

Summary

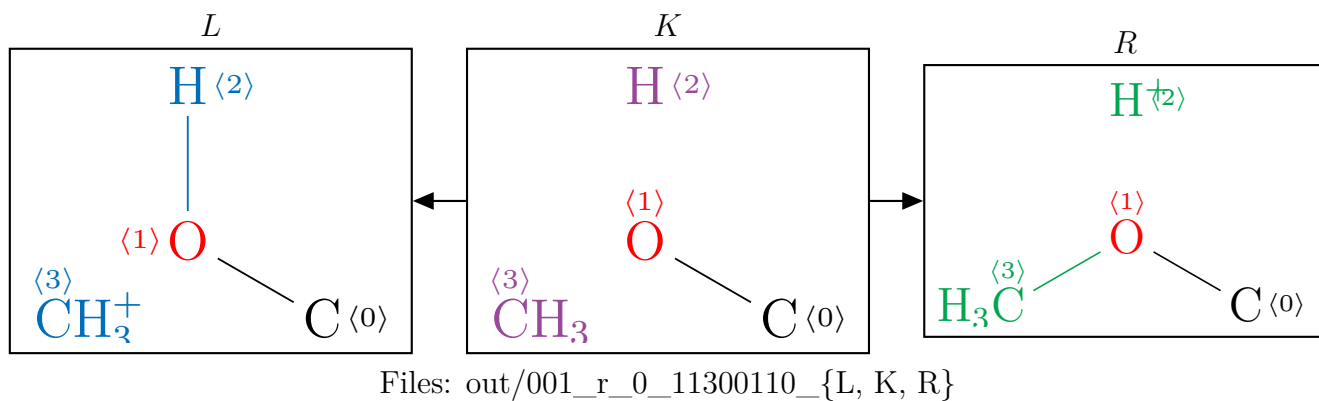
November 13, 2023

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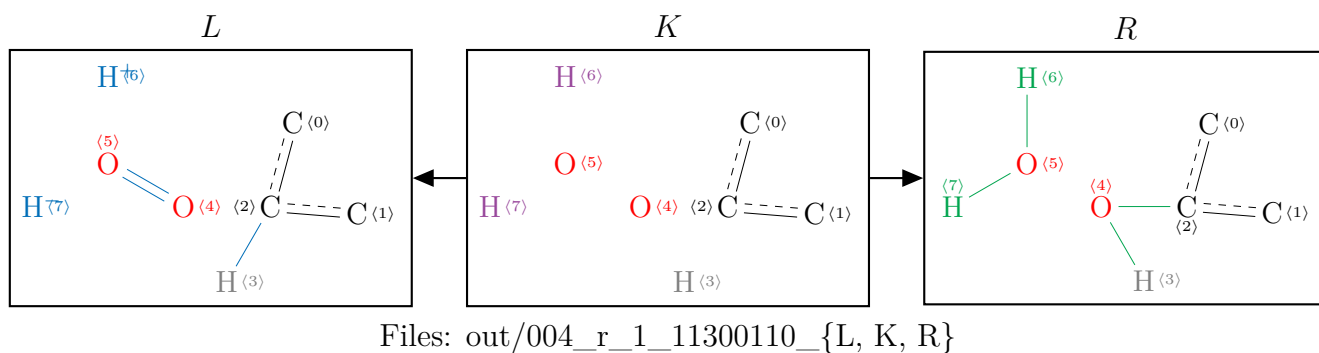
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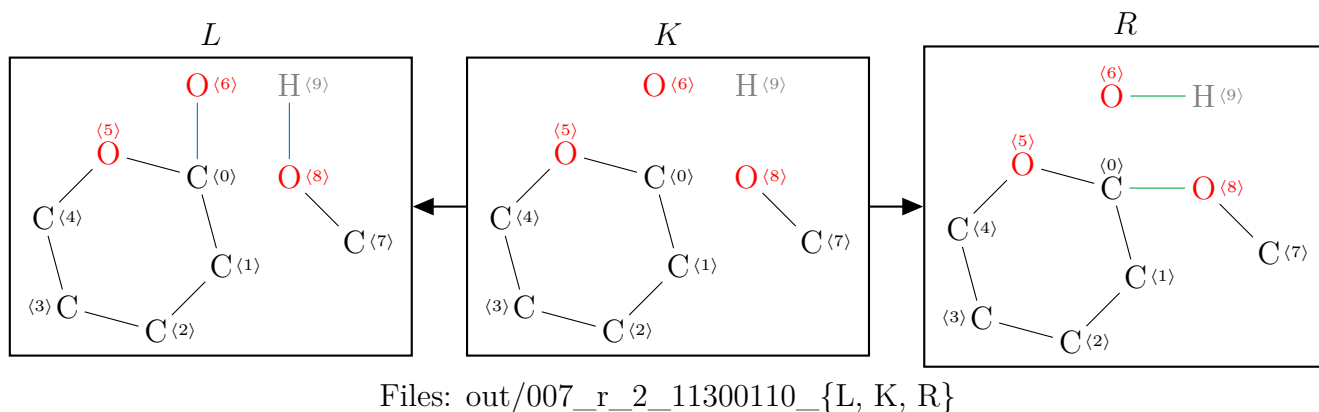
0.0.1 O-Methylation



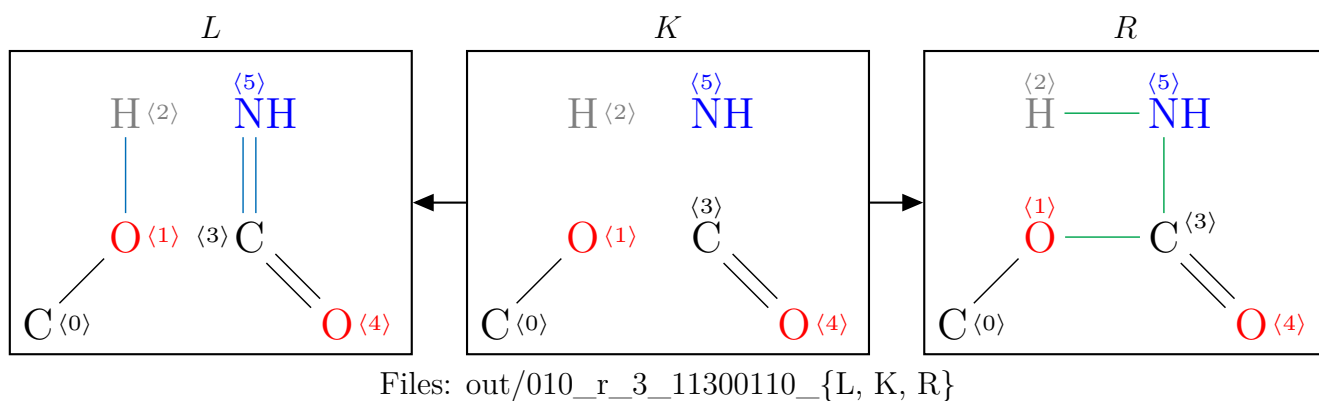
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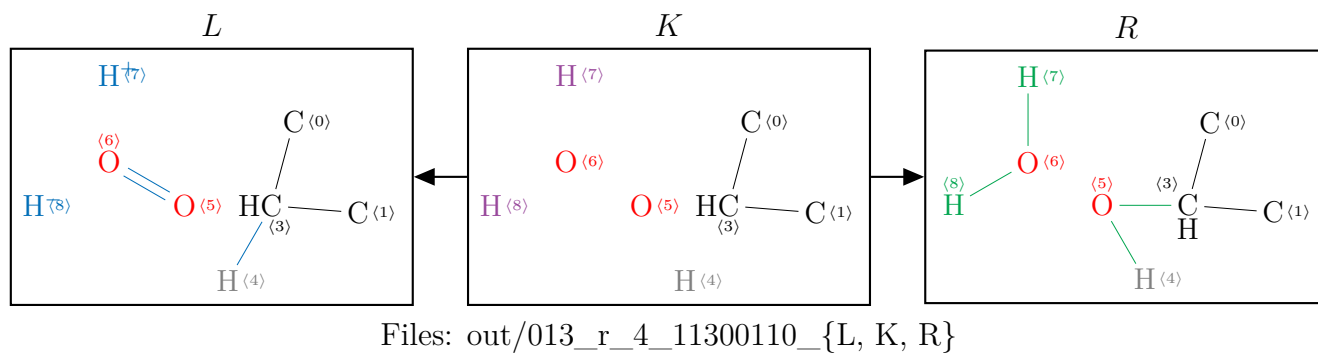
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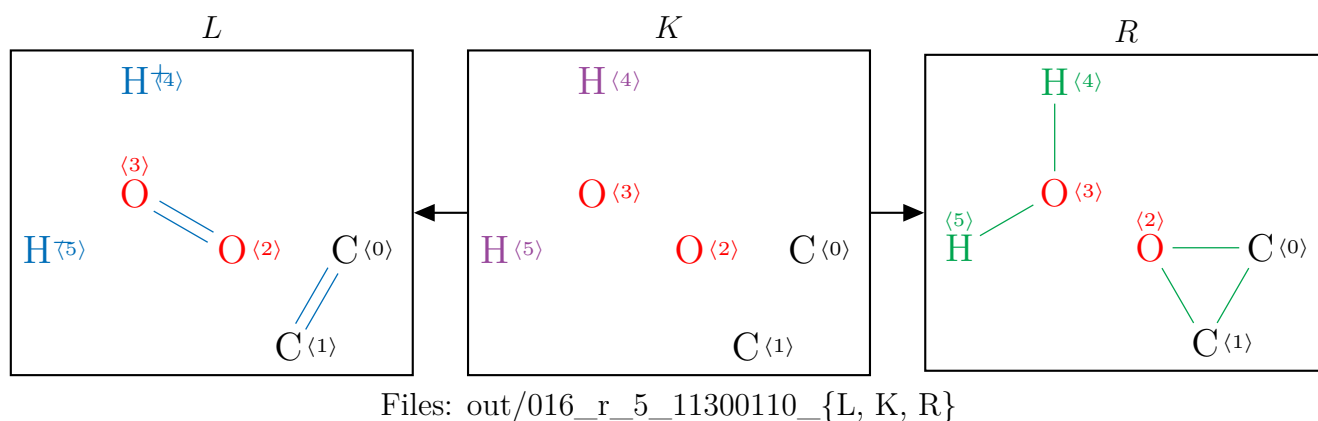
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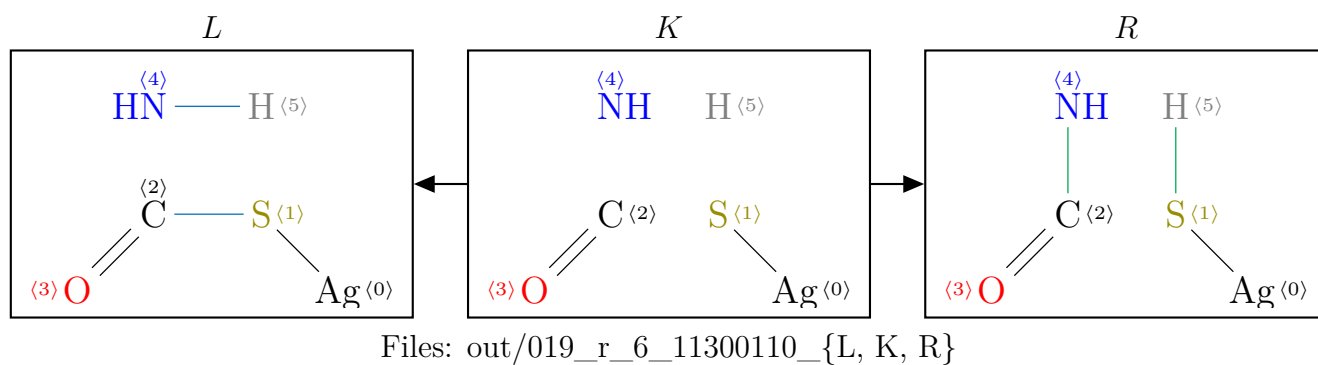
0.0.5 Aliphatic double bond oxidation



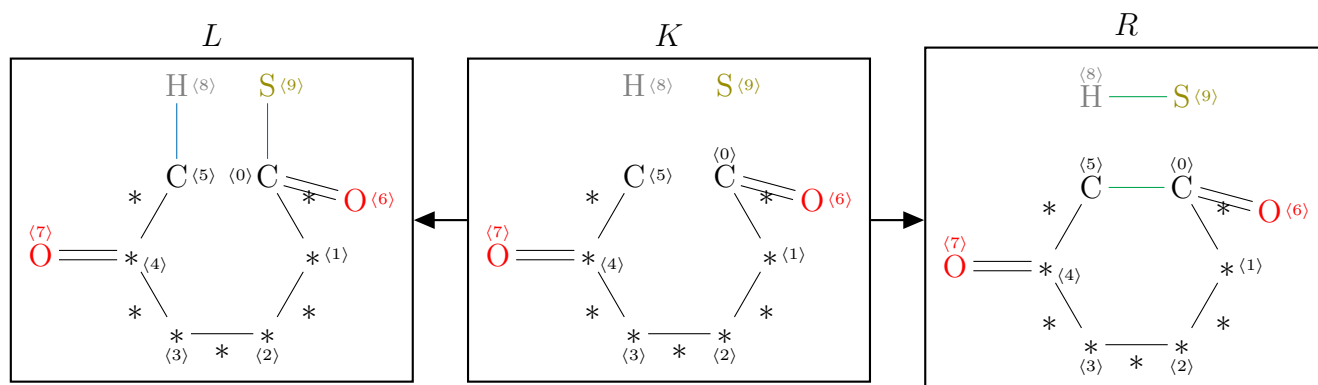
0.0.6 Epoxidation



0.0.7 Release of a polyketide from the PKS by nucleophilic attack of a primary amino group



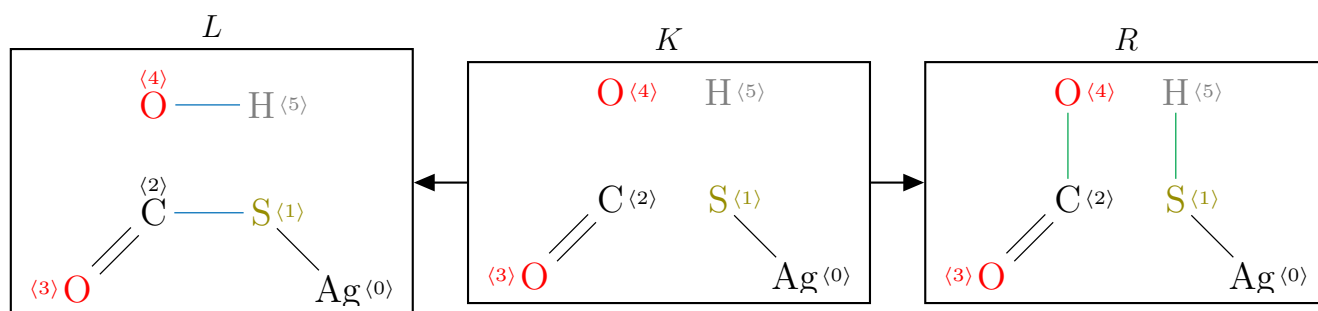
0.0.8 Intramolecular Claisen thioester condensation via near carbonyl group, ringsize 6



Files: out/022_r_7_11300110_{L, K, R}

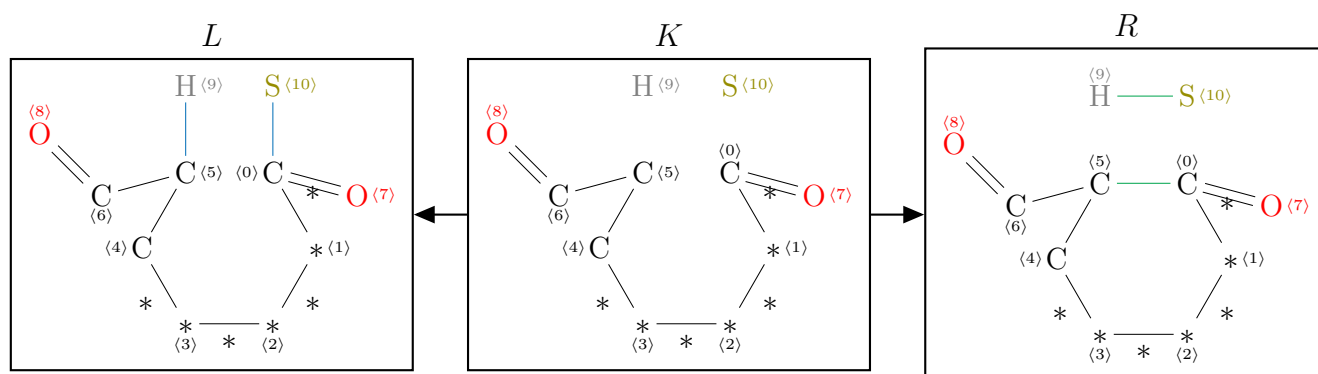
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0.0.9 Release from the synthase by nucleophilic attack of a hydroxyl group



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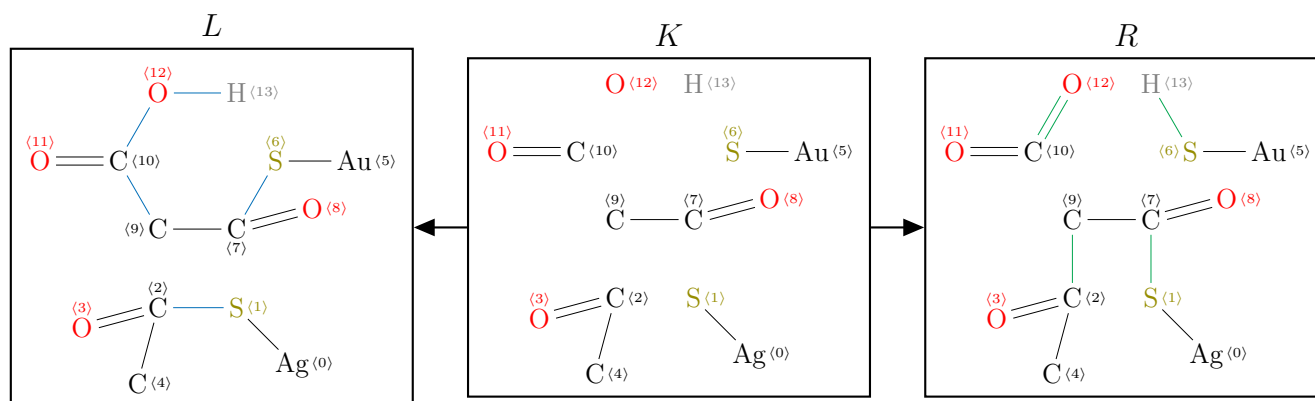
0.0.10 Intramolecular Claisen thioester condensation via near carbonyl group, ringsize 6



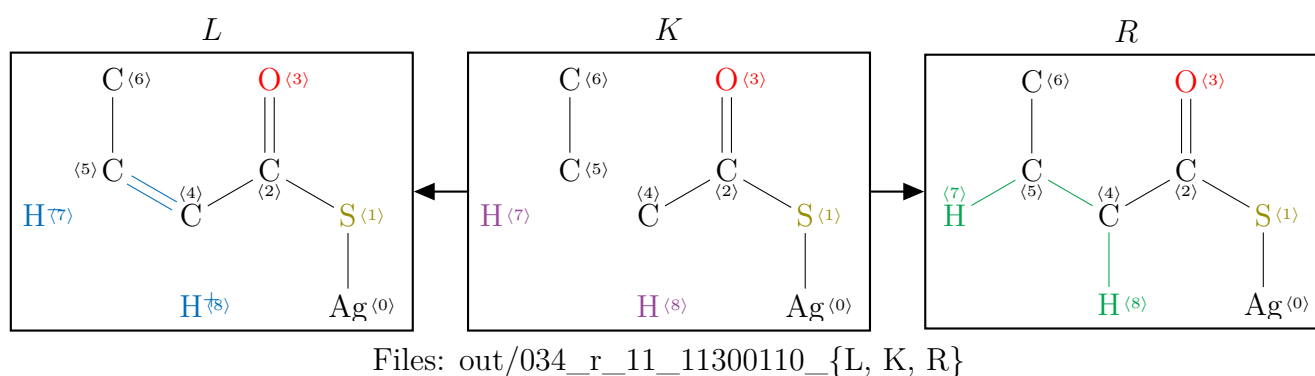
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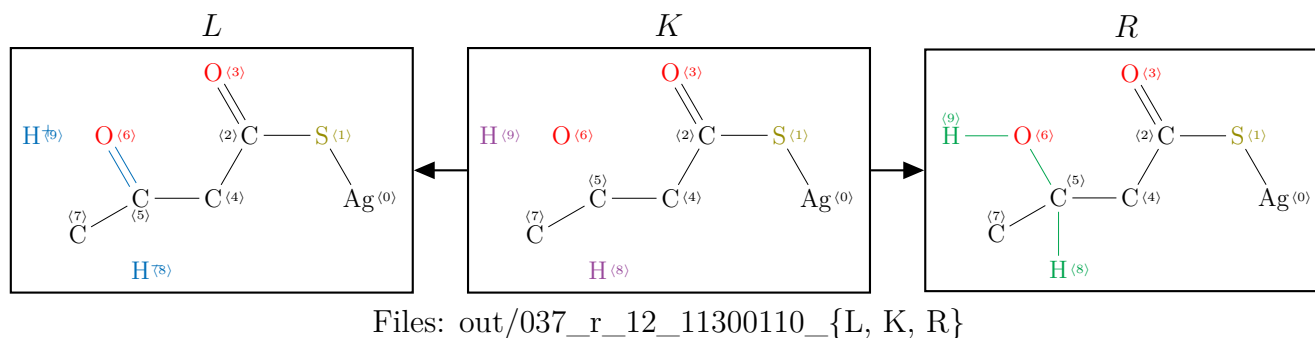
0.0.11 Intermolecular decarboxylative Claisen thioester condensation



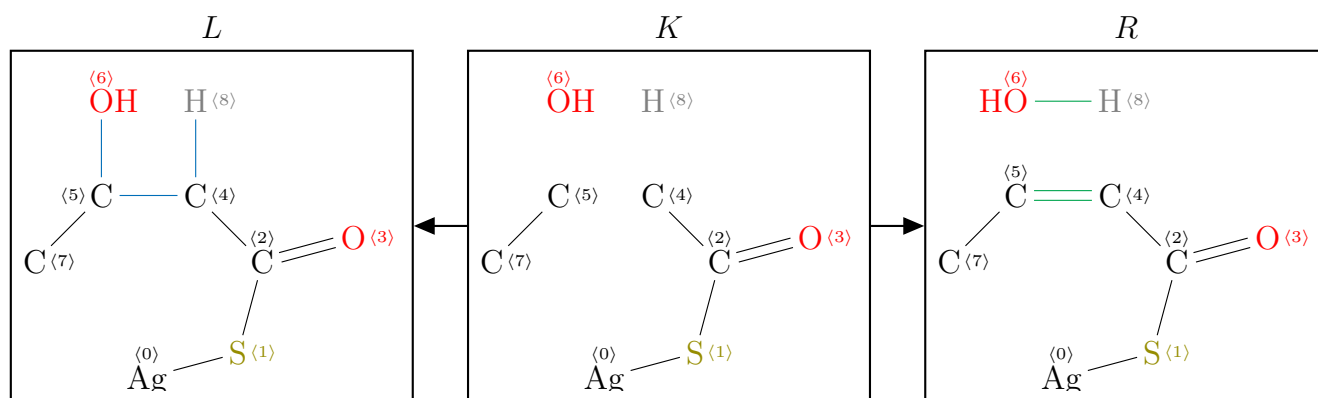
0.0.12 Reduction of enoyl group



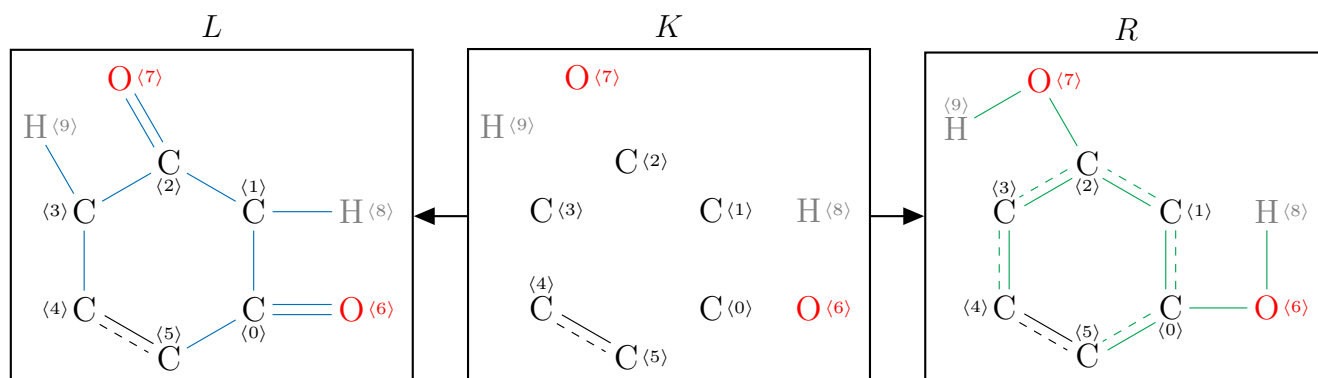
0.0.13 Reduction of beta carbonyl group



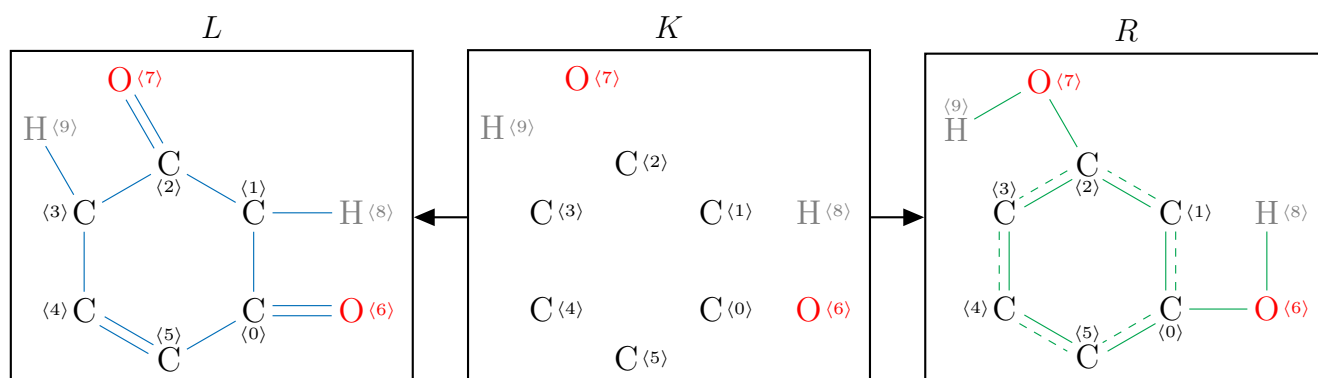
0.0.14 Dehydration of beta hydroxyl group



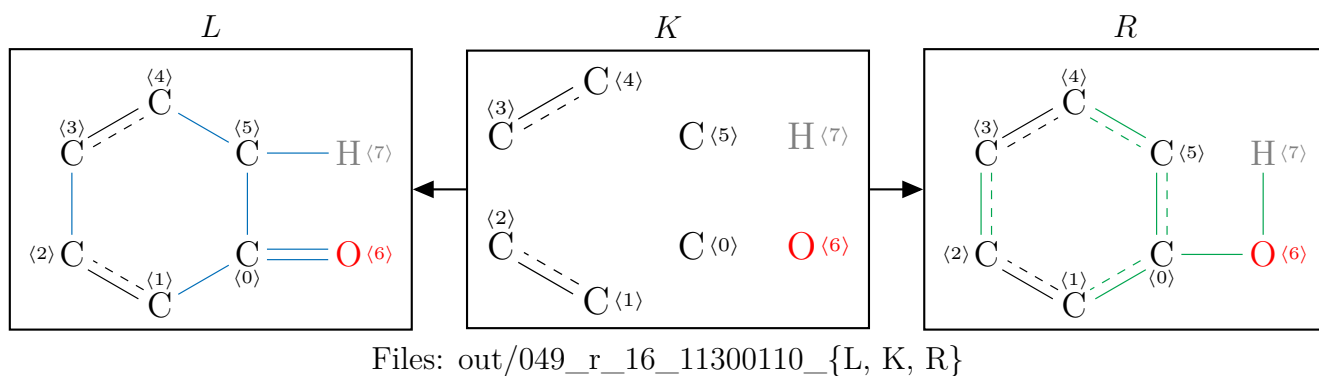
0.0.15 Aromatization of a 6-membered ring with 2 carbonyl groups and 1 aromatic bond



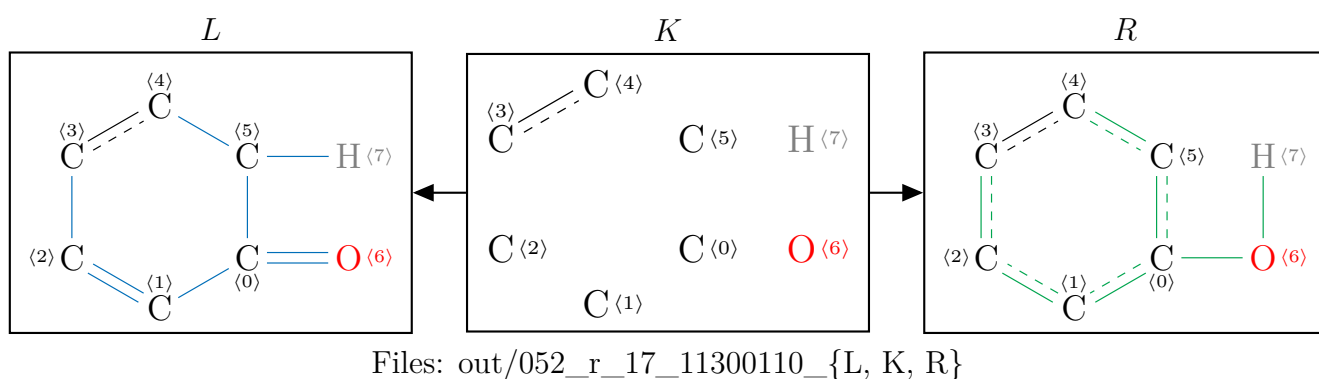
0.0.16 Aromatization of a 6-membered ring with 2 carbonyl groups and 1 double bond



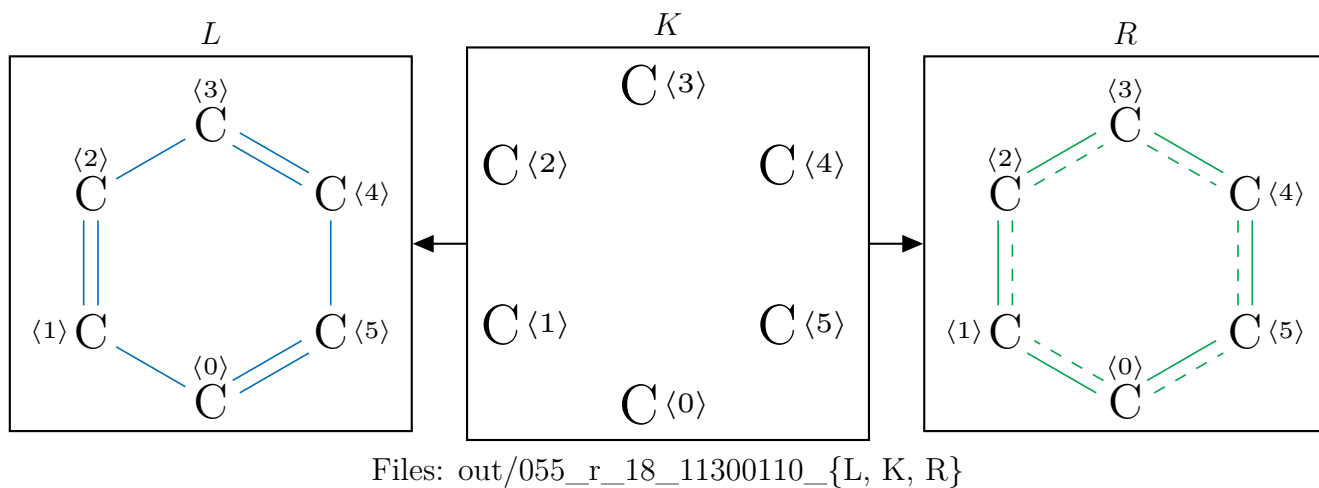
0.0.17 Aromatization of a 6-membered ring with 1 carbonyl group and 2 aromatic bonds



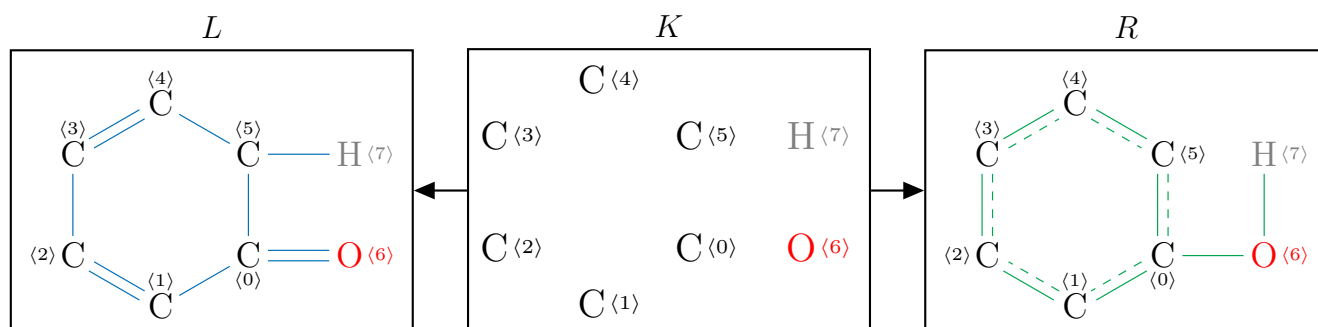
0.0.18 Aromatization of a 6-membered ring with 1 carbonyl group, 1 double bond and 1 aromatic bond - orientation 2



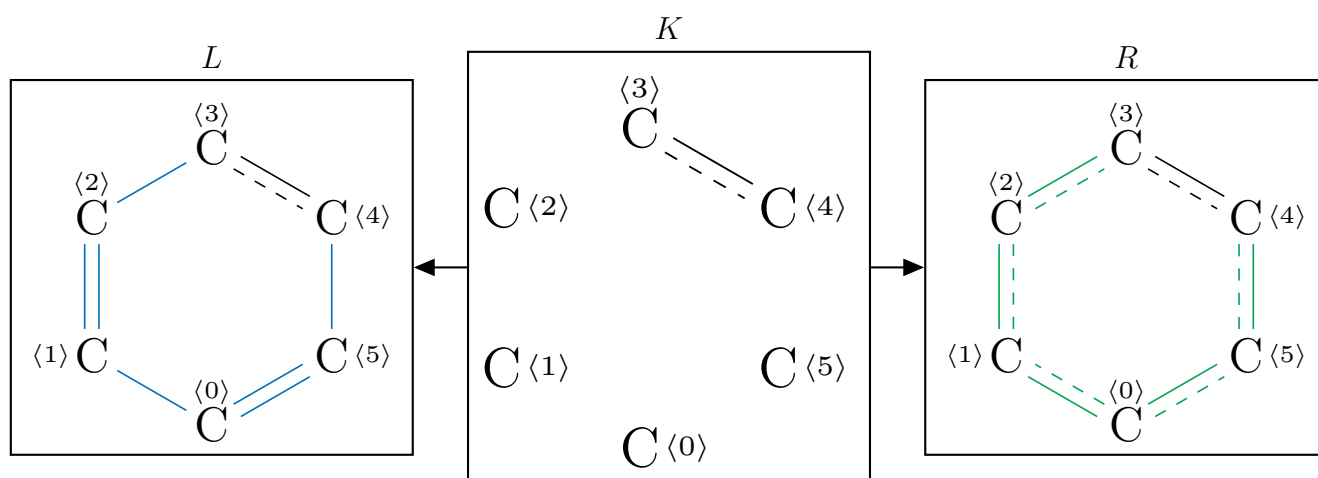
0.0.19 Aromatization of a 6-membered ring with 3 double bonds



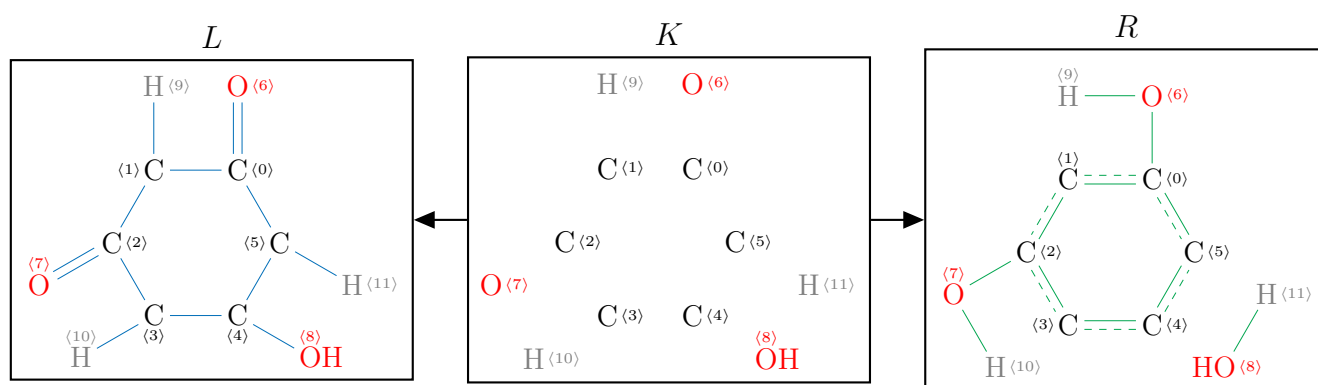
0.0.20 Aromatization of a 6-membered ring with 1 carbonyl group and 2 double bonds - orientation 1



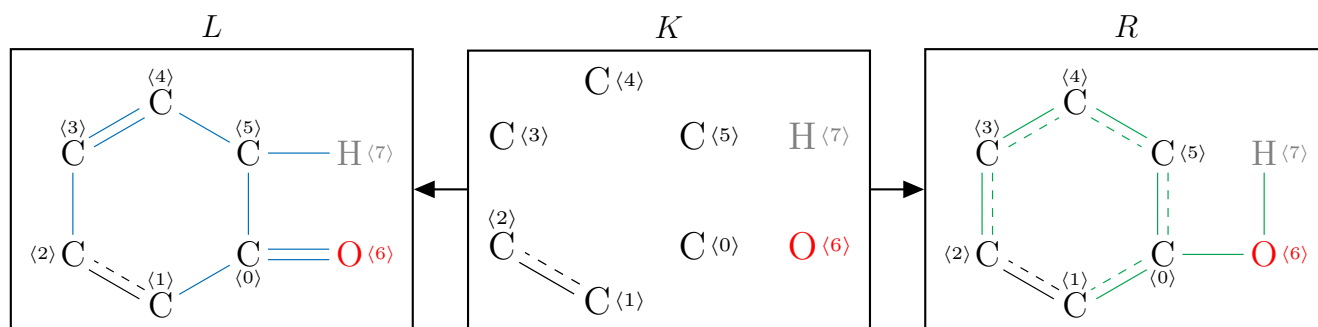
0.0.21 Aromatization of a 6-membered ring with 2 double bonds and 1 aromatic bond



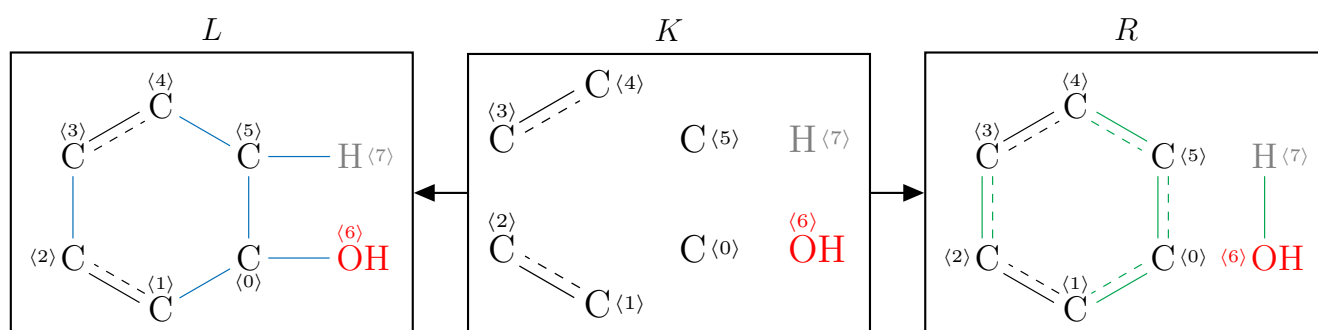
0.0.22 Aromatization of a 6-membered ring with 2 carbonyl groups and 1 hydroxyl group



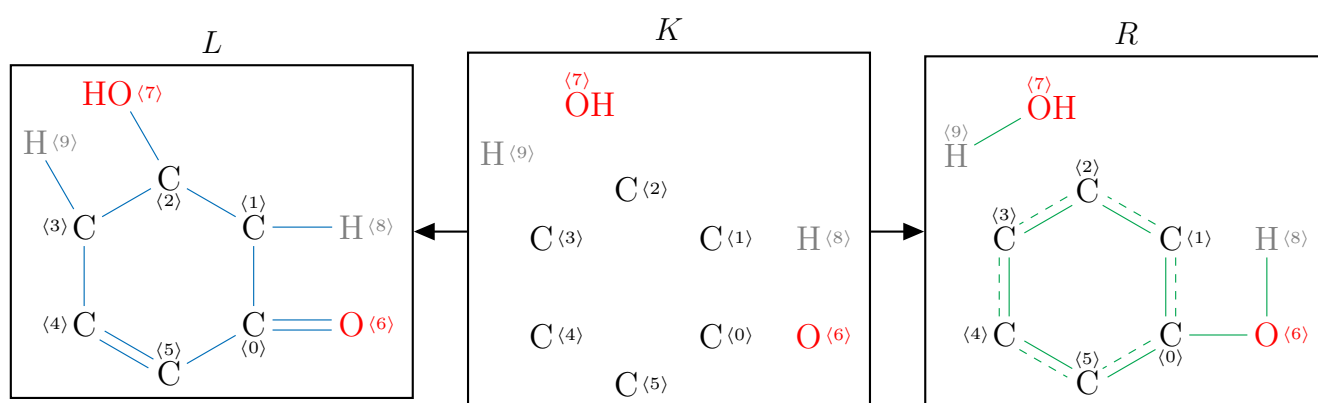
0.0.23 Aromatization of a 6-membered ring with 1 carbonyl group, 1 double bond and 1 aromatic bond - orientation 1



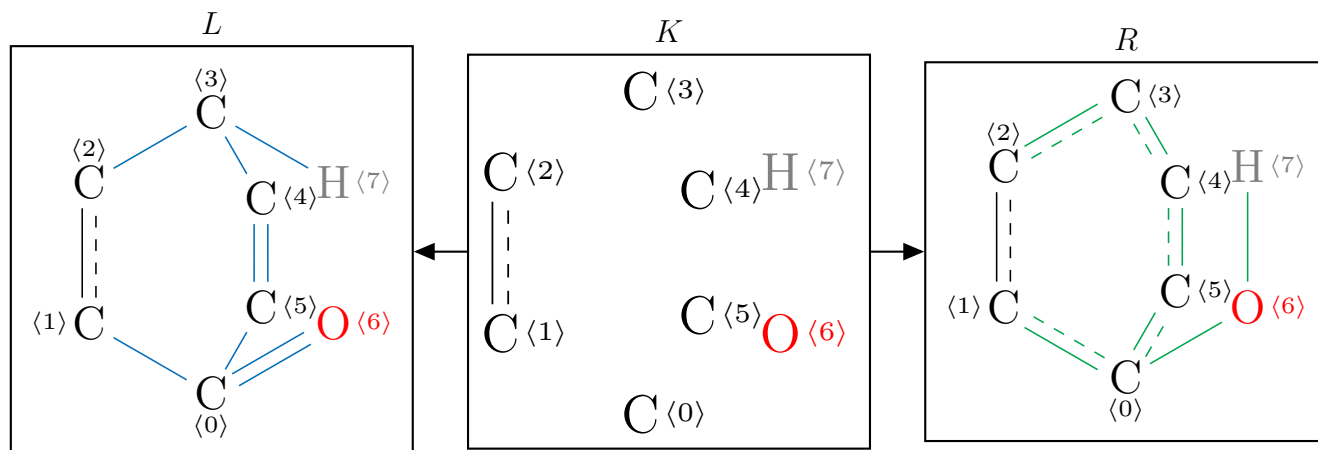
0.0.24 Aromatization of a 6-membered ring with 1 hydroxyl group and 2 aromatic bonds



0.0.25 Aromatization of a 6-membered ring with 1 carbonyl group, 1 hydroxyl group and 1 double bond - orientation 1

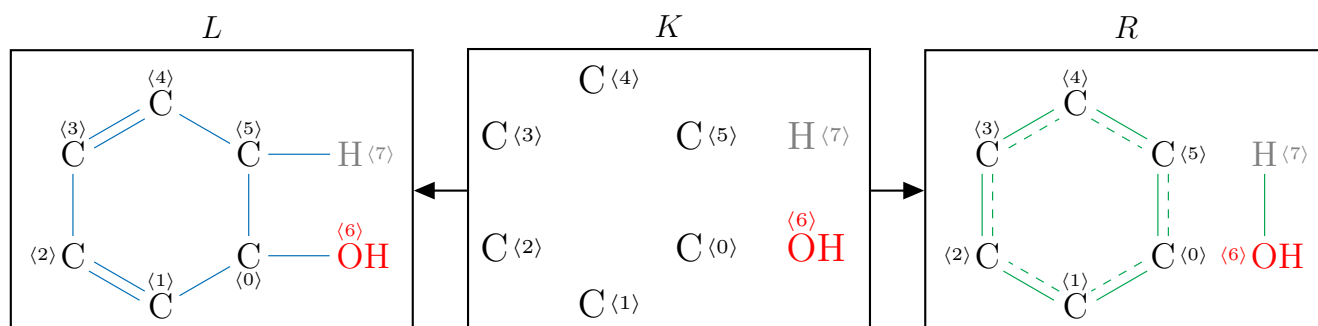


0.0.26 Aromatization of a 6-membered ring with 1 carbonyl group, 1 double bond and 1 aromatic bond - orientation 3



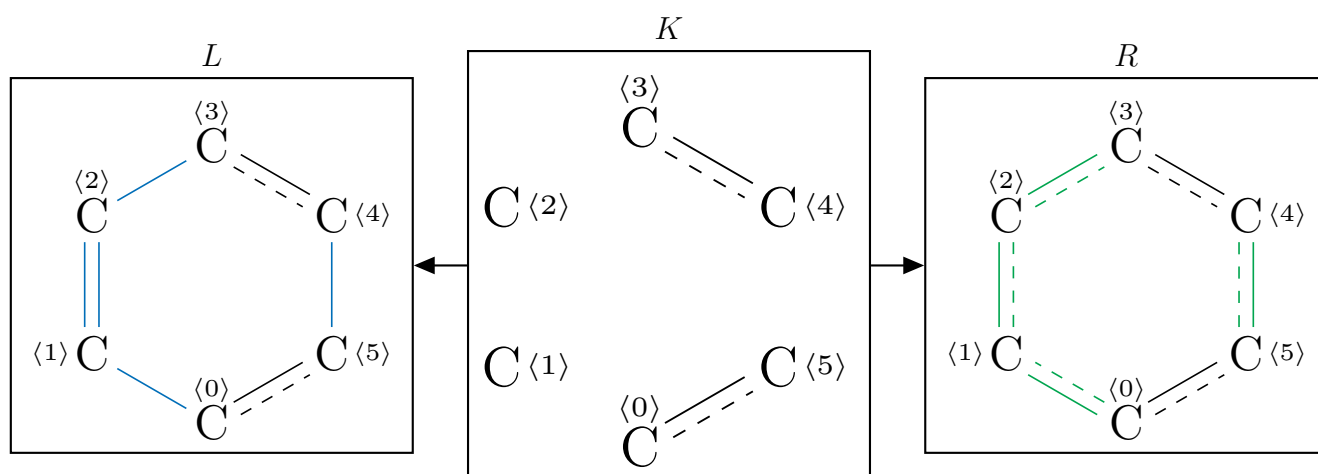
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0.0.27 Aromatization of a 6-membered ring with 1 hydroxyl group and 2 double bonds - orientation 1



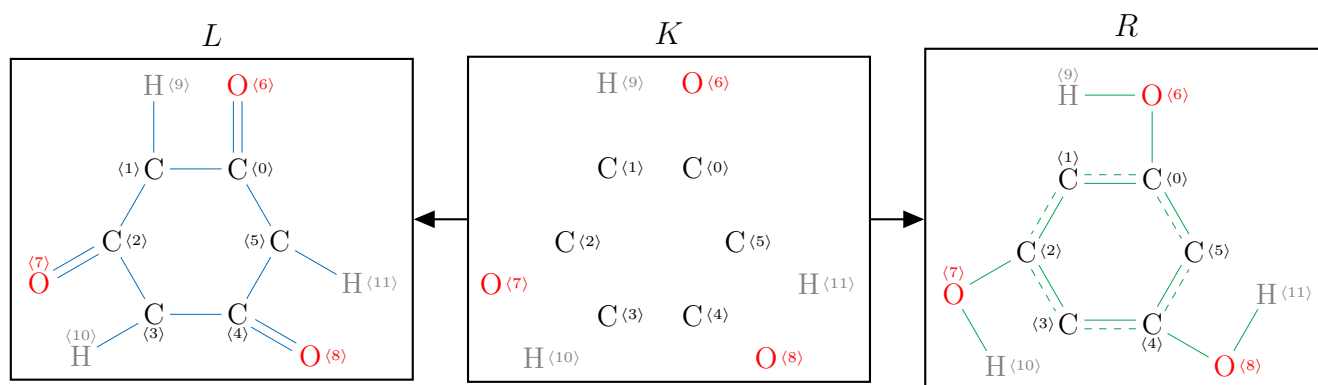
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0.0.28 Aromatization of a 6-membered ring with 1 double bond and 2 aromatic bonds

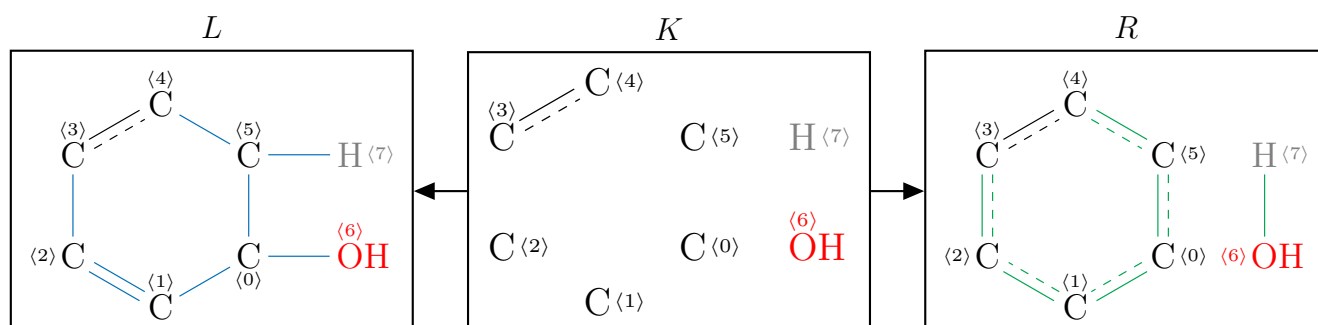


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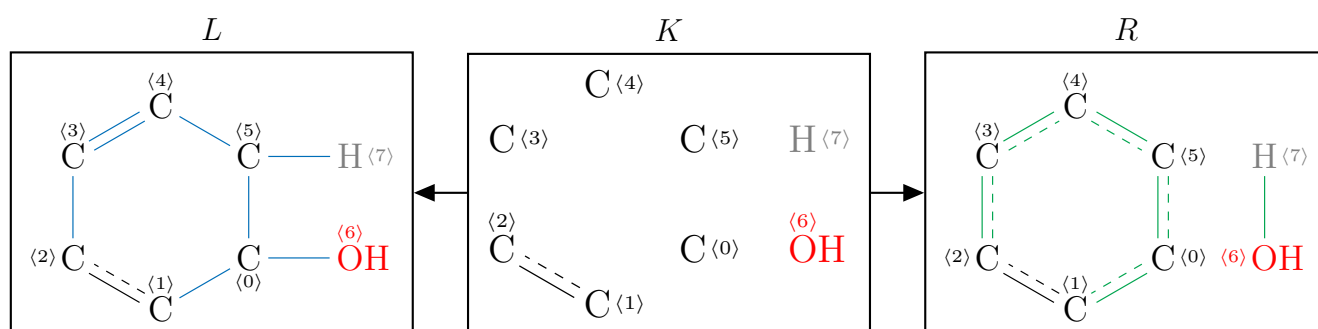
0.0.29 Aromatization of a 6-membered ring with 3 carbonyl groups



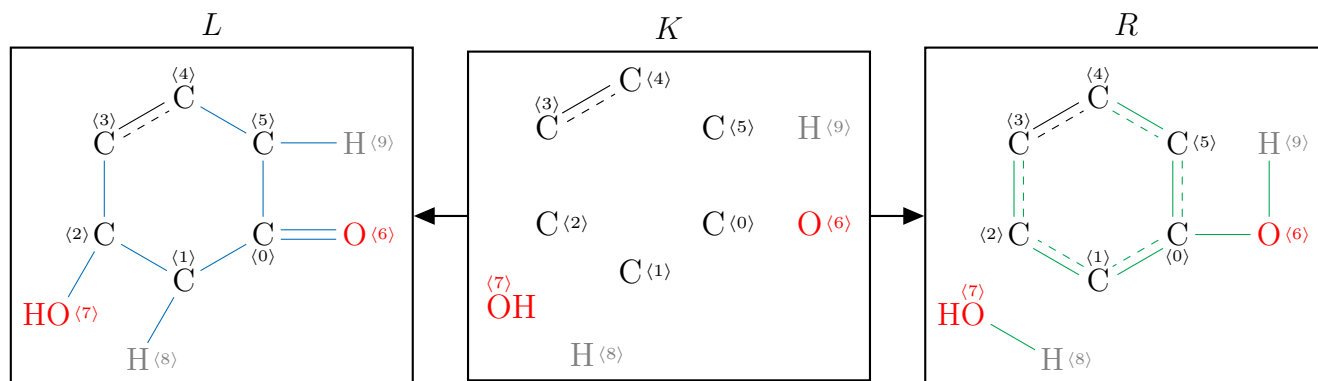
0.0.30 Aromatization of a 6-membered ring with 1 hydroxyl group, 1 double bond and 1 aromatic bond - orientation 2



0.0.31 Aromatization of a 6-membered ring with 1 hydroxyl group, 1 double bond and 1 aromatic bond - orientation 1

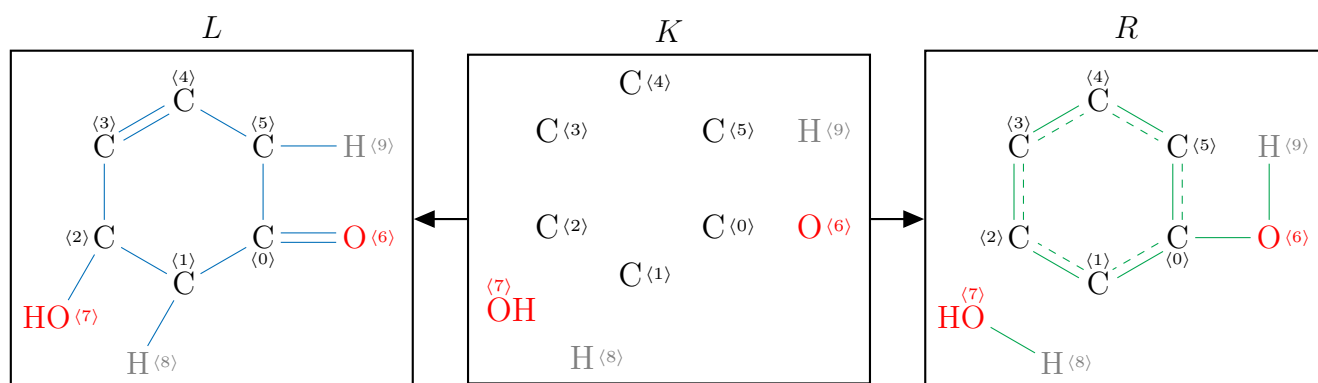


0.0.32 Aromatization of a 6-membered ring with 1 carbonyl group, 1 hydroxyl group and 1 aromatic bond - orientation 2



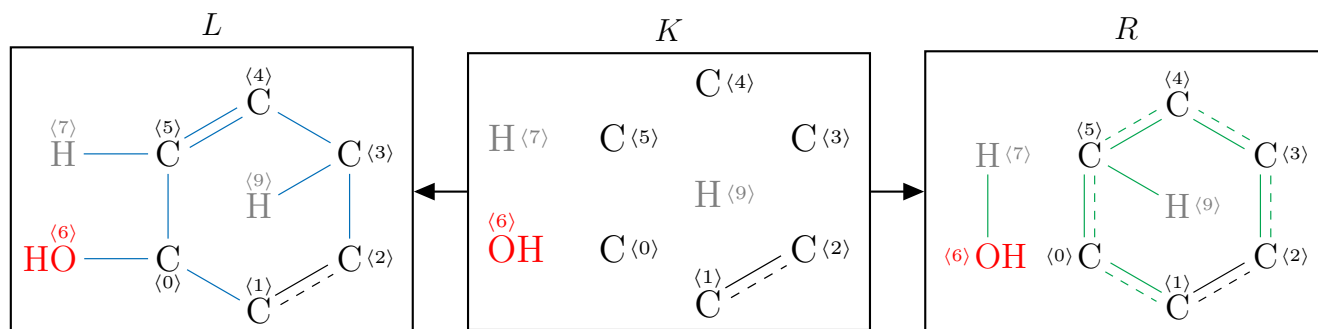
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0.0.33 Aromatization of a 6-membered ring with 1 carbonyl group, 1 hydroxyl group and 1 double bond - orientation 2



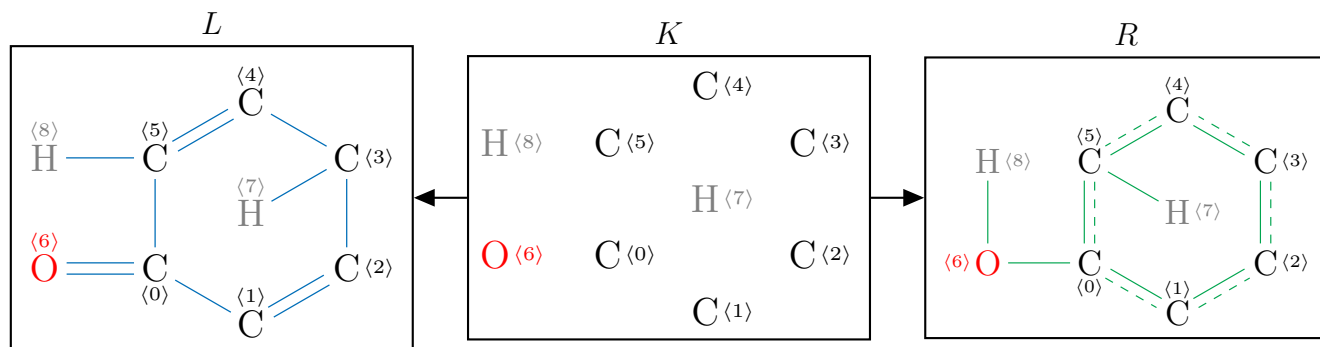
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0.0.34 Aromatization of a 6-membered ring with 1 hydroxyl group, 1 double bond and 1 aromatic bond - orientation 3



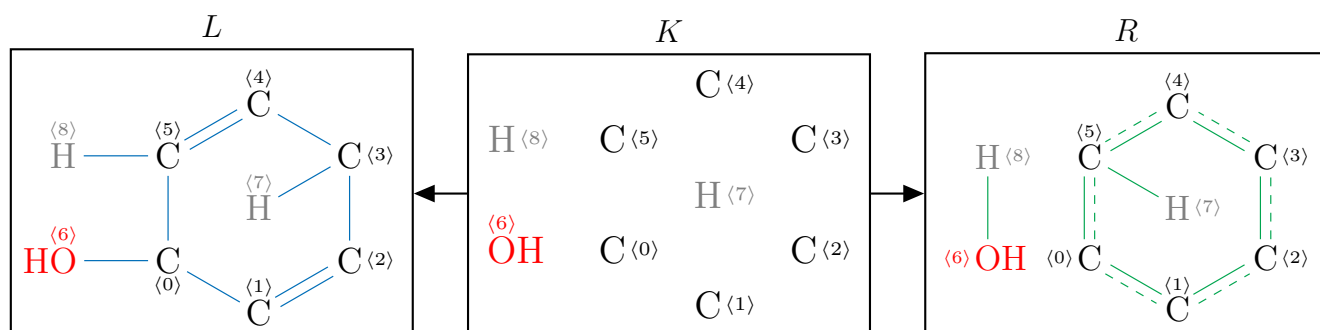
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0.0.35 Aromatization of a 6-membered ring with 1 carbonyl group and 2 double bonds - orientation 2



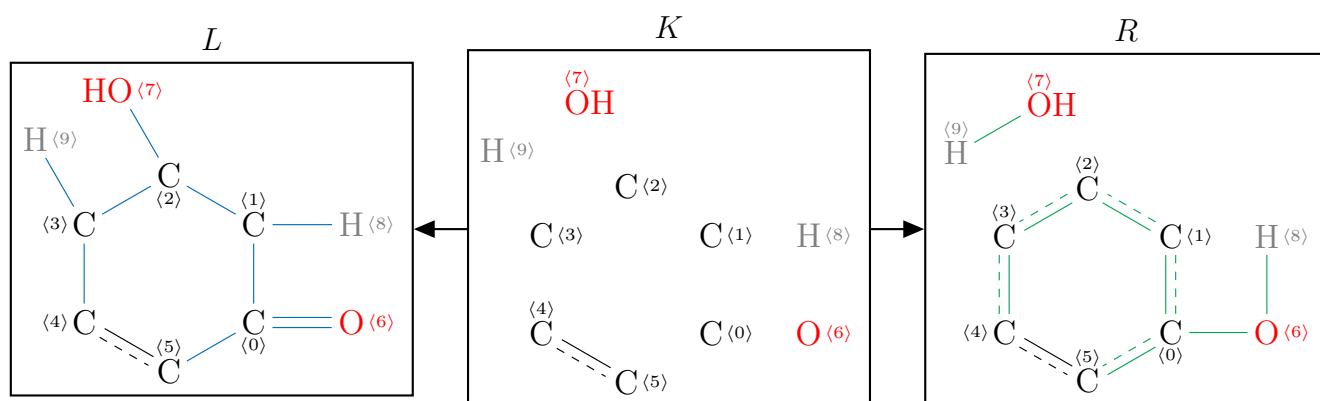
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0.0.36 Aromatization of a 6-membered ring with 1 hydroxyl group and 2 double bonds - orientation 2



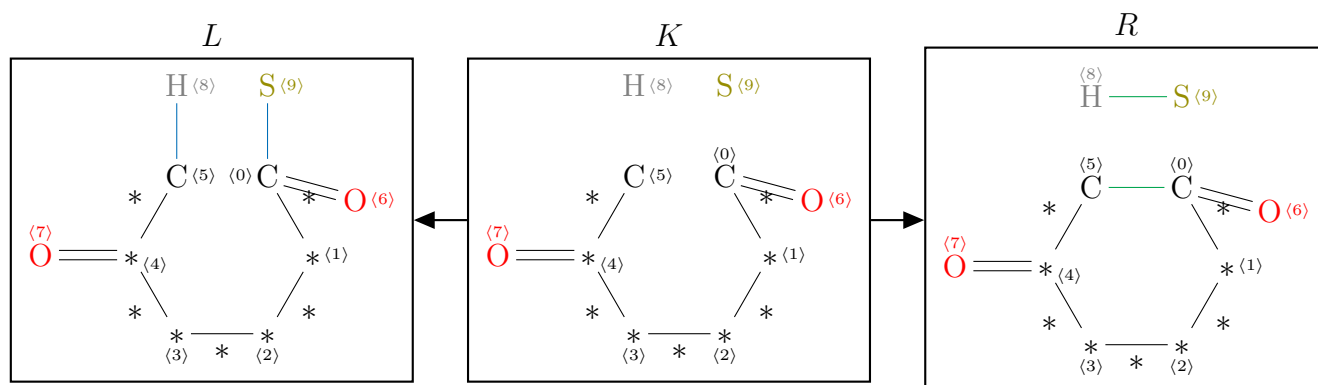
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0.0.37 Aromatization of a 6-membered ring with 1 carbonyl group, 1 hydroxyl group and 1 aromatic bond - orientation 1



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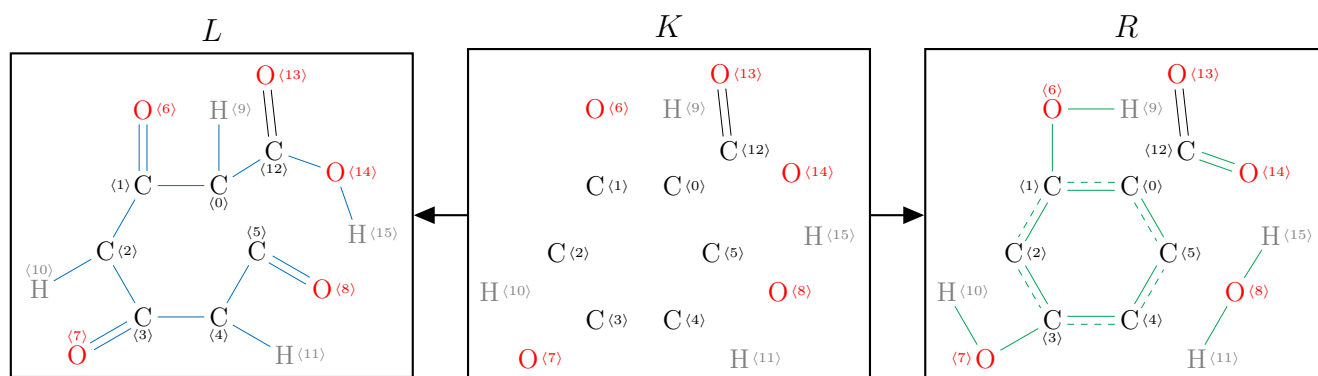
0.0.38 Intramolecular Claisen thioester condensation - ringsize 6 - near carbonyl group



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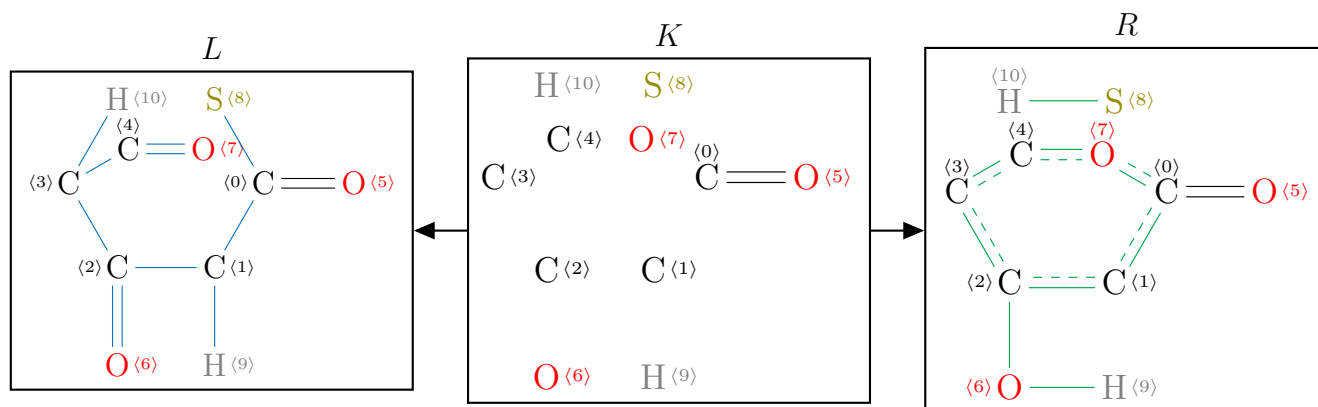
0.0.39 Intramolecular aldol condensation with decarboxylation and aromatization - ringsize 6 - 1 carboxyl group and 3 carbonyl groups



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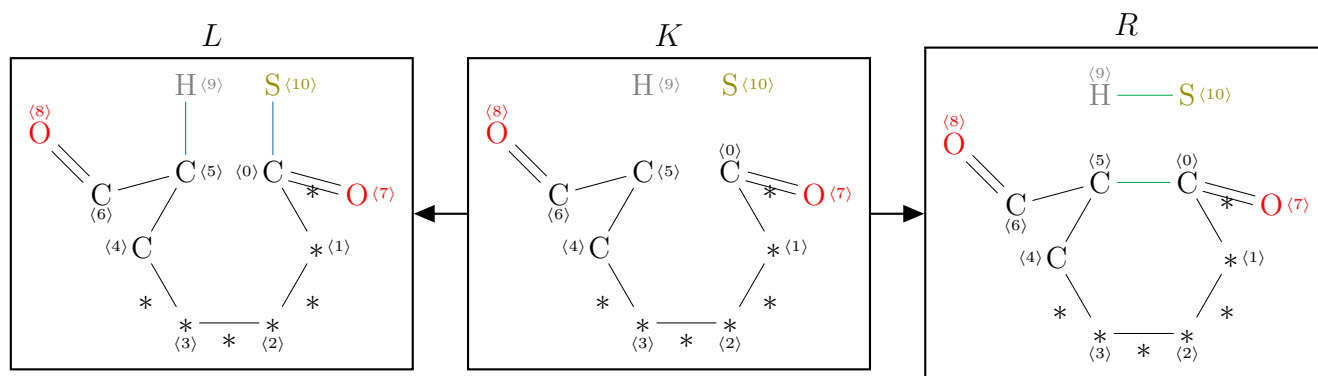
0.0.40 Lactonization with aromatization - ringsize 6



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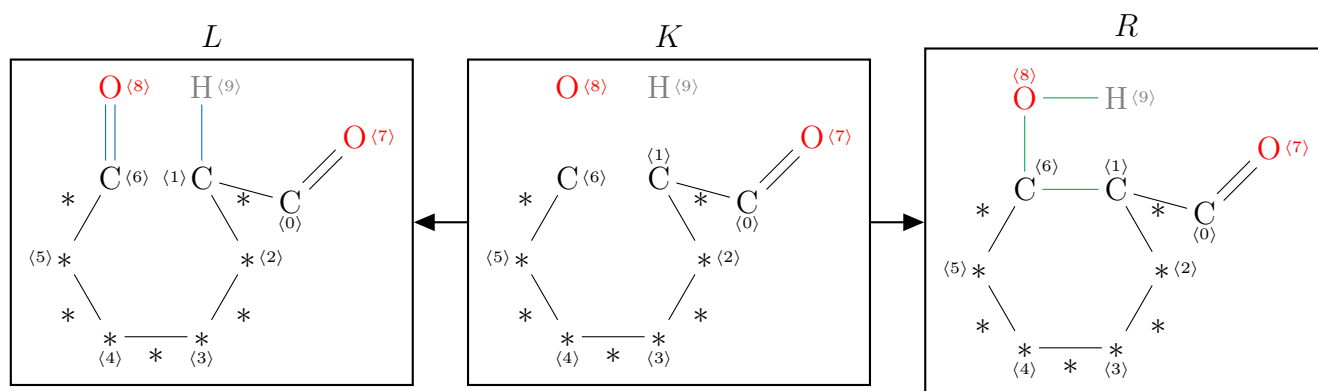
0.0.41 Intramolecular Claisen thioester condensation - ringsize 6 - distant carbonyl group



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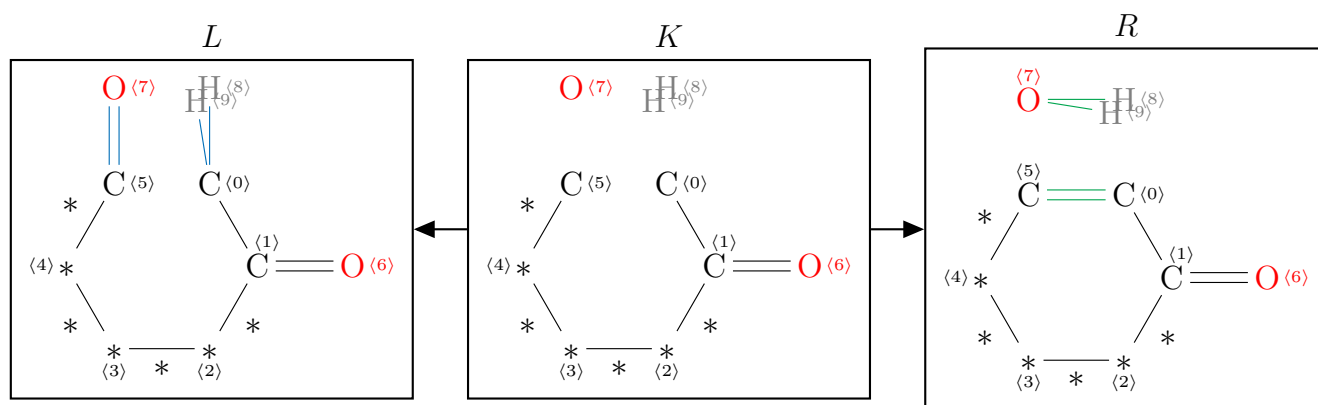
0.0.42 Intramolecular aldol addition - ringsize 6 - distant carbonyl group



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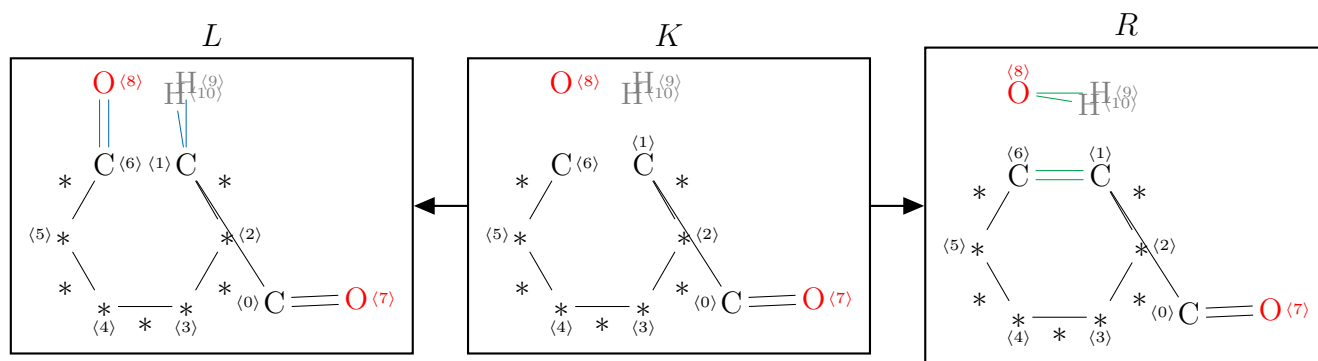
0.0.43 Intramolecular aldol condensation - ringsize 6 - near carbonyl group



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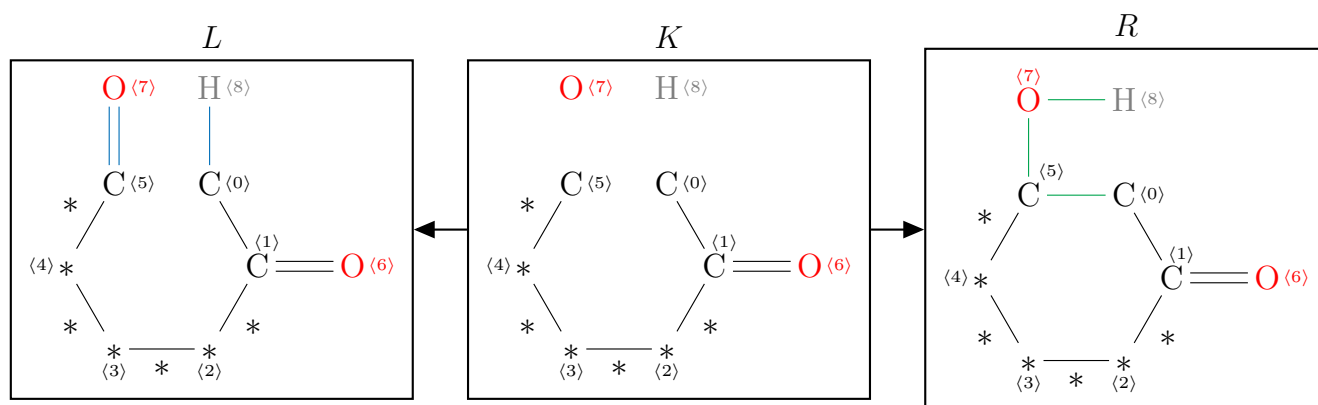
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0.0.44 Intramolecular aldol condensation - ringsize 6 - distant carbonyl group



shortestPath(1,6) = 5

0.0.45 Intramolecular aldol addition - ringsize 6 - near carbonyl group



shortestPath(0,5) = 5