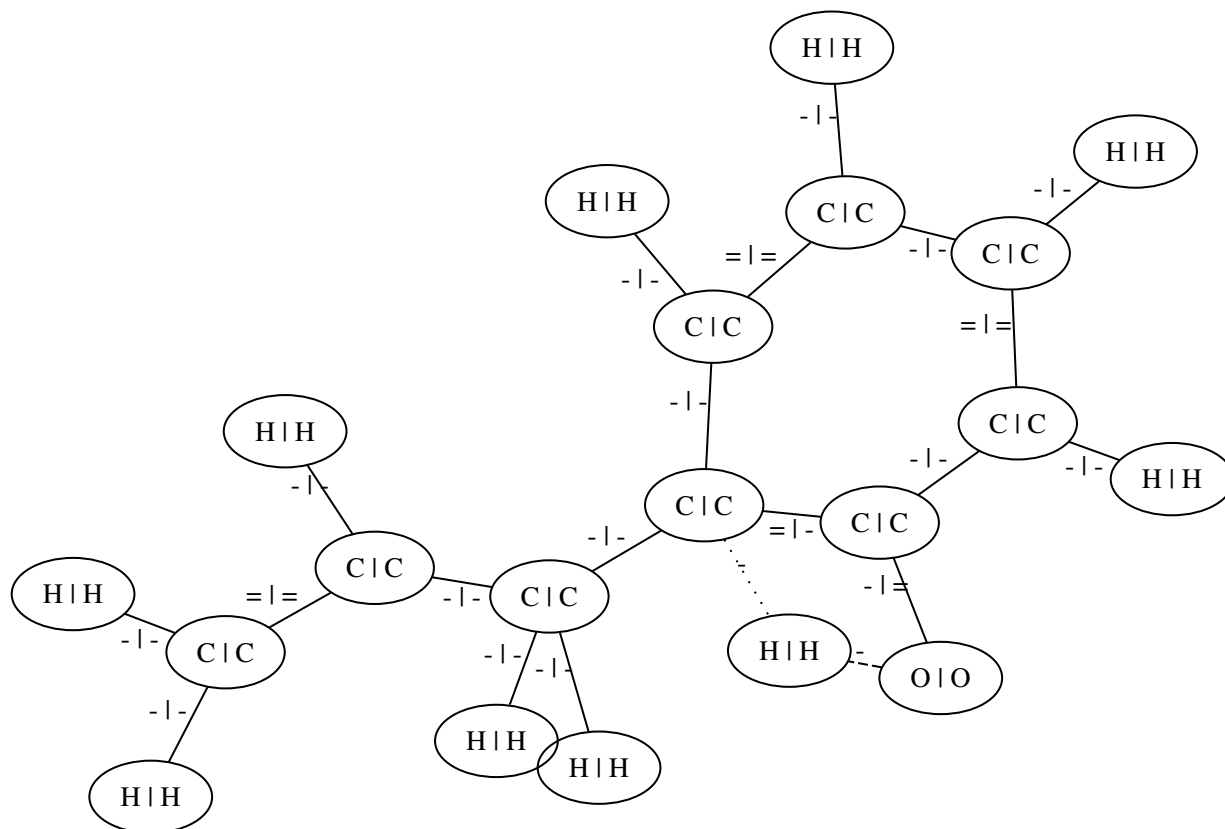
0.2.46 4.7. Claisen-Umlagerung 4



Files: out/239_r_45.10100000.{L, K, R}

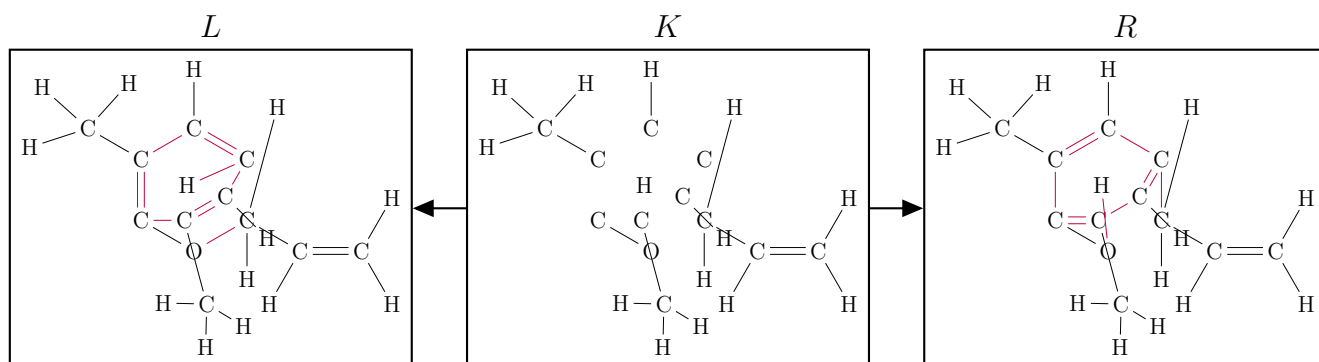


Files: out/240_r_45.11100100.{L, K, R}

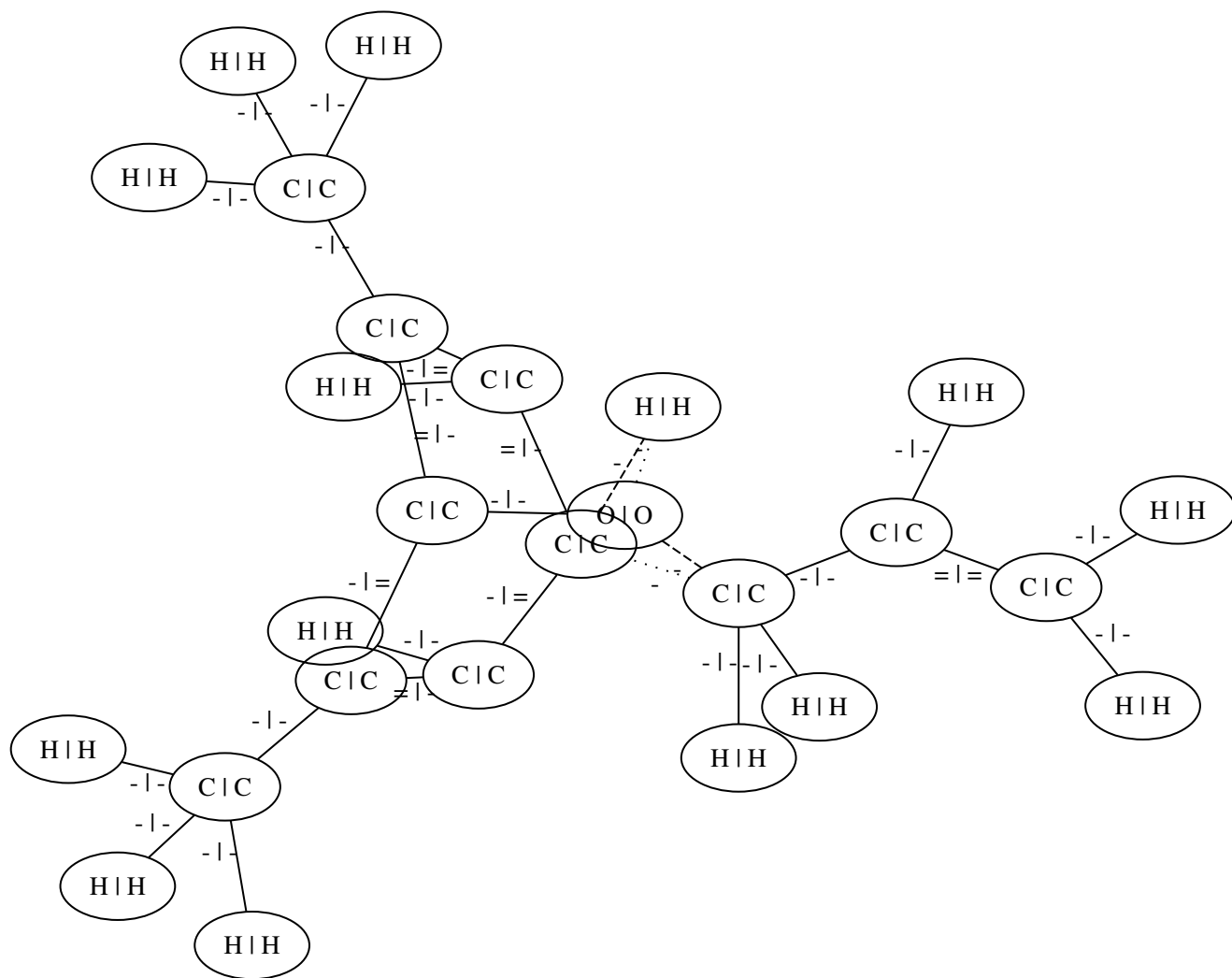
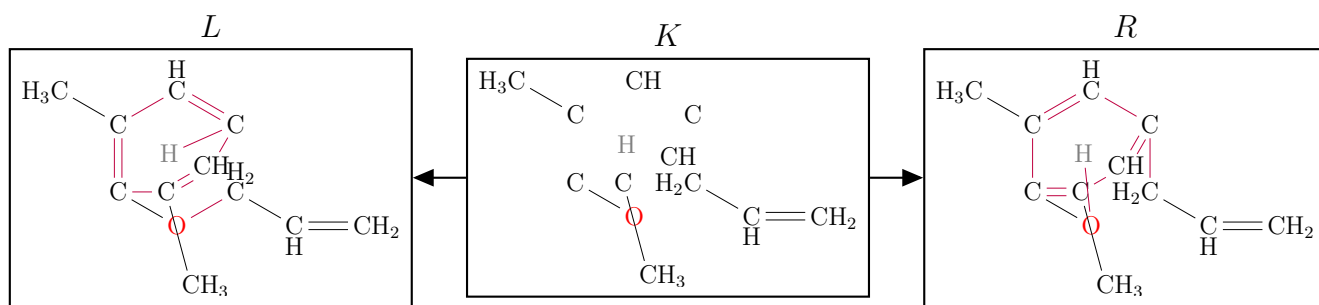


File: out/241_r_45_combined

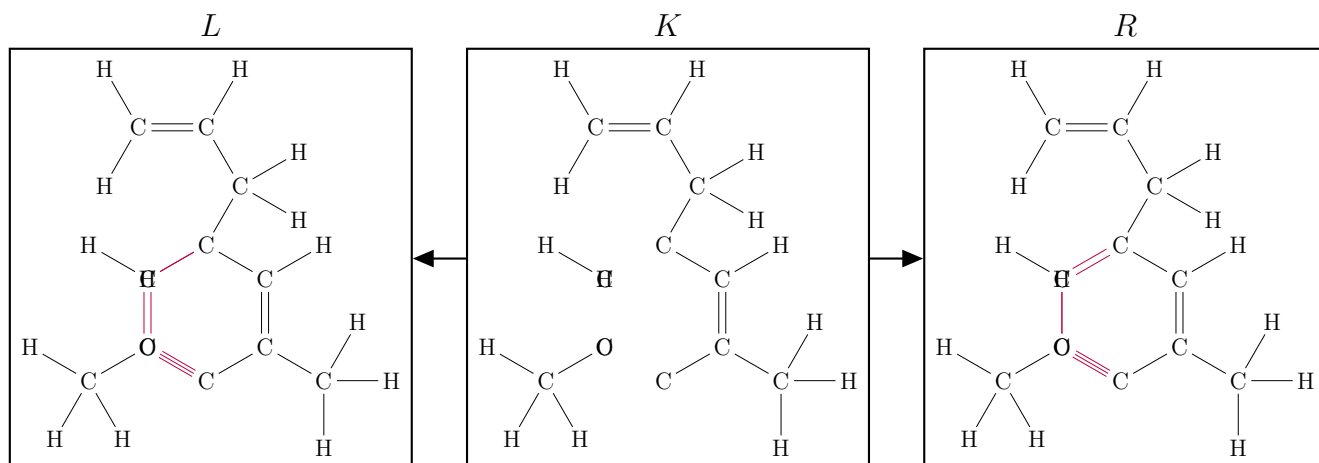
0.2.47 4.7. Claisen-Umlagerung 5



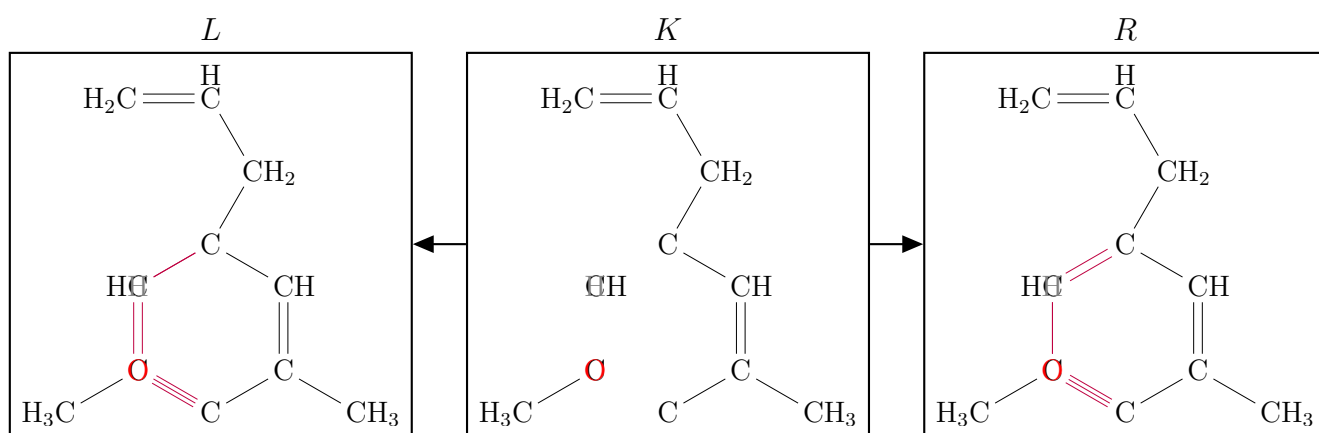
Files: out/244_r_46.10100000.{L, K, R}



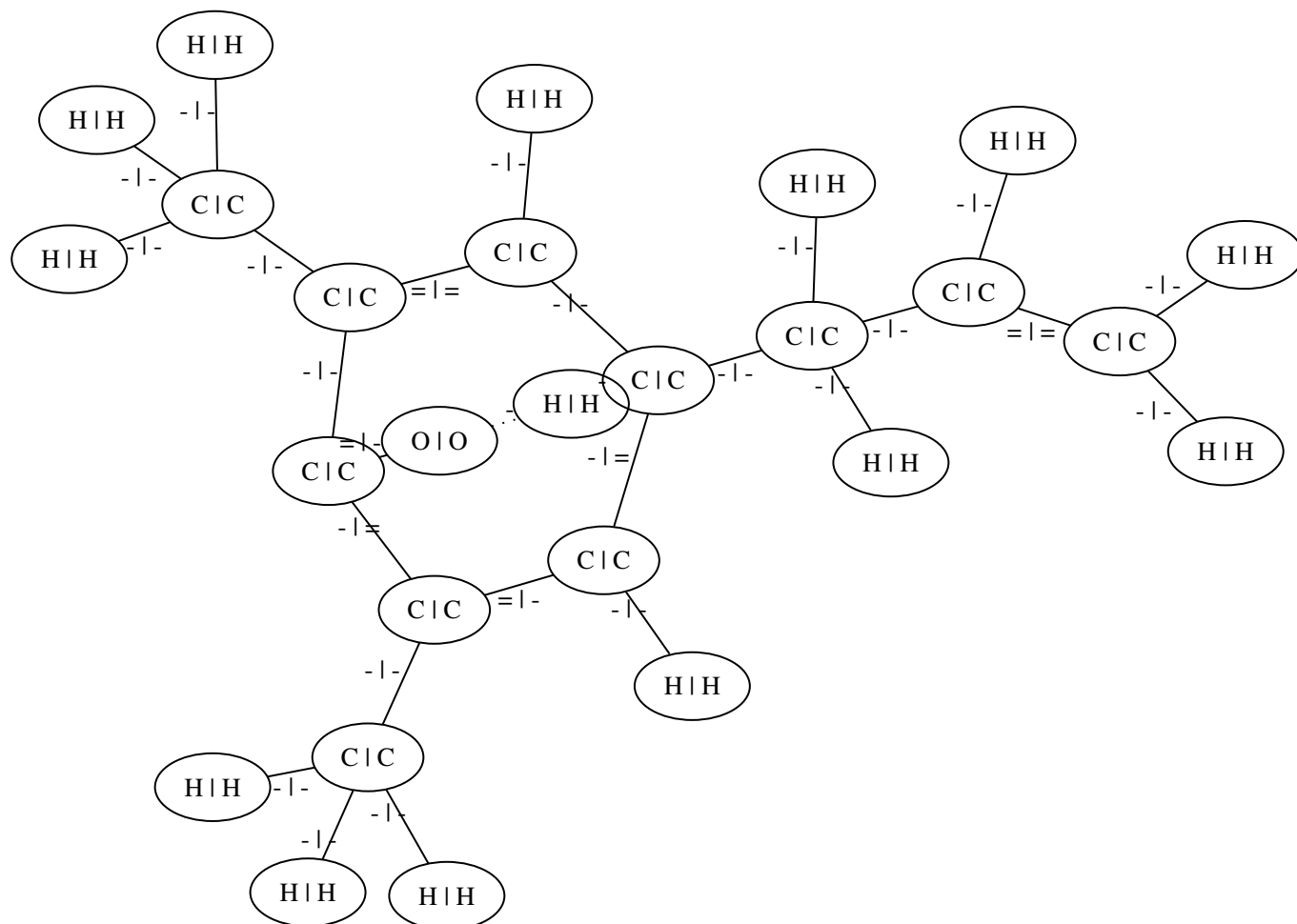
0.2.48 4.7. Claisen-Umlagerung 6



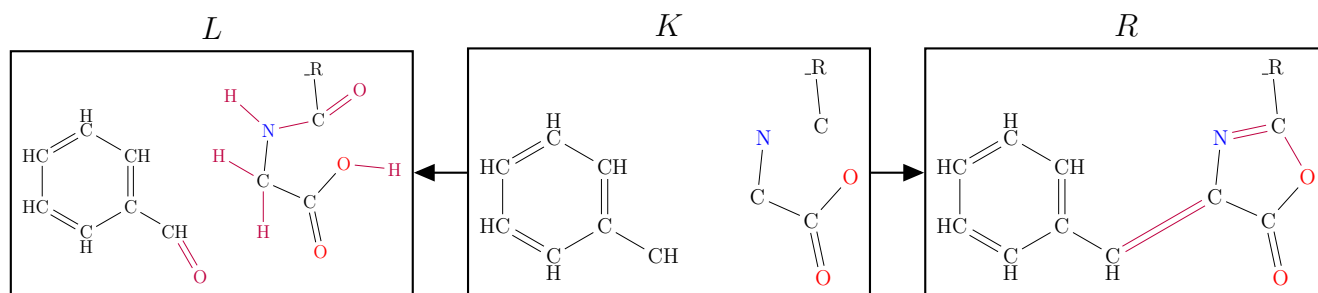
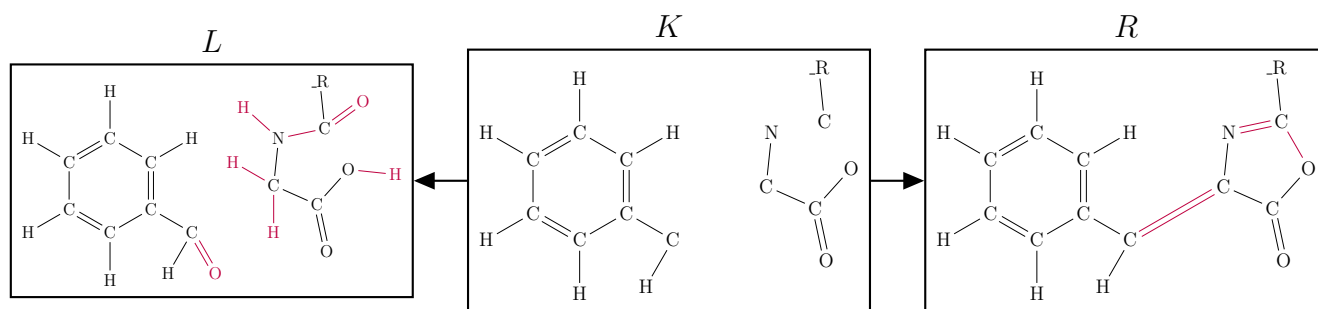
Files: out/249_r_47.10100000.{L, K, R}

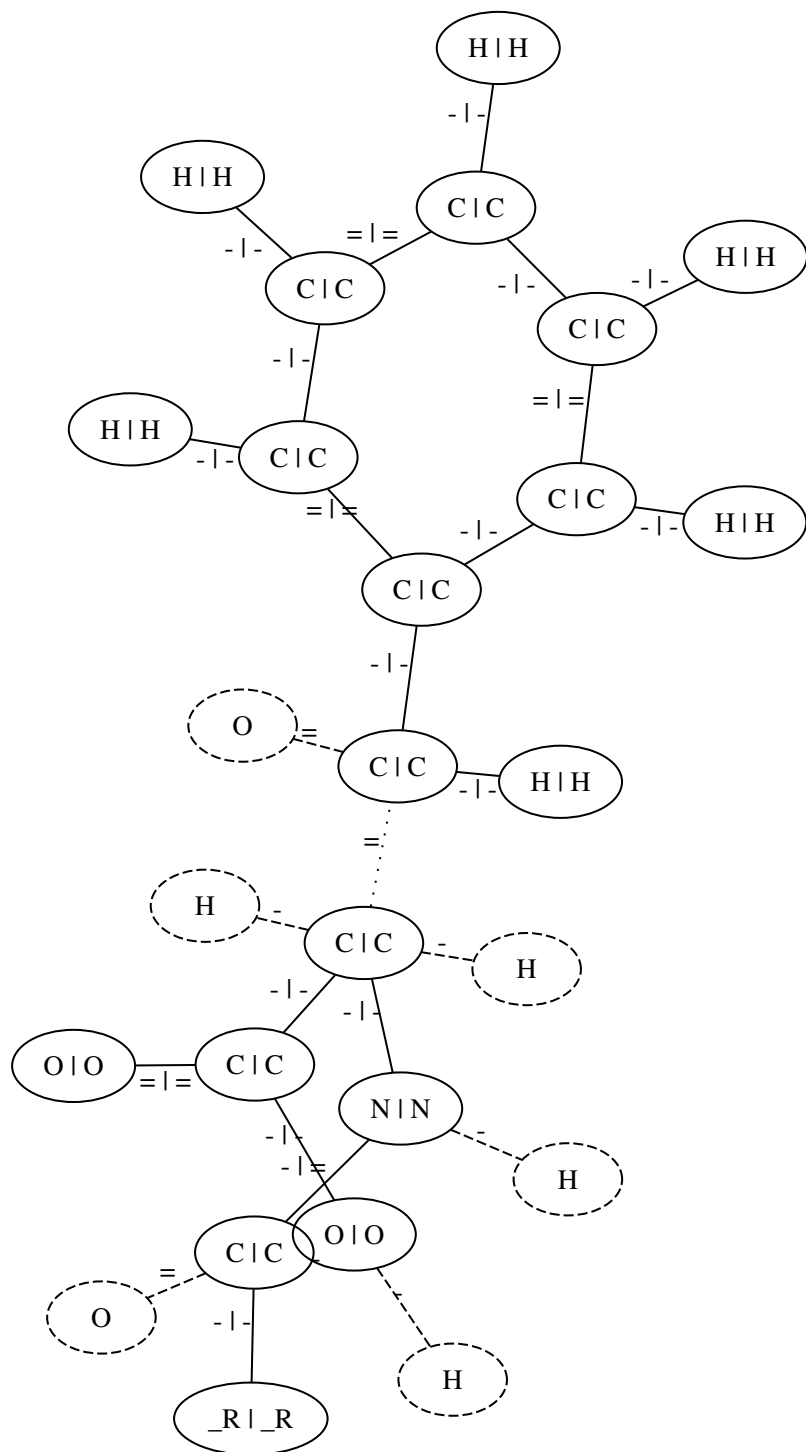


Files: out/250_r_47.11100100.{L, K, R}



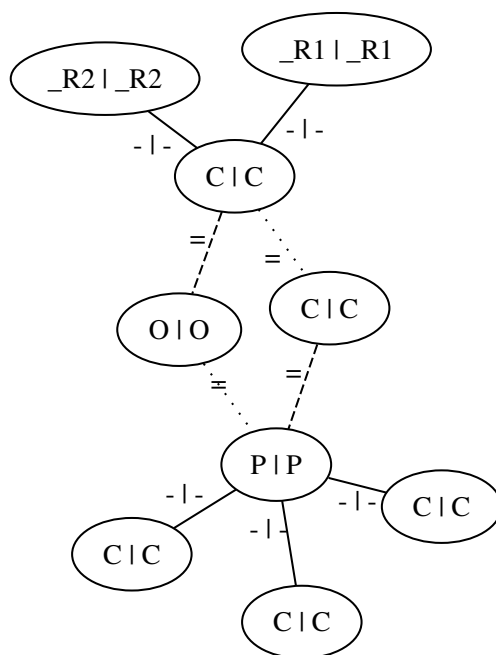
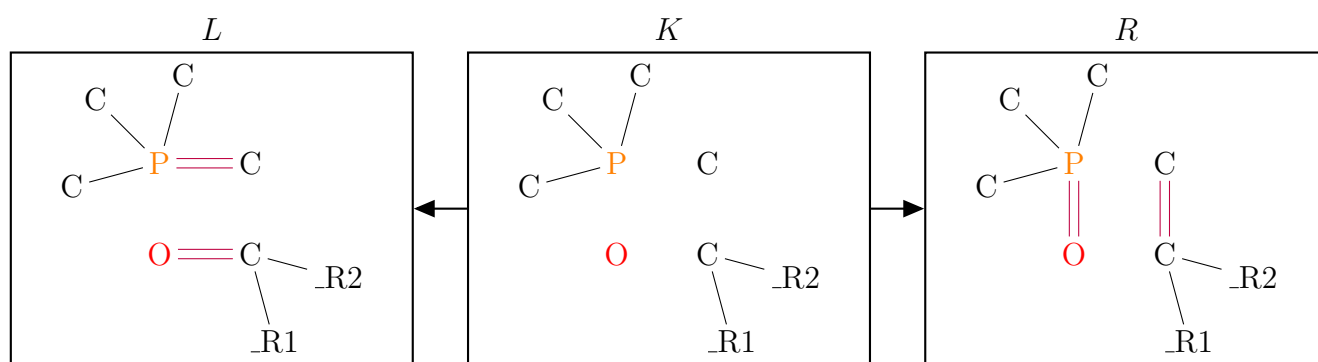
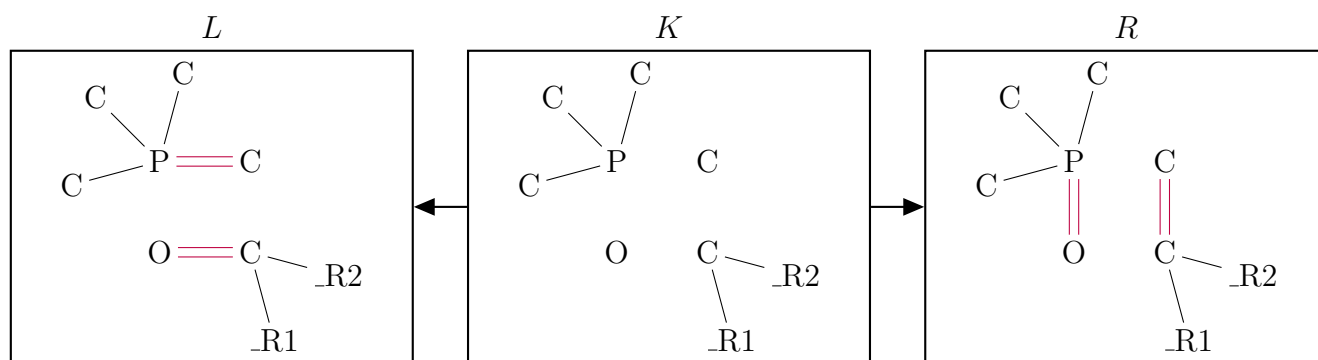
0.2.49 5.1 Erlenmaeyer-Ploechl-Azlacton-Synthese





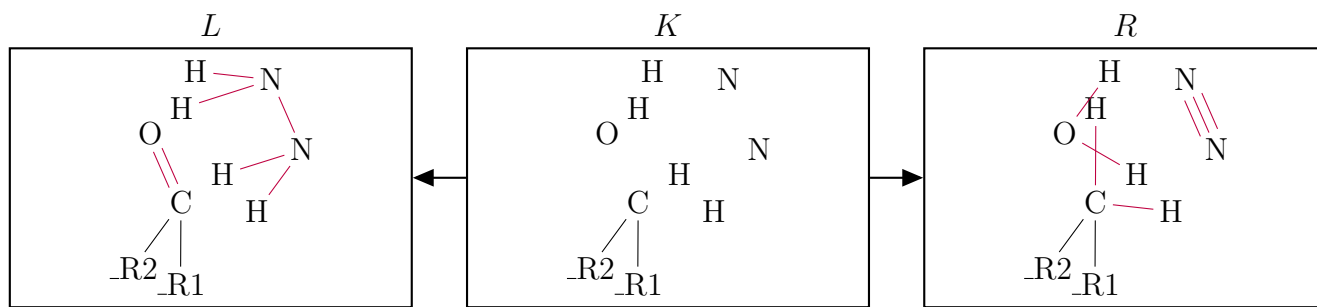
File: out/256_r_48_combined

0.2.50 Wittig1

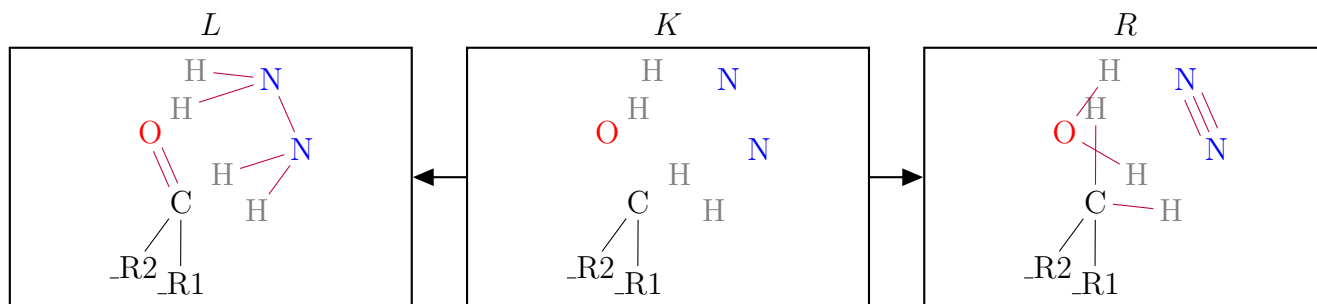


File: out/261_r_49_combined

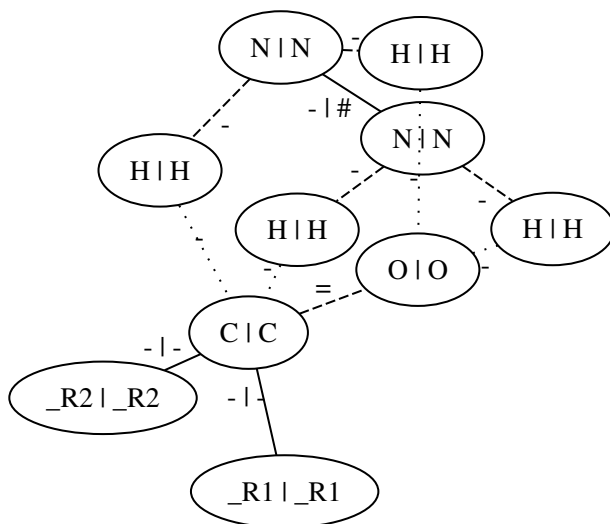
0.2.51 5.3 Wolff-Kishner-Rule



Files: out/264_r_50.10100000.{L, K, R}

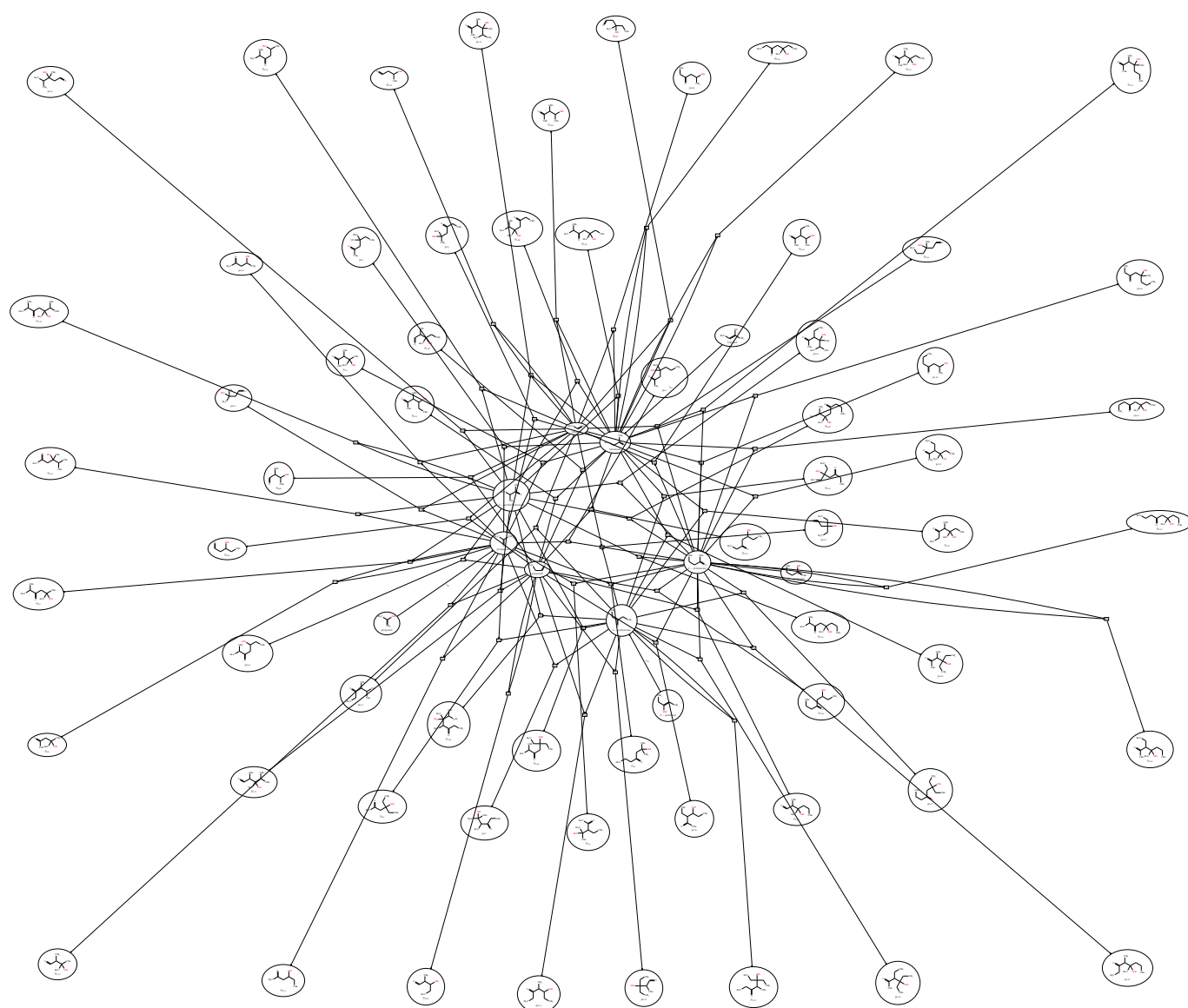


Files: out/265_r_50.11100100.{L, K, R}



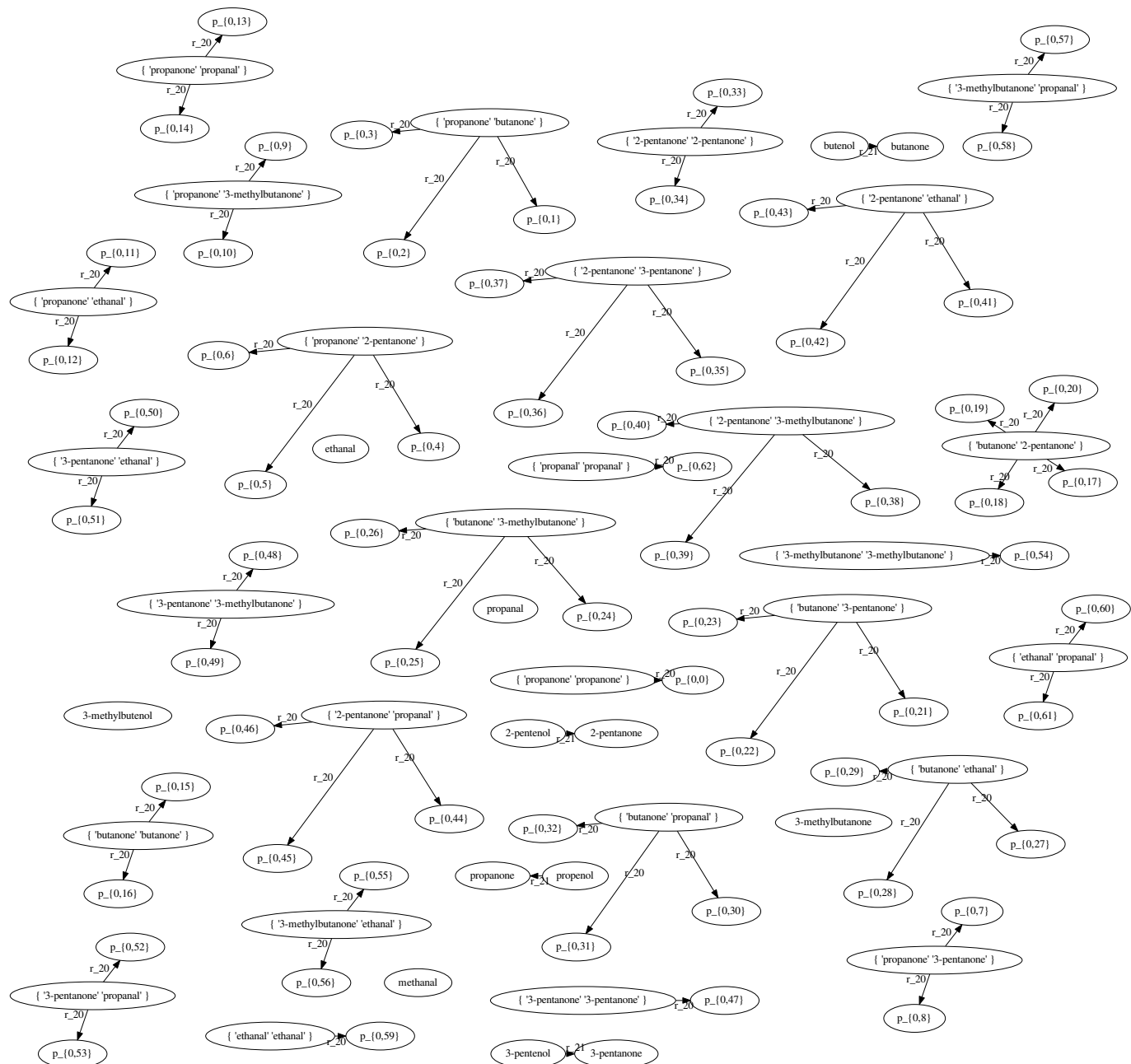
File: out/266_r_50_combined

0.2.52 DG Hyper, dg_0



File: out/332_dg_0_1110

0.2.53 DG NonHyper, dg_0



File: out/333_dgNonHyper_0